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Reusable operators for irreducible Cartesian tensor decomposition and coupling

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ABSTRACT

Molecular and material properties, from the polarizability to the elastic constants, are described by tensors. Their behavior under rotations is made explicit when a tensor is decomposed into irreducible parts that transform independently. In Cartesian form, these parts are the symmetric and traceless irreducible Cartesian tensors (ICTs), whose decomposition and coupling underlie selection rules, orientational averages, and the use of symmetry. The decomposition is a textbook result at rank two, but higher rank and the intrinsic symmetry of physical tensors make it nontrivial. What has been lacking, unlike in the well-established spherical formalism, is a general construction for a given intrinsic symmetry, together with reusable operators that extract the ICTs and rebuild the original tensor exactly. Here, we develop such a construction and obtain these operators explicitly. These operators depend on rank and symmetry alone, and therefore, each need only be built once and then applied to any tensor of that class. Building on them, we further obtain the Cartesian harmonics of a vector and the operators that couple two ICTs into a third, both central to equivariant machine learning. The construction is demonstrated on the elastic tensor, in both its second-order form of rank four and its third-order form of rank six. The ICTs of the rank-4 tensor also define a rotation- and scale-invariant measure of anisotropy, which we evaluate across the first-principles elastic tensors of crystalline materials from the Materials Project. The construction is implemented in the open-source package `natto`, which produces the operators in both exact symbolic and numerical form.

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I. INTRODUCTION

Many physical quantities are tensors of rank two or higher, among them the rank-2 polarizability[1] and nuclear magnetic shielding tensor,[2] the rank-3 piezoelectric tensor,[3] and the rank-4 second-order elastic tensor.[4] Each decomposes into parts that transform independently under rotations, and each part can be written as a symmetric and traceless tensor, an irreducible Cartesian tensor (ICT), whose rank is its *weight*.[5–7] For example, a rank-2 tensor decomposes as $T_{ij} = \delta_{ij}X_0 + \epsilon_{ijk}X_k + X_{ij}$, where δ_{ij} is the Kronecker delta and ϵ_{ijk} is the Levi–Civita symbol. Repeated indices are summed throughout. Here, $X_0 = \frac{1}{3}T_{kk}$ is a scalar, $X_k = \frac{1}{2}\epsilon_{kij}T_{ij}$ is a vector, and $X_{ij} = \frac{1}{2}(T_{ij} + T_{ji}) - \frac{1}{3}T_{kk}\delta_{ij}$ is a symmetric traceless rank-2 tensor; these are the ICTs of weight 0, 1, and 2. The separated parts have long played distinct roles across applications. In spectroscopy, the weights determine which irreducible parts can interact, allowing forbidden contributions to be excluded through selection rules.[8,9] For molecules with random orientations, rotational averages can be reduced to scalar combinations of irreducible parts instead of being evaluated orientation by orientation.[10–12] For material property tensors, the scalar parts describe isotropic response, while the remaining parts distinguish different forms of anisotropy and help identify material symmetry.[13] The same separation is now used in equivariant machine learning, where features and predictions are organized by their weight so that rotations act correctly by construction.[14–19]

In the spherical-tensor formalism, the irreducible decomposition is long established, with angular momentum theory supplying the spherical harmonics, the Wigner rotation matrices, and the Clebsch–Gordan coefficients.[20] Both formalisms carry the same irreducible content, and a Cartesian tensor can always be converted to the spherical basis, decomposed, and converted back. We instead work directly in the Cartesian basis. Property tensors are computed, tabulated, and consumed in Cartesian components, and their intrinsic index symmetries, such as the exchange symmetry $\alpha_{ij} = \alpha_{ji}$ of the polarizability, are statements about those components; staying

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in that basis avoids the conversion and its phase and normalization conventions. A brief comparison of the two formalisms is given in Sec. S11 of the supplementary material.

Cartesian tensor reduction has been approached from several directions, each supplying part of what a general construction needs: an independent set of operators at any rank, an orthonormal form of that set, and a way to impose a prescribed intrinsic symmetry. One line begins with Coope and co-workers, who built the reduction from isotropic tensors, with natural projections and mapping tensors that extract the irreducible parts,[5,6] and fixed Cartesian coupling tensors.[7] Jerphagnon and co-workers carried the reduction to physical property tensors, resolving repeated weights and treating intrinsic symmetry one class at a time.[3] In these reductions, the independent mappings are chosen by hand for each rank in turn. Andrews and Ghoul then worked out the rank-4 decomposition in full,[21] and Lehman and Parke derived closed formulas for the Cartesian harmonics of a unit vector and for coupling two irreducible tensors.[22] These formulas express the result directly in the components of the vector or tensors and require repeated evaluation of a sum of terms, once for each input. Bonvicini automated the selection, identifying independent operators at arbitrary rank by computation and demonstrating the method through rank five.[23] Shao and co-workers obtained orthonormal decomposition matrices of the full tensor-product space, from chain contractions of Clebsch–Gordan matrices following the parentage scheme of Coope *et al.*,[5] by way of a change of basis to the spherical spaces.[24] Other lines reached high rank by importing structure from elsewhere: geometric and material symmetry arguments tailored to elasticity,[4,13,25] and invariant theory giving recursive orthogonal decompositions.[26–28]

These works supply most of the ingredients of a general construction. Independence has been settled by a matrix computation; orthonormality has been settled by invariant theory, by an existence argument, or by a spherical change of basis; and intrinsic symmetry has been settled by hand one class at a time, while the harmonic and coupling operators come from derivations of their own. What has not been done is to carry the construction through for a tensor with a prescribed intrinsic index symmetry, with the independent mappings, their orthonormal form, the symmetry-adapted combinations, and the harmonic and coupling operators all coming from a single mechanism. Such a decomposition of the full tensor-product space might be restricted to a tensor with an intrinsic symmetry, but we are not aware that this has been done.

Here, we develop a general, linear-algebraic construction that, for any rank and prescribed intrinsic symmetry, produces a complete and independent set of reusable operators for extracting every irreducible part and reconstructing the tensor exactly. Starting from all possible operators, an exact matrix calculation selects the independent ones. We then retain the combinations that obey the prescribed intrinsic symmetry and provide both an extraction–reconstruction pair and an orthonormal form. The orthonormal form is self-dual, so one set of operators serves both directions, and the squared magnitude splits into contributions from the individual ICTs without cross terms. The resulting operators depend only on rank, weight, and intrinsic symmetry. They can therefore be stored as numerical arrays and reused, reducing the decomposition of any tensor in the class to contractions with fixed coefficients. The natural projector, the mapping tensors, and the extraction and reconstruction summarized in Sec. II are those of Refs. 5 and 6; the selection of the independent mappings, the orthonormal operators, the symmetry adaptation, and the implementation are developed here.

We demonstrate the construction on elastic tensors. At rank four, it reproduces the known decomposition without using an elasticity-specific derivation.[4,13,25] The same construction then gives the decomposition of the third-order elastic tensor at rank six, including an irreducible part of weight three that is absent at rank four. Across first-principles elastic tensors from the Materials Project,[29,30] the irreducible parts also separate the anisotropy of each material into contributions with different angular dependence. This gives information that is not available from a single scalar measure of anisotropy.

Beyond the reduction itself, the construction provides operators for two related tasks. Applied to repeated products of a vector, the operators produce Cartesian harmonics, which describe angular dependence in terms of ICTs. Applied to a product of two ICTs, the same construction gives an operator that couples them into a third ICT.[7,22] Both sets of operators are therefore obtained from the same decomposition rather than from separate derivations. Such couplings are central to equivariant machine learning, and the Cartesian natural tensor networks of Ref. 19 already use a condensed form of

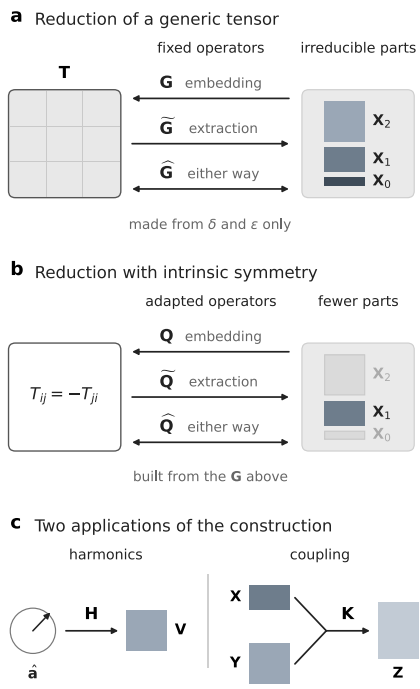


FIG. 1. One construction reduces a Cartesian tensor, adapts to its intrinsic symmetry, and yields the harmonic and coupling operators. (a) Fixed operators carry a generic tensor **T** to its irreducible parts $\mathbf{X}_\ell$ and back: **G** embeds a part, its dual $\widetilde{\mathbf{G}}$ extracts one, and the orthonormal $\widehat{\mathbf{G}}$ does either (Secs. II and III). (b) An intrinsic symmetry, here $T_{ij} = -T_{ji}$, replaces them with symmetry-adapted operators **Q**; the weights the symmetry excludes are shown greyed (Sec. IV). (c) The same construction gives the harmonic operator **H**, which carries a direction $\hat{\mathbf{a}}$ to a Cartesian harmonic **V** (Sec. VI), and the coupling operator **K**, which couples two ICTs into a third (Sec. VII).

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the present construction to predict properties from dipole moments to elastic constants.

Figure 1 summarizes the construction, and the remainder of this paper is organized as follows. Section II defines ICTs and summarizes the classical reduction and embedding operators. Section III counts the candidate operators, selects an independent set among them, and orthonormalizes it. Section IV extends it to tensors with intrinsic symmetry, with the elastic tensor worked out in detail in Sec. V. Section VI constructs the Cartesian harmonics, and Sec. VII constructs the coupling operators. Appendixes A–G collect tables of notations and mathematical support. The complete construction is implemented in the open-source package `natto`,[31] which builds the operators in exact symbolic as well as numerical form.

II. FOUNDATIONS OF CARTESIAN TENSOR REDUCTION

This section summarizes the classical Cartesian construction for tensor reduction developed in Refs. 3, 5–7, and 21. We state the results and illustrate them by example rather than reproduce their proofs, for which the reader is referred to those references. We work with tensors in three-dimensional Euclidean space. A rank-n Cartesian tensor $\mathbf{T}_n$ has components $T_{i_1 i_2 \dots i_n}$, where each index runs over the three Cartesian directions, giving 3^n components in total. We call a tensor *generic* if no relation is assumed among its components so that all 3^n of them are independent; physical property tensors usually carry intrinsic symmetries that lower this count, a case treated in Sec. IV.

Throughout, boldface symbols denote tensors and indexed symbols their Cartesian components, and we simply write $\mathbf{T}$ when the rank is unimportant. Einstein summation over repeated indices is implied unless otherwise stated. Two operation symbols are used heavily: $\otimes$ denotes a tensor product, and $\odot^{\ell}$ denotes a contraction over ℓ pairs of indices. A compact list of all symbols and tensor operations is collected in Appendix A.

A. Irreducible and isotropic Cartesian tensors

Definition 1 (Irreducible Cartesian tensor). A rank-n tensor $\mathbf{X}_n$ with components $X_{i_1 i_2 \dots i_n}$ is an *irreducible Cartesian tensor* (ICT) if it is (i) *symmetric*, $X_{i_{\pi(1)} \dots i_{\pi(n)}} = X_{i_1 \dots i_n}$ for every permutation $\pi \in S_n$ of its n indices, and (ii) *traceless*, $\delta_{i_a i_b} X_{i_1 \dots i_a \dots i_b \dots i_n} = 0$ for every pair of indices $1 \le a < b \le n$, where S_n is the permutation group on n indices and δ_{ij} is the Kronecker delta.[5–7]

Tracelessness applies for $n \ge 2$; scalars and vectors are treated as rank-0 and rank-1 ICTs. Such tensors are also called *natural* tensors, after Ref. 5, and elsewhere irreducible[6] or harmonic[13] tensors. We use *irreducible Cartesian tensors* throughout.

Two properties of ICTs are central to what follows. The first is that, in three dimensions, a rank-n ICT has $2n+1$ independent components,[3] far fewer than the 3^n of a generic tensor; Section S1 of the supplementary material derives the count. The second is irreducibility: under a rotation, the $2n+1$ independent components of a rank-n ICT transform among themselves, and no smaller set of linear combinations of them transforms only among itself.[32] This is what makes ICTs the endpoint of the reduction: they cannot be split further into pieces that transform independently.

All the reduction and embedding operators in this paper are built from two isotropic tensors: the Kronecker delta $\boldsymbol{\delta}$, whose components δ_{ij} equal 1 if $i = j$ and 0 otherwise, and the Levi–Civita symbol $\boldsymbol{\epsilon}$, whose components ϵ_{ijk} equal +1 (−1) if (i,j,k) is an even (odd) permutation of (1, 2, 3) and 0 otherwise. A tensor is *isotropic* when its components are the same in every rotated frame, and both $\boldsymbol{\delta}$ and $\boldsymbol{\epsilon}$ are, so every operator built from them is the same in every frame. They are moreover the elementary isotropic tensors, in that every isotropic Cartesian tensor is a linear combination of products of them, and products of two $\boldsymbol{\epsilon}$'s reduce to $\boldsymbol{\delta}$'s, so at most one $\boldsymbol{\epsilon}$ is ever needed. Contracted with a pair of indices of an arbitrary tensor, $\boldsymbol{\delta}$ takes the trace in that pair and $\boldsymbol{\epsilon}$ retains only the antisymmetric part, the two rank-lowering operations on which the reduction rests. Applied to an ICT, however, both come up empty: $\boldsymbol{\delta} \odot^2 \mathbf{X} = 0$ because an ICT is traceless and $\boldsymbol{\epsilon} \odot^2 \mathbf{X} = 0$ because it is symmetric, so neither operation lowers an ICT any further. Section S2 of the supplementary material collects the identities used throughout.

B. Reduction spectrum

Definition 2 (Reduction spectrum). A generic rank-n Cartesian tensor $\mathbf{T}_n$ decomposes into ICTs as[3,21]

$$\mathbf{T}_n = \bigoplus_{\ell} \bigoplus_{p} \mathbf{X}_{\ell}^{p}. \tag{1}$$

Here, $\ell = 0, 1, \dots, n$ is the *weight*. For each weight ℓ, its *multiplicity* N_ℓ is the number of independent ICTs of that weight. We call each of them a *channel* of weight ℓ, and the *multiplicity index* $p = 1, 2, \dots, N_\ell$ labels the channels. The collection of ICTs $\mathbf{X}_{\ell}^{p}$ is the *reduction spectrum* of $\mathbf{T}_n$.

The symbol $\oplus$ signals that Eq. (1) is a direct sum rather than an ordinary one: ICTs of different weights have different ranks and cannot literally be added, and those of the same weight are kept as separate pieces rather than added. Each ICT of weight ℓ carries $2\ell+1$ components, and the spectrum accounts for the whole rank-n tensor space, $\sum_{\ell=0}^{n} N_\ell (2\ell+1) = 3^n$. The multiplicities N_ℓ are determined in Sec. III A.

At rank two, every weight occurs once, $\mathbf{T}_2 = \mathbf{X}_0 \oplus \mathbf{X}_1 \oplus \mathbf{X}_2$, and the multiplicity index is then omitted. Multiplicity first appears at rank three, $\mathbf{T}_3 = \mathbf{X}_0 \oplus \mathbf{X}_1^1 \oplus \mathbf{X}_1^2 \oplus \mathbf{X}_1^3 \oplus \mathbf{X}_2^1 \oplus \mathbf{X}_2^2 \oplus \mathbf{X}_3$, whose seven ICTs are written out in Sec. S6 of the supplementary material. Both spectra can be obtained systematically through the following procedure:

Procedure 1. A weight-ℓ ICT $\mathbf{X}_{\ell}^{p}$ can be obtained from a generic rank-n Cartesian tensor $\mathbf{T}_n$ $(\ell \le n)$ as follows:[3,21]

(i) lower the rank of $\mathbf{T}_n$ to ℓ by contracting it with the isotropic tensors $\boldsymbol{\delta}$ and/or $\boldsymbol{\epsilon}$;
(ii) symmetrize the rank-lowered tensor by averaging over all index permutations; and
(iii) remove traces by subtracting tensors formed from pairwise contractions.

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Steps (ii) and (iii) impose the two defining conditions of an ICT: symmetry and tracelessness, respectively.

Subsections II C–II F formulate the three steps as explicit operators and show how these operators perform extraction and embedding. The rank-2 reduction serves as a running example: although simple, it contains the essential elements of the general construction. Table I summarizes its operators and results and is referenced at the relevant points below.

C. Rank-lowering tensors

We take the three steps of Procedure 1 in turn, beginning with step (i). To reach a weight-ℓ ICT from a generic tensor $\mathbf{T}_n$ $(T_{i_1 i_2 \ldots i_n})$ of higher rank $n \geq \ell$, the rank must first be lowered from n to ℓ, which is done by contracting the surplus indices of $\mathbf{T}_n$ in pairs against $\boldsymbol{\delta}$ and, when the parity requires it, one $\boldsymbol{\epsilon}$. Which indices are paired is a choice, and different choices leave different information behind. Collecting the $\boldsymbol{\delta}$'s and $\boldsymbol{\epsilon}$ of one choice into a single *rank-lowering tensor* $\mathbf{F}^p_{n\to\ell}$, labeled by p, step (i) reads[21]

$$\mathbf{T}'_\ell = \mathbf{F}^p_{n\to\ell} \odot^m \mathbf{T}_n, \tag{2}$$

with m being the number of contracted indices. Each p gives its own rank-ℓ tensor $\mathbf{T}'_\ell$, and it is this freedom of choice that lets a single rank-n tensor carry several ICTs of the same weight. The form of $\mathbf{F}^p_{n\to\ell}$ depends on the parity of $n-\ell$.

When $n-\ell$ is even, the pairing is carried out by $\boldsymbol{\delta}$'s alone,

$$F^p_{n\to\ell} = \prod_{(a,b)\,\in\,\mathcal{D}_p} \delta_{i_a i_b}, \tag{3}$$

where $\mathcal{D}_p$ is a set of $k = (n-\ell)/2$ disjoint pairs of indices, one pair per $\boldsymbol{\delta}$, so that $\delta_{i_a i_b}$ contracts with the pair i_a, i_b in $\mathbf{T}_{i_1 \ldots i_a \ldots i_b \ldots i_n}$. All $m = 2k = n-\ell$ paired indices are contracted away, leaving a tensor of rank ℓ. Here, the label p is simply the label of $\mathcal{D}_p$.

As an example, for $n = 3$ and $\ell = 1$, $\mathbf{F}^p_{3\to1}$ is a rank-2 tensor made of a single $\boldsymbol{\delta}$. Then, $\mathcal{D}_1 = \{(1,2)\}$, $\mathcal{D}_2 = \{(1,3)\}$, and $\mathcal{D}_3 = \{(2,3)\}$, resulting in three different rank-lowering tensors,

$$F^1_{3\to1} = \delta_{i_1 i_2}, \quad F^2_{3\to1} = \delta_{i_1 i_3}, \quad F^3_{3\to1} = \delta_{i_2 i_3}, \tag{4}$$

one for each index of $\mathbf{T}_3$ left free.

When $n-\ell$ is odd, one pair is taken by $\boldsymbol{\epsilon}$ instead,

$$F^p_{n\to\ell} = \epsilon_{j\, i_u i_v} \prod_{(a,b)\,\in\,\mathcal{D}_p} \delta_{i_a i_b}, \tag{5}$$

with $k = (n-\ell-1)/2$ of $\boldsymbol{\delta}$'s left. All $m = 2(k+1) = n-\ell+1$ paired indices are contracted away, and $\boldsymbol{\epsilon}$ restores one through its free index j, again leaving a tensor of rank ℓ. Here, the label p records two things: which pair $\boldsymbol{\epsilon}$ takes, and how the remaining indices are paired in $\mathcal{D}_p$.

As an example, for $n = 3$ and $\ell = 2$, the rank drop is one, so $k = 0$ and $\mathbf{F}^p_{3\to2}$ is a single $\boldsymbol{\epsilon}$, again one for each index of $\mathbf{T}_3$ left free,

$$F^1_{3\to2} = \epsilon_{j\, i_1 i_2}, \quad F^2_{3\to2} = \epsilon_{j\, i_1 i_3}, \quad F^3_{3\to2} = \epsilon_{j\, i_2 i_3}. \tag{6}$$

Note that $\ell = 0$ is a special case, in which $\boldsymbol{\epsilon}$ has no free index left over and contracts all three of its indices with $\mathbf{T}_n$. Across both cases, the distinct assignments for a given rank n and weight ℓ are indexed by $p = 1, 2, \ldots, N^{\mathrm{c}}_\ell$, so N^{c}_ℓ counts the distinct rank-lowering tensors. See Appendix B for a closed-form count of the number of distinct assignments N^{c}_ℓ and more examples.

D. Natural projector

The rank-lowered tensor $\mathbf{T}'_\ell$ of Eq. (2) has the right rank but is, in general, neither symmetric nor traceless. Steps (ii) and (iii) of Procedure 1 remain and are carried out together here by a single operator, fixed by the weight ℓ alone.

Definition 3 (Natural projector). The *natural projector* $\mathbf{E}_{(\ell|\ell)}$ is the rank-2ℓ tensor,[6]

$$E_{(\ell|\ell)} = \sum_{t=0}^{\lfloor \ell/2 \rfloor} c_t \left\langle \delta^{\ell-2t}_{\alpha i} \delta^t_{\alpha\alpha} \delta^t_{ii} \right\rangle, \tag{7}$$

with no sum over the repeated indices, the upper limit being $\lfloor \ell/2 \rfloor = \ell/2$ when ℓ is even and $(\ell-1)/2$ when ℓ is odd. Written in full, it is $\mathbf{E}_{(\alpha_1\alpha_2\ldots\alpha_\ell|i_1 i_2 \ldots i_\ell)}$, where the Greek indices belong to the ICT space $\mathcal{X}^\ell$ and the Roman indices belong to the Cartesian tensor space $\mathcal{T}^\ell$. The coefficients c_t depend only on ℓ and t and are fixed by requiring that $\mathbf{E}_{(\ell|\ell)}$ returns a traceless tensor,[6,7]

$$c_t = (-1)^t \, \frac{(\ell!)^2 \, (2\ell-2t)!}{(2\ell)! \; t! \; (\ell-t)! \; (\ell-2t)!}. \tag{8}$$

TABLE I. Reduction of a generic rank-2 tensor T_2, operator by operator. Because each weight occurs once, g denotes the single Gram coefficient at that weight.

Quantity	$\ell = 0$	$\ell = 1$	$\ell = 2$
X_ℓ	$\frac{1}{3} T_{kk}$	$\frac{1}{2}\epsilon_{\alpha_1 i_1 i_2} T_{i_1 i_2}$	$\frac{1}{2}(T_{\alpha_1\alpha_2} + T_{\alpha_2\alpha_1}) - \frac{1}{3}\delta_{\alpha_1\alpha_2} T_{kk}$
S^ℓ_n	$\frac{1}{3} T_{kk}\delta_{i_1 i_2}$	$\frac{1}{2}(T_{i_1 i_2} - T_{i_2 i_1})$	$\frac{1}{2}(T_{i_1 i_2} + T_{i_2 i_1}) - \frac{1}{3}\delta_{i_1 i_2} T_{kk}$
$F_{n\to\ell}$	$\delta_{i_1 i_2}$	$\epsilon_{j\, i_1 i_2}$	1
$E_{(\ell\|\ell)}$	1	$\delta_{\alpha_1 j}$	$\frac{1}{2}(\delta_{\alpha_1 i_1}\delta_{\alpha_2 i_2} + \delta_{\alpha_1 i_2}\delta_{\alpha_2 i_1}) - \frac{1}{3}\delta_{\alpha_1\alpha_2}\delta_{i_1 i_2}$
$G_{(\ell\|n)}$	$\delta_{i_1 i_2}$	$\epsilon_{\alpha_1 i_1 i_2}$	Same as $E_{(2\|2)}$
g	3	2	1
$\widetilde{G}_{(\ell\|n)}$	$\frac{1}{3}\delta_{i_1 i_2}$	$\frac{1}{2}\epsilon_{\alpha_1 i_1 i_2}$	Same as $E_{(2\|2)}$

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The shorthand $\langle \delta_{\alpha i}^{\ell-2t} \delta_{\alpha\alpha}^{t} \delta_{ii}^{t} \rangle$ denotes the average of a product of ℓ Kronecker deltas, the exponents counting the factors of each type. The average is taken over all $\ell!$ permutations of the α indices and, separately, all $\ell!$ permutations of the i indices. Many of those $(\ell!)^2$ products coincide, and each distinct product occurs the same number of times, so the average may equally be taken over the distinct products alone. For example, when $\ell = 2$, the two symmetrized products appearing in Eq. (7) are

$$\begin{aligned} \langle \delta_{\alpha i}^{2} \rangle &= \frac{1}{2} (\delta_{\alpha_1 i_1} \delta_{\alpha_2 i_2} + \delta_{\alpha_1 i_2} \delta_{\alpha_2 i_1}), \\ \langle \delta_{\alpha\alpha} \delta_{ii} \rangle &= \delta_{\alpha_1 \alpha_2} \delta_{i_1 i_2}. \end{aligned} \tag{9}$$

See Sec. S3 of the supplementary material for more examples of the symmetrized products and Sec. S4 of the supplementary material for explicit expressions for $\mathbf{E}_{(\ell|\ell)}$ for $\ell \leq 3$.

The terms of Eq. (7) fall into two groups, which give the projection its two functions. The $t = 0$ term, $\langle \delta_{\alpha i}^{\ell} \rangle$, fully symmetrizes the tensor, as required in step (ii) of Procedure 1, whereas the $t \geq 1$ terms remove all traces, as required in step (iii). The $t \geq 1$ terms do so by contracting t pairs of the i indices, those of the tensor being projected, with δ_{ii}^{t}, extracting traces, and re-expanding them with $\delta_{\alpha\alpha}^{t}$, while the remaining $\delta_{\alpha i}^{\ell-2t}$ carries the uncontracted indices over from the i block to the α block.

The natural projector has several properties that the rest of this paper rests on. First, Eq. (7) is built from $\boldsymbol{\delta}$'s alone, so $\mathbf{E}_{(\ell|\ell)}$ is isotropic (Sec. II A).

Second, by construction in Eq. (7), it is symmetric under any permutation of its α indices and, separately, of its i indices, and it is unchanged when the two blocks are exchanged, so it is self-adjoint.

Third, it is traceless within each block,

$$\delta_{\alpha_1\alpha_2} E_{(\alpha_1\alpha_2\ldots\alpha_\ell|i_1\ldots i_\ell)} = \delta_{i_1 i_2} E_{(\alpha_1\ldots\alpha_\ell|i_1 i_2\ldots i_\ell)} = 0, \tag{10}$$

for $\ell \geq 2$, because the projection must return a traceless tensor for every rank-ℓ tensor, the requirement that fixes the c_t in Eq. (8).

Fourth, it is *idempotent* under the ℓ-fold contraction,[6]

$$E_{(\alpha_1\ldots\alpha_\ell|k_1\ldots k_\ell)}\, E_{(k_1\ldots k_\ell|i_1\ldots i_\ell)} = E_{(\alpha_1\ldots\alpha_\ell|i_1\ldots i_\ell)}, \tag{11}$$

so that applying it twice is the same as applying it once: a tensor that is already an ICT of weight ℓ is its own weight-ℓ part, and the projection returns it unchanged. Its trace therefore counts the components it keeps,[6] $\mathrm{tr}\, \mathbf{E}_{(\ell|\ell)} = E_{(i_1\ldots i_\ell|i_1\ldots i_\ell)} = 2\ell + 1$, the number of independent components of an ICT of weight ℓ. This trace pairs each Greek index with a Roman one and so is a different contraction from those of Eq. (10), which are taken within a block and vanish.

Finally, acting on a generic rank-ℓ tensor $\mathbf{T}_\ell$ $(T_{i_1 i_2\ldots i_\ell})$, the natural projector extracts the ICT $\mathbf{X}_\ell$ of weight ℓ,

$$\mathbf{X}_\ell = \mathbf{E}_{(\ell|\ell)} \odot^{\ell} \mathbf{T}_\ell, \quad X_{\alpha_1\ldots\alpha_\ell} = E_{(\alpha_1\ldots\alpha_\ell|i_1\ldots i_\ell)}\, T_{i_1\ldots i_\ell}. \tag{12}$$

By the second property, this contraction is independent of how the i-index slots of the projector are paired with the indices of $\mathbf{T}_\ell$.

Evaluating Eq. (7) at $\ell = 0, 1, 2$ gives the three natural projectors of the rank-2 reduction, listed in Table I. In particular, the $\ell = 2$ result follows by substituting $c_0 = 1$ and $c_1 = -\frac{1}{3}$ from Eq. (8). At $\ell = 2$, there is no rank to lower, so Eq. (12) applies directly and returns the symmetric traceless $\mathbf{X}_2$ of Table I. At $\ell = 0$ and $\ell = 1$, the projector must be preceded by the rank-lowering tensors listed there, and the two are combined in Subsection II E.

E. Mapping tensors between ranks

Applying $\mathbf{F}^{p}_{n\to\ell}$ and then $\mathbf{E}_{(\ell|\ell)}$ carries out all three steps, so the two can be combined into a single operator $\mathbf{G}^{p}_{(\ell|n)}$, the *mapping tensor* between the spaces $\mathcal{X}^{\ell}$ and $\mathcal{T}^{n}$,

$$\mathbf{G}^{p}_{(\ell|n)} = \mathbf{E}_{(\ell|\ell)}\ \mathbf{F}^{p}_{n\to\ell}. \tag{13}$$

See Appendix C for the index form of Eq. (13), written out for even and odd $n - \ell$. The resulting $\mathbf{G}^{p}_{(\ell|n)}$ is a rank-$(\ell + n)$ tensor with ℓ Greek indices associated with $\mathcal{X}^{\ell}$ and n Roman indices associated with $\mathcal{T}^{n}$. Contracting it with a generic rank-n tensor $\mathbf{T}_n$ gives an ICT $\mathbf{D}^{p}_{\ell} = \mathbf{G}^{p}_{(\ell|n)} \odot^{n} \mathbf{T}_n$ of weight ℓ, with components $D^{p}_{\alpha_1\ldots\alpha_\ell} = G^{p}_{(\alpha_1\ldots\alpha_\ell|i_1\ldots i_n)} T_{i_1\ldots i_n}$.

For a rank-2 tensor, combining the $F_{n\to\ell}$ and $E_{(\ell|\ell)}$ rows of Table I gives the $G_{(\ell|n)}$ row listed there, completing the weight-0 and weight-1 cases left open in Sec. II D. Each weight has a single mapping tensor at this rank. Several appear per weight from rank three on. For example, for $n = 3$ and $\ell = 2$, the three rank-lowering tensors of Eq. (6) give three candidate mapping tensors,

$$\begin{aligned} G^{1}_{(2|3)} &= E_{(\alpha_1\alpha_2|i_3 j)}\ \epsilon_{j i_1 i_2}, \\ G^{2}_{(2|3)} &= E_{(\alpha_1\alpha_2|i_2 j)}\ \epsilon_{j i_1 i_3}, \\ G^{3}_{(2|3)} &= E_{(\alpha_1\alpha_2|i_1 j)}\ \epsilon_{j i_2 i_3}. \end{aligned} \tag{14}$$

Each $\boldsymbol{\epsilon}$ passes its free index j to the projector, which also receives the one index of $\mathbf{T}_3$ that $\boldsymbol{\epsilon}$ does not take. See Appendix C for Eq. (14) expanded in $\boldsymbol{\delta}$ and $\boldsymbol{\epsilon}$ and for further examples.

F. Extraction and embedding

A complete reduction must both extract the ICTs and reconstruct $\mathbf{T}_n$ from them. Here, we complete the dual pair of mapping tensors: $\mathbf{G}^{p}_{(\ell|n)}$ for embedding and $\widetilde{\mathbf{G}}^{p}_{(\ell|n)}$ for extraction.

The construction begins with the pairwise contractions of mapping tensors of the same weight. Contracting $\mathbf{G}^{p}_{(\ell|n)}$ and $\mathbf{G}^{q}_{(\ell|n)}$ over all n Roman indices leaves a rank-2ℓ tensor, carrying one group of ℓ ICT indices from each factor. Being built from $\boldsymbol{\delta}$ and $\boldsymbol{\epsilon}$ alone, the mapping tensors are isotropic (Sec. II A), and so is their contraction. In Eq. (13), the rank-lowering tensor supplies Roman indices only, so the ℓ Greek indices of $\mathbf{G}^{p}_{(\ell|n)}$ are the α indices of $\mathbf{E}_{(\ell|\ell)}$, which are symmetric among themselves and traceless by Eq. (10). The contraction between $\mathbf{G}^{p}_{(\ell|n)}$ and $\mathbf{G}^{q}_{(\ell|n)}$ runs over Roman indices alone and so leaves both Greek groups as they are, making the result symmetric and traceless within each of them. Up to a scalar, the only isotropic tensor with these properties is the natural projector,[6]

$$\mathbf{G}^{p}_{(\ell|n)} \odot^{n} \mathbf{G}^{q}_{(\ell|n)} = g_{pq} \mathbf{E}_{(\ell|\ell)}, \tag{15}$$

where the scalar g_{pq} measures the overlap between $\mathbf{G}^{p}_{(\ell|n)}$ and $\mathbf{G}^{q}_{(\ell|n)}$. The values of g_{pq} form a symmetric Gram matrix $\mathbf{g}$, which is invertible for a linearly independent set of mapping tensors.[33]

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The *dual mapping tensors* $\widetilde{\mathbf{G}}^{p}_{(\ell|n)}$ are defined, as in Ref. 6, by

$$\widetilde{\mathbf{G}}^{p}_{(\ell|n)} = \sum_{q} (\mathbf{g}^{-1})_{pq}\mathbf{G}^{q}_{(\ell|n)}. \tag{16}$$

Each $\widetilde{\mathbf{G}}^{p}_{(\ell|n)}$ has the same rank and index structure as $\mathbf{G}^{p}_{(\ell|n)}$. Combining Eqs. (15) and (16) gives the duality relation (see Appendix D for the derivation),

$$\widetilde{\mathbf{G}}^{p}_{(\ell|n)} \odot^{n} \mathbf{G}^{q}_{(\ell|n)} = \delta_{pq}\mathbf{E}_{(\ell|\ell)}. \tag{17}$$

The two sets now have complementary roles. Acting on $\mathbf{T}_n$, $\widetilde{\mathbf{G}}^{p}_{(\ell|n)}$ extracts the ICT $\mathbf{X}^{p}_{\ell}$ of weight ℓ and multiplicity index p,

$$\mathbf{X}^{p}_{\ell} = \widetilde{\mathbf{G}}^{p}_{(\ell|n)} \odot^{n} \mathbf{T}_n. \tag{18}$$

Conversely, $\mathbf{G}^{p}_{(\ell|n)}$ embeds $\mathbf{X}^{p}_{\ell}$ into $\mathcal{T}^{n}$,

$$\mathbf{S}^{\ell,p}_{n} = \mathbf{G}^{p}_{(\ell|n)} \odot^{\ell} \mathbf{X}^{p}_{\ell}. \tag{19}$$

The embedded tensors reconstruct the original tensor through the ordinary sum,

$$\mathbf{T}_n = \sum_{\ell=0}^{n} \sum_{p=1}^{N_\ell} \mathbf{S}^{\ell,p}_{n}. \tag{20}$$

Equations (1) and (20) are the same decomposition in two forms: a direct sum of the ICTs $\mathbf{X}^{p}_{\ell}$, each of rank ℓ, or an ordinary sum of their embeddings $\mathbf{S}^{\ell,p}_{n}$, each of rank n. Although $\mathbf{S}^{\ell,p}_{n}$ has 3^n components, only $2\ell + 1$ are independent, since it carries no information beyond $\mathbf{X}^{p}_{\ell}$. For example, the three embedded tensors for a rank-2 tensor are provided in Table I.

III. INDEPENDENT AND ORTHONORMAL MAPPING TENSORS

The reduction and embedding operators of Sec. II generate candidate mapping tensors $\mathbf{G}^{p}_{(\ell|n)}$. At rank two, nothing further is needed, as Table I shows: each weight occurs once, its single candidate is the mapping tensor, and the familiar isotropic, antisymmetric, and symmetric traceless parts follow at once. From rank three on, a weight can occur more than once, and Eq. (13) may then generate more candidates than there are independent ones (Table II): of the three weight-2 candidates in Eq. (14), only two are needed. This is the obstacle, and it surfaces in the Gram matrix $\mathbf{g}$ of Eq. (15), which a linearly dependent set makes singular, so that the inverse-Gram construction of Eq. (16) cannot be applied to the full candidate set. An independent subset must therefore be selected first.

The selected subset is independent but generally not orthonormal, $\mathbf{g} \neq \mathbf{I}$. Nothing breaks: the reduction goes through the dual pair $\mathbf{G}^{p}_{(\ell|n)}$ and $\widetilde{\mathbf{G}}^{p}_{(\ell|n)}$, at the cost of building and storing two operator sets, one for extraction and one for embedding. An orthonormal set is the more convenient basis, as an orthonormal basis usually is: it is self-dual, so a single set serves in both directions, and it leaves the ICTs on an equal footing, none scaled differently from another by the choice of mappings.

We address both in this section. We first count the candidates and determine the multiplicity of each weight, then select an independent subset by an exact QR factorization, and finally orthonormalize the selected subset using the Gram matrix. Everything stays within the operator formalism of Sec. II: the independent subset and the orthonormal set are again constant operators, precomputable for a given rank and weight and reusable for every tensor of that class.

TABLE II. Numbers N_ℓ of independent mapping tensors by rank n and weight ℓ. Parentheses give the number N^{c}_{ℓ} of candidate mapping tensors when $N^{c}_{\ell} \neq N_\ell$.

	Rank n						
Weight ℓ	0	1	2	3	4	5	6
0	1		1	1	3	6(10)	15
1		1	1	3	6	15	36(45)
2			1	2(3)	6	15(30)	40(45)
3				1	3(6)	10	29(90)
4					1	4(10)	15
5						1	5(15)
6							1

A. Number of independent mapping tensors

In Eq. (13), the natural projector is fixed by the weight alone, so at a given rank n and weight ℓ, the candidates differ only through the rank-lowering tensor. Each $\mathbf{F}^{p}_{n\to\ell}$ yields one $\mathbf{G}^{p}_{(\ell|n)}$, so there are N^{c}_{ℓ} candidates, indexed by $p = 1, 2, \ldots, N^{c}_{\ell}$. A closed-form expression for N^{c}_{ℓ} is derived in Appendix B, and the values through rank six are listed in Table II.

The number of these candidates that are linearly independent is the multiplicity N_ℓ of that weight in the reduction spectrum of a rank-n tensor. Following Ref. 3, N_ℓ is determined recursively using the angular-momentum addition rule: ICTs of weights ℓ_1 and ℓ_2 combine into ICTs of every weight ℓ satisfying $|\ell_1 - \ell_2| \le \ell \le \ell_1 + \ell_2$. Since each Cartesian index has weight one, the weight content of the rank-2 reduction spectrum is $1 \otimes 1 = 0 \oplus 1 \oplus 2$. That of rank three is $1 \otimes 1 \otimes 1 = 1 \otimes (0 \oplus 1 \oplus 2) = 0 \oplus 1_3 \oplus 2_2 \oplus 3$, where the subscripts denote multiplicities. Repeating this tensor-product decomposition gives the multiplicities at higher ranks. The resulting multiplicities are listed alongside N^{c}_{ℓ} in Table II.

For ranks $n \le 2$, each weight has multiplicity $N_\ell = 1$. Moreover, $N_\ell = N^{c}_{\ell}$ at every weight, so every candidate mapping tensor is independent. At higher ranks, however, $N_\ell > 1$ in general, while $N^{c}_{\ell} > N_\ell$ for some weights. At the top weight $\ell = n$, $N_n = N^{c}_{n} = 1$ for every rank because no rank lowering is needed there and Eq. (13) reduces to $\mathbf{G}_{(n|n)} = \mathbf{E}_{(n|n)}$. A generic tensor of any rank n therefore has exactly one ICT of weight n.

B. Selection of an independent set

For a given rank n and weight ℓ, we now determine the linear dependencies among the N^{c}_{ℓ} candidate mapping tensors $\mathbf{G}^{p}_{(\ell|n)}$ and identify a subset of N_ℓ linearly independent ones. A linear

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ALGORITHM 1. Identification of linearly independent mapping tensors.

Input: Candidate mapping tensors $\{\mathbf{G}^{p}_{(\ell|n)}\}_{p=1}^{N_\ell^{\mathrm{c}}}$
Output: Index set $\mathcal{I}$ of linearly independent mapping tensors
for $p = 1$ to N_ℓ^{c} **do**
  $\mathbf{v}^p \leftarrow \mathrm{reshape}\,(\mathbf{G}^{p}_{(\ell|n)})$ ▷ Length $d = 3^{\ell+n}$
end for
$\mathbf{A} \leftarrow [\mathbf{v}^1, \mathbf{v}^2, \ldots, \mathbf{v}^{N_\ell^{\mathrm{c}}}]$ ▷ $d \times N_\ell^{\mathrm{c}}$ matrix
$\tilde{\mathbf{Q}}, \mathbf{U} \leftarrow \mathrm{exactQR}\,(\mathbf{A})$ ▷ rational; columns of $\tilde{\mathbf{Q}}$ orthogonal
$\mathcal{I} \leftarrow \emptyset$
for $k = 1$ to N_ℓ^{c} **do**
  if $\|\tilde{\mathbf{q}}_k\|^2 \neq 0$ **then** ▷ Exact, in rational arithmetic
    $\mathcal{I} \leftarrow \mathcal{I} \cup \{k\}$
  end if
end for
return $\mathcal{I}$

dependence among them is specified by a nonzero coefficient vector $\mathbf{w} = (w_1, w_2, \ldots, w_{N_\ell^{\mathrm{c}}})^{\mathsf{T}}$ satisfying $\sum_{p=1}^{N_\ell^{\mathrm{c}}} w_p \mathbf{G}^{p}_{(\ell|n)} = \mathbf{0}$. Reshaping each $\mathbf{G}^{p}_{(\ell|n)}$ into a vector $\mathbf{v}^p$ of length $d = 3^{\ell+n}$ is linear and one-to-one, so the relation becomes $\mathbf{A}\mathbf{w} = \mathbf{0}$ once the $\mathbf{v}^p$ are stacked as the columns of a matrix $\mathbf{A}$. The problem is therefore to determine the column rank of $\mathbf{A}$ and select N_ℓ independent columns. A QR factorization of $\mathbf{A}$ provides this selection,[34] as set out in Algorithm 1. The entries of $\mathbf{A}$ are rational, since the candidates are built from $\boldsymbol{\delta}$ and $\boldsymbol{\epsilon}$ alone, and we factorize $\mathbf{A} = \tilde{\mathbf{Q}}\mathbf{U}$ in rational arithmetic, where the columns $\tilde{\mathbf{q}}_k$ of $\tilde{\mathbf{Q}}$ are mutually orthogonal and not normalized and $\mathbf{U}$ is unit upper triangular. A column of $\mathbf{A}$ that is a linear combination of the earlier ones gives $\tilde{\mathbf{q}}_k = \mathbf{0}$, so the independent columns are those with $\|\tilde{\mathbf{q}}_k\|^2 \neq 0$.

From here on, $\mathbf{G}^{p}_{(\ell|n)}$ denotes the selected independent set, with $p = 1, 2, \ldots, N_\ell$. We note that the set is not unique; any basis of the weight-ℓ mapping space is valid. The three candidates of Eq. (14), for instance, span a two-dimensional space, and any two of them (or two independent linear combinations) may serve. The worked examples and `natto` fix one choice by the conventions of Sec. S5 of the supplementary material, which also explains why some choice cannot be avoided.

C. Orthonormal mapping tensors

An orthonormal choice of the mappings always exists, as noted in Ref. 6, and we now construct it explicitly. The mapping tensors selected in Sec. III B are independent, so their Gram matrix $\mathbf{g}$ of Eq. (15) is positive definite as well as symmetric and therefore has a unique symmetric positive-definite inverse square root,[33] which we denote by $\mathbf{g}^{-1/2}$. It can be obtained by diagonalizing $\mathbf{g}$ and taking the inverse square roots of its eigenvalues, as detailed in Appendix D. The *orthonormal mapping tensors* are then defined by

$$\widehat{\mathbf{G}}^{p}_{(\ell|n)} = \sum_{q=1}^{N_\ell} (\mathbf{g}^{-1/2})_{pq} \mathbf{G}^{q}_{(\ell|n)}. \tag{21}$$

The orthonormal set is not unique; the symmetric inverse square root selects one basis within each repeated weight. The $\widehat{\mathbf{G}}^{p}_{(\ell|n)}$ satisfy the relation (derived in Appendix D)

$$\widehat{\mathbf{G}}^{p}_{(\ell|n)} \odot^{n} \widehat{\mathbf{G}}^{q}_{(\ell|n)} = \delta_{pq} \mathbf{E}_{(\ell|\ell)}. \tag{22}$$

They are therefore orthonormal and self-dual, so the same $\widehat{\mathbf{G}}^{p}_{(\ell|n)}$ performs both extraction, replacing $\widetilde{\mathbf{G}}^{p}_{(\ell|n)}$ in Eq. (18), and embedding, replacing $\mathbf{G}^{p}_{(\ell|n)}$ in Eq. (19),

$$\mathbf{X}^{p}_{\ell} = \widehat{\mathbf{G}}^{p}_{(\ell|n)} \odot^{n} \mathbf{T}_n, \quad \mathbf{S}^{\ell,p}_{n} = \widehat{\mathbf{G}}^{p}_{(\ell|n)} \odot^{\ell} \mathbf{X}^{p}_{\ell}. \tag{23}$$

Substituting Eq. (23) into Eq. (20) reconstructs $\mathbf{T}_n$ using only the orthonormal mapping tensors,

$$\mathbf{T}_n = \sum_{\ell=0}^{n} \sum_{p=1}^{N_\ell} \widehat{\mathbf{G}}^{p}_{(\ell|n)} \odot^{\ell} \left(\widehat{\mathbf{G}}^{p}_{(\ell|n)} \odot^{n} \mathbf{T}_n \right). \tag{24}$$

The reduction can therefore be carried out in either of two ways: with the dual pair $\mathbf{G}^{p}_{(\ell|n)}$ and $\widetilde{\mathbf{G}}^{p}_{(\ell|n)}$ of Sec. II F or with the single self-dual $\widehat{\mathbf{G}}^{p}_{(\ell|n)}$. Both span the same weight-ℓ mapping space, so both recover the same total weight-ℓ content $\sum_p \mathbf{S}^{\ell,p}_{n}$ of $\mathbf{T}_n$; the individual $\mathbf{X}^{p}_{\ell}$ are not the same, the two differing in how the N_ℓ channels within a repeated weight are apportioned. The dual pair keeps every entry rational, as $\mathbf{g}^{-1}$ is rational whenever $\mathbf{g}$ is. The orthonormal set needs only a single operator, and by Eq. (22), it makes the reduction an isometry: $\|\mathbf{T}_n\|^2 = \sum_{\ell,p} \|\mathbf{X}^{p}_{\ell}\|^2$, with no cross terms between channels of the same weight. Its coefficients are, in general, irrational, however, since $\mathbf{g}^{-1/2}$ is. Computing the mapping tensors is fast: with `natto`, all orthonormal mapping tensors of a rank-n tensor take 10 ms at rank four and 1.5 s at rank six on one central processing unit (CPU) core (Apple M4 Pro), and they are built once for all tensors of that rank. The timings, and those with an intrinsic symmetry, are given in Sec. S12 of the supplementary material.

IV. REDUCTION OF TENSORS WITH INTRINSIC SYMMETRY

Having established how to select and orthonormalize mappings for generic tensors, we now extend the construction to tensors with intrinsic symmetry, sketched in Fig. 1(b). Physical property tensors almost always carry an intrinsic symmetry: certain permutations of their indices leave the components unchanged or reverse their sign. Table III lists common examples with their symmetries and reduction spectra.[3] The symmetry-free construction of Sec. III cannot be applied directly because a symmetry-constrained tensor no longer distinguishes all of its ICTs. What survives at each weight is, in general, not a subset of the candidate mappings but a subspace of their span: those linear combinations that transform under the prescribed index permutations with the prescribed sign. The multiplicity therefore drops from N_ℓ to the dimension of that subspace, which may be anything from N_ℓ down to zero.

To make this concrete, let us look at some examples. A weight may lose all of its channels: in three dimensions, an antisymmetric index pair transforms like a single vector index under rotations, so the rank-2 rotation-rate tensor, $W_{ij} = -W_{ji}$, keeps only its weight-1

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TABLE III. Reduction spectrum of some physical tensors. Intrinsic symmetries are denoted using parentheses and square brackets: indices inside parentheses are symmetric, whereas indices inside square brackets are antisymmetric so that (ij) represents $T_{ij} = T_{ji}$ and $[ij]$ represents $T_{ij} = -T_{ji}$, and nested groups are exchanged as a unit, as in $((ij)(kl))$ for the elastic tensor. N_{ind} is the number of independent components, and the entries under weight ℓ are the multiplicities: N_ℓ for the unconstrained classes, and the symmetry-restricted $N_\ell^{\mathcal{S}}$ of Sec. IV once an intrinsic symmetry is imposed. SHG: second-harmonic generation.

				Weight ℓ						
Rank n	Symmetry	Example	N_{ind}	0	1	2	3	4	5	6
0		Pressure	1	1						
1	i	Spontaneous polarization	3		1					
2	ij	Optical activity	9	1	1	1				
	(ij)	Stress and strain	6	1		1				
	$[ij]$	Rotation rate	3		1					
3	ijk	Second-order optical mixing	27	1	3	2	1			
	$i(jk)$	Piezoelectric effect	18		2	1	1			
	(ijk)	Kleinman symmetry in SHG	10		1		1			
	$[ij]k$	Hall effect	9	1	1	1				
4	$ijkl$	Third-order optical mixing	81	3	6	6	3	1		
	$(ij)kl$	Photoelastic effect	54	2	3	4	2	1		
	$(ij)(kl)$	Kerr effect	36	2	1	3	1	1		
	$i(jkl)$	Third-harmonic generation	30	1	1	2	1	1		
	$((ij)(kl))$	Second-order elasticity	21	2		2		1		
	$(ijkl)$	Cauchy relations	15	1		1		1		
6	$ijklmn$		729	15	36	40	29	15	5	1
	$((ij)(kl)(mn))$	Third-order elasticity	56	3		3	1	2		1

channel, with the weight-0 and weight-2 multiplicities of a general rank-2 tensor both falling to zero.[35] The rank-3 piezoelectric tensor, symmetric in its last two indices, $d_{ijk} = d_{ikj}$, loses its weight-0 channel the same way, with the single weight-0 channel of a general rank-3 tensor not surviving the symmetry. A weight can also lose only some of its channels: a general rank-4 tensor has three weight-0 channels, T_{iijj}, T_{ijij}, and T_{ijji}, and for an elastic tensor, the minor symmetry $C_{ijkl} = C_{ijlk}$ makes the last two coincide, so the weight-0 multiplicity drops from three to two. The rest of this section builds a systematic construction for an arbitrary intrinsic symmetry, one that covers them all: the rotation-rate and piezoelectric tensors are worked through in Sec. S7 of the supplementary material and the elastic tensor in Sec. V.

An intrinsic symmetry is prescribed by a set of generators, each consisting of an index-permutation operator Π_a and a sign η_a, $a = 1, 2, \ldots, N_\Pi$,

$$\Pi_a \mathbf{T}_n = \eta_a \mathbf{T}_n, \quad \eta_a \in \{+1, -1\}. \tag{25}$$

Together, these generators define the intrinsic-symmetry class $\mathcal{S}$. Only a generating set needs to be prescribed: a tensor invariant under the Π_a is automatically invariant under every permutation they generate, with the sign given by the corresponding product of the η_a. The elastic tensor C_{ijkl} has $N_\Pi = 2$ generators: a minor symmetry, exchanging the indices within the leading pair, and the major symmetry, exchanging the two pairs,

$$(\Pi_1 \mathbf{C})_{ijkl} = C_{jikl}, \ (\Pi_2 \mathbf{C})_{ijkl} = C_{klij}, \ \eta_1 = \eta_2 = +1. \tag{26}$$

The remaining minor symmetry, $C_{ijkl} = C_{ijlk}$, follows by composing them as $\Pi_2\Pi_1\Pi_2$.

The construction rests on one observation: an intrinsic symmetry constrains how the operators may be built, not how the ICTs behave. Because every mapping that respects it lies in the span of the symmetry-free ones already at hand, the constraint becomes a linear condition on N_ℓ coefficients, and the tensor itself never enters. The procedure below carries that out in three steps.

Procedure 2. At each weight ℓ, the symmetry-adapted mapping tensors $\mathbf{Q}^p_{(\ell|n)}$ are obtained from the set of independent mapping tensors $\{\mathbf{G}^p_{(\ell|n)}\}_{p=1}^{N_\ell}$ of Sec. III as follows:

(i) write each $\mathbf{Q}$ as a general combination of $\mathbf{G}$, Eq. (27), and require it to carry the prescribed symmetry, Eq. (28);
(ii) evaluate how that symmetry transforms $\mathbf{G}$, Eq. (29); and
(iii) select the combinations that survive, giving $\mathbf{Q}$, Eq. (31).

Starting with step (i), each $\mathbf{Q}^p_{(\ell|n)}$, $p = 1, 2, \ldots, N_\ell^{\mathcal{S}}$, lies in the weight-$\ell$ mapping space, so it can be written as a linear combination of the mapping tensors $\{\mathbf{G}^q_{(\ell|n)}\}$,

$$\mathbf{Q}^p_{(\ell|n)} = \sum_{q=1}^{N_\ell} c_q^p \mathbf{G}^q_{(\ell|n)}, \tag{27}$$

where $\mathbf{c}^p = (c_1^p, c_2^p, \ldots, c_{N_\ell}^p)^{\mathsf{T}}$ is a coefficient vector to be determined, as is $N_\ell^{\mathcal{S}}$, the number of independent symmetry-adapted mappings

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at weight ℓ. Permuting the indices of $\mathbf{T}_n$ permutes those of the mapping tensors and leaves the ICTs untouched, so the symmetry is imposed on the $\mathbf{Q}^p_{(\ell|n)}$: each must transform as $\mathbf{T}_n$ does in Eq. (25),

$$\Pi_a \mathbf{Q}^p_{(\ell|n)} = \eta_a \mathbf{Q}^p_{(\ell|n)}. \tag{28}$$

Turning to step (ii), imposing this condition requires the action of each generator on the mapping tensors $\mathbf{G}^q_{(\ell|n)}$, since $\Pi_a \mathbf{Q}^p_{(\ell|n)} = \sum_q c^p_q \, \Pi_a \mathbf{G}^q_{(\ell|n)}$. The permuted mapping $\Pi_a \mathbf{G}^q_{(\ell|n)}$ remains in the same weight-ℓ mapping space and can therefore be expanded uniquely in the same basis,

$$\Pi_a \mathbf{G}^q_{(\ell|n)} = \sum_{p=1}^{N_\ell} M^a_{pq} \mathbf{G}^p_{(\ell|n)}. \tag{29}$$

The duals isolate its entries (Appendix E),

$$M^a_{pq} = \frac{\widetilde{\mathbf{G}}^p_{(\ell|n)} \odot^{\ell+n} \left(\Pi_a \mathbf{G}^q_{(\ell|n)} \right)}{2\ell + 1}. \tag{30}$$

Hence, $\mathbf{M}^a$, which records how generator a mixes the N_ℓ mappings, is built from operators already in hand.

In step (iii), substituting Eqs. (27) and (29) into the requirement Eq. (28) gives the linear system (see Appendix E),

$$\left(\mathbf{M}^a - \eta_a \mathbf{I} \right) \mathbf{c}^p = \mathbf{0}. \tag{31}$$

In words, the surviving mappings are those the permutation leaves alone up to the prescribed sign: they are the eigenvectors of $\mathbf{M}^a$ at eigenvalue η_a, and N^S_ℓ is the dimension of that eigenspace.

A weight loses a channel whenever some combination of its candidates extracts nothing from any tensor of the class, and the constraint discards exactly those combinations. The extremes are the ones easiest to recognize: the combination can be the difference of two candidates that extract the same ICT, as T_{ijij} and T_{ijji} do for an elastic tensor, or a single candidate that extracts nothing on its own, as the trace W_{ii} does for the rotation-rate tensor. Both are special cases of the same rule: the combination may run over any number of candidates, which is why Eq. (31) is solved as a linear system rather than found by inspection. This is not the reduction carried out in Sec. III B, where candidates were cut because some were redundant for any tensor; here, they stay independent, in general, and lose their independence only against the intrinsic symmetry.

Solving Eq. (31), for example, by Gaussian elimination, gives N^S_ℓ independent coefficient vectors $\{\mathbf{c}^p\}_{p=1}^{N^S_\ell}$, which Eq. (27) turns into the symmetry-adapted mapping tensors. Which basis of solutions is taken, and how it is scaled and ordered, is again a choice, fixed in Sec. S5 of the supplementary material. These carry the prescribed symmetry on their Cartesian indices and span every weight-ℓ mapping compatible with that symmetry. For several generators, the conditions for $\Pi_1, \Pi_2, \ldots, \Pi_{N_\Pi}$ are imposed simultaneously so that every $\mathbf{c}^p$ satisfies all the prescribed symmetries. The combined system and its exact solution are detailed in Appendix E.

The $\mathbf{Q}^p_{(\ell|n)}$ are again independent mapping tensors between $\mathcal{X}^\ell$ and $\mathcal{T}^n$, being combinations of the $\mathbf{G}^q_{(\ell|n)}$. Sections II F and III C assumed no more than this, so the Gram matrix, the duals, the extraction and embedding, and the orthonormalization all carry over with the $\mathbf{Q}^p_{(\ell|n)}$ in place of the $\mathbf{G}^p_{(\ell|n)}$ and N^S_ℓ in place of N_ℓ. Either route may therefore be taken: the dual pair $\mathbf{Q}^p_{(\ell|n)}$ and $\widetilde{\mathbf{Q}}^p_{(\ell|n)}$ or the self-dual orthonormal $\widehat{\mathbf{Q}}^p_{(\ell|n)}$, with the reconstruction of Eq. (24) holding in either case.

This completes the construction: given the generators of an intrinsic symmetry, Procedure 2 yields the symmetry-adapted mapping tensors at every weight, and with them the reduction spectrum of the symmetry class, at any rank. Section V applies the construction to the rank-4 elastic tensor.

V. APPLICATION TO THE ELASTIC TENSOR

Elastic tensors describe how a material responds to mechanical load. A small deformation is measured by the symmetric strain ε_{ij} and the internal force it generates by the symmetric stress σ_{ij}, and expanding one in powers of the other gives a hierarchy of response tensors,[36]

$$\sigma_{ij} = C_{ijkl} \, \varepsilon_{kl} + \frac{1}{2} \, C_{ijklmn} \, \varepsilon_{kl} \varepsilon_{mn} + \cdots. \tag{32}$$

The leading term defines the second-order elastic tensor C_{ijkl} of rank four (also called the stiffness tensor), the linear response of Hooke's law that fixes the moduli, the sound velocities, and the mechanical stability of a crystal;[37,38] the next defines the third-order elastic tensor C_{ijklmn} of rank six, the leading anharmonic correction. Because the strain is symmetric, each tensor is symmetric within every index pair, and because each derives from the strain energy, each is also symmetric under permutation of its pairs, giving the symmetry classes $((ij)(kl))$ and $((ij)(kl)(mn))$ with 21 and 56 independent components.

The construction treats the two in the same way, one symmetry class in place of another. Complete reductions of both, with the symmetry-restricted multiplicities, mapping bases, Gram matrices, and duals at every surviving weight, are given in Sec. S7 of the supplementary material. The rest of this section follows the rank-4 tensor: its decomposition, the weight fractions that partition its anisotropy, and what they reveal across computed elastic tensors.

A. Reduction of the elastic tensor

The symmetry class $((ij)(kl))$ of the second-order elastic tensor $\mathbf{C}$ collects the minor symmetries $C_{ijkl} = C_{jikl} = C_{ijlk}$ and the major symmetry $C_{ijkl} = C_{klij}$. Its two generators are those of Eq. (26).

Applying the construction to this symmetry class yields the reduction spectrum listed in Table III,

$$\mathbf{C} = 2 \, \mathbf{X}_0 \oplus 2 \, \mathbf{X}_2 \oplus \mathbf{X}_4. \tag{33}$$

The 21 independent components are recovered by summing the dimensions of the ICTs, $2 \times 1 + 2 \times 5 + 1 \times 9 = 21$. Physically, the two scalars $\mathbf{X}_0$ capture the isotropic response (the two rotational invariants that fix the orientation-averaged bulk and shear moduli), while the weight-2 ICTs $\mathbf{X}_2$ and the weight-4 ICT $\mathbf{X}_4$ encode finer angular dependence of the anisotropic elastic response successively.[3]

We now construct the operators behind this spectrum. The candidates follow from Eq. (13): the rank-lowering tensors of Eq. (3)

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pair the four Cartesian indices in the three possible ways, and $E_{(0|0)} = 1$, so

$$G^1_{(0|4)} = \delta_{i_1 i_2}\delta_{i_3 i_4},$$
$$G^2_{(0|4)} = \delta_{i_1 i_3}\delta_{i_2 i_4}, \tag{34}$$
$$G^3_{(0|4)} = \delta_{i_1 i_4}\delta_{i_2 i_3}.$$

Algorithm 1 finds these $N_0^c = 3$ candidates linearly independent, so none is discarded and the multiplicity is $N_0 = 3$. Each symmetry-adapted mapping is then a combination $\mathbf{Q}^p_{(0|4)} = \sum_q c^p_q \mathbf{G}^q_{(0|4)}$ of these three, Eq. (27), with the coefficients still to be found.

The minor symmetry gives $\Pi_1 \mathbf{G}^1_{(0|4)} = \mathbf{G}^1_{(0|4)}$, $\Pi_1 \mathbf{G}^2_{(0|4)} = \mathbf{G}^3_{(0|4)}$, and $\Pi_1 \mathbf{G}^3_{(0|4)} = \mathbf{G}^2_{(0|4)}$, while the pair exchange Π_2 leaves all three unchanged. Expanding these in the basis through Eq. (30) gives

$$\mathbf{M}^1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{M}^2 = \mathbf{I}, \tag{35}$$

so the major symmetry imposes nothing at this weight. With $\eta_1 = \eta_2 = +1$, the conditions in Eq. (31) reduce to $c_2 = c_3$ with c_1 free, giving $N_0^S = 2$ and the sparse solution basis $\mathbf{c}^1 = (1,0,0)^\mathsf{T}$, $\mathbf{c}^2 = (0,1,1)^\mathsf{T}$, and hence, via Eq. (27),

$$Q^1_{(0|4)} = \delta_{i_1 i_2}\delta_{i_3 i_4}, \quad Q^2_{(0|4)} = \delta_{i_1 i_3}\delta_{i_2 i_4} + \delta_{i_1 i_4}\delta_{i_2 i_3}. \tag{36}$$

The remaining steps are those of Sec. II F, applied to the $\mathbf{Q}^p_{(0|4)}$: their Gram matrix and its inverse, Eq. (15), are

$$\mathbf{g}^Q = \begin{pmatrix} 9 & 6 \\ 6 & 24 \end{pmatrix}, \quad (\mathbf{g}^Q)^{-1} = \begin{pmatrix} \frac{2}{15} & -\frac{1}{30} \\ -\frac{1}{30} & \frac{1}{20} \end{pmatrix}. \tag{37}$$

Combining the duals of Eq. (16) with the extraction of Eq. (18), and using Eqs. (36) and (37), gives

$$X^1_0 = \frac{2}{15}C_{iijj} - \frac{1}{15}C_{ijij}, \quad X^2_0 = -\frac{1}{30}C_{iijj} + \frac{1}{10}C_{ijij}. \tag{38}$$

Embedding them back with Eq. (19), with the symmetry-adapted $\mathbf{Q}^p_{(0|4)}$ in place of the $\mathbf{G}^p_{(\ell|n)}$, gives the weight-0 part of $\mathbf{C}$,

$$X^1_0\ \delta_{i_1 i_2}\delta_{i_3 i_4} + X^2_0(\delta_{i_1 i_3}\delta_{i_2 i_4} + \delta_{i_1 i_4}\delta_{i_2 i_3}), \tag{39}$$

in which we recognize the classical isotropic elastic tensor of the Lamé decomposition.[37] The two scalars the construction extracts are the Lamé constants themselves, $\lambda = X^1_0$ and $\mu = X^2_0$.

The weight-0 sector exercises the full machinery: the candidates of Eq. (13), the multiplicity from Algorithm 1, the symmetry adaptation of Procedure 2, and the Gram matrix, duals, extraction, and embedding of Sec. II F. Weights 2 and 4 follow the same route, with larger matrices at each step and nothing new in kind. The complete reduction of $\mathbf{C}$ is collected in Sec. S7 of the supplementary material, which adds to the weight-0 construction above the weight-2 and weight-4 mappings, their Gram matrices and duals, and the resulting ICTs. The third-order elastic tensor, at rank six, is reduced there by the same route.

B. Weight-resolved anisotropy

The reduction of Sec. V A says which ICTs an elastic tensor has; the ICTs themselves say how much of the elastic response each one carries. Elastic anisotropy thereby becomes measurable in a resolved way: each weight has a definite angular dependence, so the response separates into an isotropic part and anisotropic parts of weight two and weight four, and the share carried by each is a physical quantity in its own right. We can thus build a single scalar index that reports how anisotropic a crystal is, while the shares also report which angular dependence that anisotropy has.

These shares are well defined because rotations do not mix different weights, so the embeddings are mutually orthogonal in the Frobenius inner product and the squared norm of $\mathbf{C}$ partitions among them,[3,39]

$$\|\mathbf{C}\|^2 = \sum_\ell \|\mathbf{C}_\ell\|^2. \tag{40}$$

Here, $\mathbf{C}_\ell$ is the weight-ℓ part of $\mathbf{C}$, assembled from its ICTs by the embedding of Eq. (19) as $\mathbf{C}_\ell = \sum_p \mathbf{Q}^p_{(\ell|4)} \odot^\ell \mathbf{X}^p_\ell$, and its norm follows from the Gram matrix of Eq. (15),

$$\|\mathbf{C}_\ell\|^2 = \mathbf{C}_\ell \odot^4 \mathbf{C}_\ell = \sum_{p,q} g_{pq}\left(\mathbf{X}^p_\ell \odot^\ell \mathbf{X}^q_\ell\right). \tag{41}$$

The share of the total carried by each weight is the weight fraction,

$$f_\ell = \frac{\|\mathbf{C}_\ell\|^2}{\|\mathbf{C}\|^2}, \quad \sum_\ell f_\ell = 1, \tag{42}$$

so f_0 is the isotropic share of the response, while f_2 and f_4 measure the anisotropy carried at each weight. The anisotropic weights together carry $1 - f_0$ of the response, and the anisotropy weight fractions,

$$\hat{f}_\ell = \frac{f_\ell}{1 - f_0}, \quad \ell \neq 0, \quad \sum_{\ell \neq 0} \hat{f}_\ell = 1, \tag{43}$$

give the weight-ℓ share of that, for any tensor that is not isotropic. For $\mathbf{C}$, there are only two anisotropic weights, so $\hat{f}_2 + \hat{f}_4 = 1$, and either one carries the division on its own. Being ratios, the weight fractions are dimensionless and invariant under rotation and under overall scaling of $\mathbf{C}$, so materials of different overall stiffness are directly comparable. Within a repeated weight, the mapping basis is fixed only up to an invertible mixing of the channels, which redistributes norm among them but leaves $\mathbf{C}_\ell$ unchanged, with the duals of Eq. (16) transforming inversely. The weight fractions are therefore the same whether $\mathbf{Q}^p_{(\ell|4)}$ or the orthonormal mappings of Sec. III C are used.

Because the weight-0 subspace is itself rotation invariant, $\mathbf{C}_0$ is the orthogonal projection of $\mathbf{C}$ onto the isotropic elastic tensors of Eq. (36), so $1 - f_0$ is the squared distance to isotropy, obtained without fitting. It is the quantity compared with established anisotropy measures in Sec. V C. The weight fractions also inherit the crystal's symmetry: because rotations do not mix weights, its point-group invariance factorizes into an independent condition on each ICT, so if the Laue class admits no invariant of weight ℓ, meaning that no nonzero ICT of weight ℓ is left unchanged by all its symmetry operations, f_ℓ vanishes, as f_2 does for cubic crystals.

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The weight fractions generalize the classical measure of cubic anisotropy. The cubic classes admit no invariant at weight two[40] (supplementary material, Sec. S8), so the entire anisotropy of a cubic crystal is the single weight-4 ICT and $f_4 = 1 - f_0$; evaluating the weight-0 norm from Eq. (41), with Eqs. (37) and (38), gives

$$f_4 = \frac{6}{5}\,\frac{(C_{11} - C_{12} - 2C_{44})^2}{\|\mathbf{C}\|^2}, \tag{44}$$

which vanishes precisely when the Zener ratio $A = 2C_{44}/(C_{11} - C_{12})$ equals unity.[41] A vanishing weight fraction therefore need not come from symmetry: the cubic classes admit an invariant of weight four, yet f_4 vanishes for a cubic crystal with $A = 1$. Together with the Lamé constants at weight zero in Eq. (38), the same operators thus reproduce classical elasticity at both ends of the cubic spectrum without elasticity-specific input. The Zener ratio, however, is defined only for cubic crystals. The weight fractions are defined for crystals of any symmetry, reproduce the cubic criterion as the special case just shown, and in addition record which weight the anisotropy occupies.

C. First-principles elastic tensors

Elastic anisotropy varies widely across crystalline materials, and the weight fractions give a resolved way to survey it. We apply them to all 10 276 second-order elastic tensors from the Materials Project,[29,30,42] asking how much of the elastic response is isotropic, how the remainder divides between weights two and four, and how that picture relates to the anisotropy measures already in use. The survey is possible at this scale because the mapping tensors are precomputed once for the $((ij)(kl))$ class, so each material costs a single contraction.

Figure 2(a) resolves the three weight fractions by the crystal system. The isotropic part dominates throughout, with its mean fraction of the squared norm being 0.88 for triclinic crystals and 0.95 for hexagonal and cubic ones, so, measured by the norm, the anisotropic part of a real crystal is relatively small. Both anisotropic

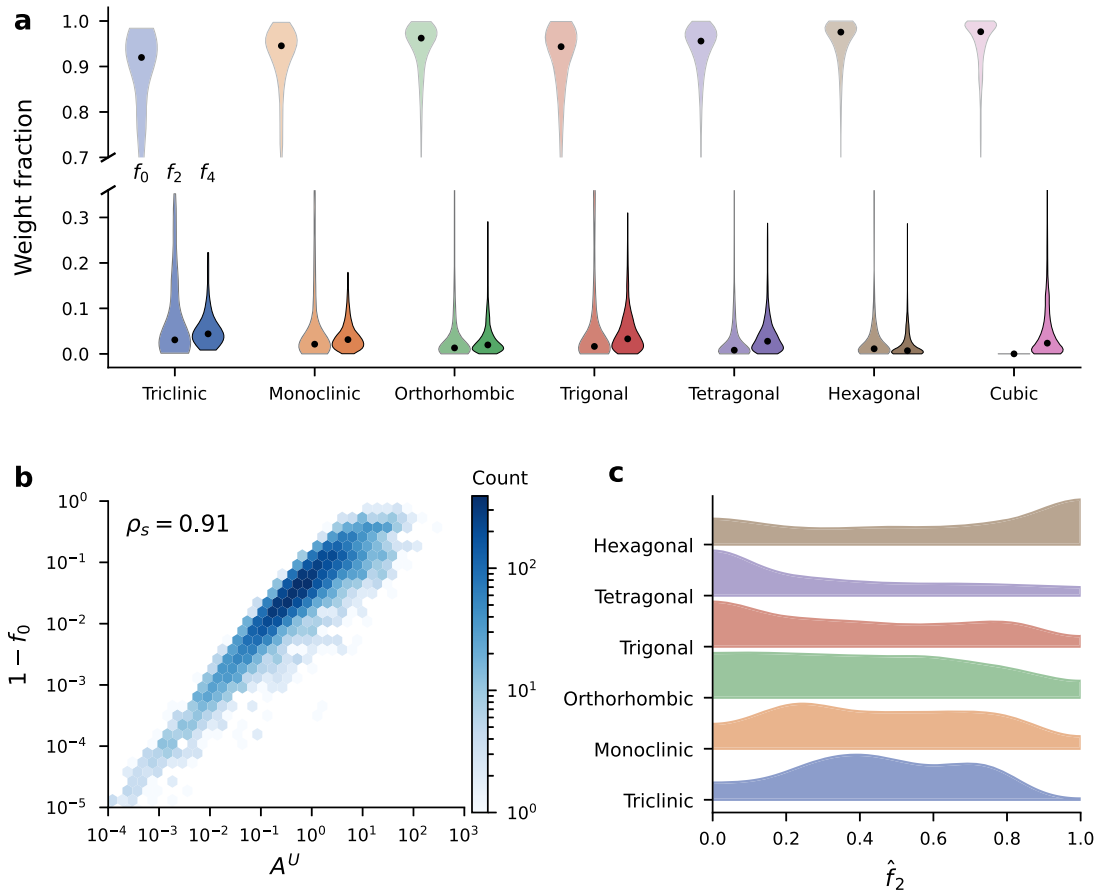


FIG. 2. Weight-resolved anisotropy of second-order elastic tensors from the Materials Project. (a) Distributions of the weight fractions f_0, f_2, and f_4 of Eq. (42) by crystal system; black dots mark the medians. The vertical axis is broken, the two segments being drawn to a common scale. (b) The squared distance to isotropy, $1 - f_0$, against the universal anisotropy index A^U, binned by material count, with ρ_s being the Spearman rank correlation. (c) Distributions of the anisotropy weight fraction $\hat{f}_2$ of Eq. (43) by the crystal system, each curve scaled to a common height. Cubic entries are omitted, with $\hat{f}_2$ vanishing identically for them.

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weights are populated in every class but the cubic one, where f_2 vanishes identically, the selection rule of Sec. V B is recovered, although the operators are built for the $((ij)(kl))$ class alone and nothing about cubic symmetry enters them.

The weight fractions measure how the squared norm of $\mathbf{C}$ is distributed over the weights, and f_0 close to unity means that the norm is almost entirely carried by the isotropic part. This, however, does not rule out a strong directional dependence of the mechanical response, for example, of the shear or Young's modulus. As shown in Sec. V A, the isotropic part $\mathbf{C}_0$ is the Lamé tensor with the Lamé constants λ and μ of Eq. (38), equivalently a bulk modulus $K = \lambda + \frac{2}{3}\mu$ and a shear modulus $G = \mu$,[37] which for these λ and μ are the Voigt averages of the moduli of the crystal.[43] Both are the same in every direction, so they carry no directional information, yet they contribute to the squared norm of the isotropic part. A material with a large bulk modulus can therefore have f_0 close to unity even when its moduli, such as the shear or Young's modulus, vary strongly with direction. Applied to the compliance, the inverse of $\mathbf{C}$, the same reduction gives the Reuss averages[43] in place of the Voigt ones for the isotropic part.

We next compare $1 - f_0$ with the measures of elastic anisotropy already in use. All of them are built from the mismatch between the Voigt and Reuss bounds on the bulk and shear moduli, a gap that closes only for an isotropic material. Writing K_V, G_V and K_R, G_R for those bounds, they are the universal index[44] $A^U = 5G_V/G_R + K_V/K_R - 6$, the log-Euclidean index[45] $A^L = ([\ln(K_V/K_R)]^2 + 5[\ln(G_V/G_R)]^2)^{1/2}$, and the Chung–Buessem shear and bulk anisotropies[46] $A_G = (G_V - G_R)/(G_V + G_R)$ and $A_B = (K_V - K_R)/(K_V + K_R)$. Because f_0 is a norm fraction rather than a bound mismatch, the comparison sets two ways of quantifying the same departure from isotropy against each other. Figure 2(b) makes it for A^U, and Table IV does this for all four. The rank correlation with A^U, A^L, and A_G is uniformly high, and resolving it by crystal system leaves it between 0.89 and 0.95 in every group, so it does not arise from pooling symmetries. Rank correlation is the appropriate comparison, the measures differing widely in scale; the lower raw Pearson value for A^U reflects its unbounded range rather than a genuinely weaker association. Since these measures encode established practice, the agreement validates f_0 rather than distinguishing it. The bulk anisotropy A_B is the exception, and the fault lies with it rather than with f_0: cubic symmetry forces $K_V = K_R$, so A_B vanishes for the 41% of the database that is cubic, although those crystals are not isotropic.

TABLE IV. Correlation of $1 - f_0$ with established scalar measures of elastic anisotropy. The measures A^U, A^L, A_G, and A_B are defined in the text. Spearman is the rank correlation; the Pearson columns are computed on the raw values and on their logarithms. Values of A_B below 10^{-12} in magnitude are rounding noise and are set to zero, which applies to the 4217 cubic crystals, for which $A_B = 0$ by symmetry; these are excluded from the logarithm, and all other quantities are positive for every crystal.

Measure	Spearman	Pearson	Pearson (log)
A^U	0.91	0.56	0.93
A^L	0.91	0.76	0.94
A_G	0.90	0.76	0.93
A_B	0.41	0.73	0.61

A scalar index reports one number, and the weight fractions add a second dimension to it. Figure 2(c) shows the distribution of the anisotropy weight fraction $\hat{f}_2$ of Eq. (43) for each crystal system, the cubic entries being omitted because the selection rule fixes $\hat{f}_2 = 0$ for them. Pooled, the fifth to ninety-fifth percentiles run from 0.02 to 0.94, and no crystal system covers less than three quarters of that interval, so how the anisotropy divides between weights two and four is a property of the material rather than of its symmetry. The established measures fix the magnitude of the departure from isotropy, on which f_0 agrees with them, while f_2 and f_4 record which weight that departure occupies.

VI. CARTESIAN HARMONICS

The construction now turns from property tensors to the ICTs themselves: building them from a vector here and coupling two of them in Sec. VII. The ICTs built from a vector $\mathbf{a}$ are the *Cartesian harmonics*, one for each weight n; their components are homogeneous polynomials of degree n in the Cartesian coordinates that satisfy Laplace's equation, that is, solid harmonics. The reduction of Secs. II–IV produces them with no new machinery and yields a single operator for each weight. The construction below uses the unit vector $\hat{\mathbf{a}} = \mathbf{a}/a$, of length $a = |\mathbf{a}|$, which fixes the scale; homogeneity restores the general case, $\mathbf{V}_n(\mathbf{a}) = a^n \mathbf{V}_n(\hat{\mathbf{a}})$.

The rank-n polyadic $\hat{\mathbf{a}}^{\otimes n}$ has components $\hat{a}_{i_1}\hat{a}_{i_2}\cdots\hat{a}_{i_n}$. Full symmetry is one of the intrinsic symmetries treated in Sec. IV, so the reduction developed in Secs. II–IV applies to it unchanged. Two properties of the polyadic simplify that reduction: $\hat{\mathbf{a}}$ has unit length, and $\hat{\mathbf{a}}^{\otimes n}$ is fully symmetric.

Unit length disposes of the rank lowering. A harmonic of weight $\ell < n$ is built from $\hat{\mathbf{a}}^{\otimes \ell}$ directly, and $\hat{a}_i\hat{a}_i = 1$ makes the weight-ℓ part of $\hat{\mathbf{a}}^{\otimes n}$ proportional to it, so nothing is lost by taking the polyadic of the weight one wants. Step (i) of Procedure 1 therefore never enters, and the mapping tensor of Eq. (13) reduces to the projector alone, $\mathbf{G}_{(n|n)} = \mathbf{E}_{(n|n)}$.

Full symmetry eliminates symmetrization and simplifies what is left. Step (ii) of Procedure 1, the average over index permutations, is already carried out in $\hat{\mathbf{a}}^{\otimes n}$, so the projector has only the traces of step (iii) to remove, and it does that in one step: the weight-n part of $\hat{\mathbf{a}}^{\otimes n}$ is $\mathbf{E}_{(n|n)} \odot^n \hat{\mathbf{a}}^{\otimes n}$. The projector itself also simplifies because each of its terms averages over all $n!$ permutations of the Greek indices and, separately, over all $n!$ permutations of the Roman ones, and the Roman permutations only change which index of $\hat{\mathbf{a}}^{\otimes n}$ each $\boldsymbol{\delta}$ meets. They therefore contribute equally; their average may be dropped, and δ^t_{ii} comes outside it, leaving

$$E_{(n|n)} \cong \sum_{t=0}^{\lfloor n/2 \rfloor} c_t \left\langle \delta_{\alpha i}^{\,n-2t} \delta^t_{\alpha\alpha} \right\rangle \delta^t_{ii}, \tag{45}$$

with the coefficients c_t of Eq. (7) unchanged. Here, $\cong$ marks an equality that holds when both sides are contracted with a fully symmetric tensor, not a generic tensor. Appendix F gives the detailed steps.

What the reduction does not fix is the normalization. The projector $\mathbf{E}_{(n|n)}$ is scaled so as to return a weight-n tensor unchanged,

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whereas harmonics are conventionally scaled by the Legendre polynomial they generate.[5,6,22] Rescaling Eq. (45) by $C = (2n-1)!!/n!$ gives the *harmonic operator*,

$$H_{(n|n)} = C \sum_{t=0}^{\lfloor n/2 \rfloor} c_t \left\langle \delta_{\alpha i}^{\,n-2t} \delta_{\alpha\alpha}^{t} \right\rangle \delta_{ii}^{t}. \tag{46}$$

Contracting it with the polyadic returns the Cartesian harmonic of weight n, $\mathbf{V}_n = \mathbf{H}_{(n|n)} \odot^n \hat{\mathbf{a}}^{\otimes n}$, which has the Legendre property,

$$\mathbf{V}_n \odot^n \hat{\mathbf{b}}^{\otimes n} = P_n(\hat{\mathbf{a}} \cdot \hat{\mathbf{b}}) \tag{47}$$

for every unit vector $\hat{\mathbf{b}}$, where P_n is the Legendre polynomial of degree n and, in particular, $\mathbf{V}_n \odot^n \hat{\mathbf{a}}^{\otimes n} = P_n(1) = 1$. Appendix G verifies Eq. (47).

The $2n+1$ independent components of $\mathbf{V}_n$ span the degree-n solid harmonics; Appendix F writes out $\mathbf{H}_{(2|2)}$ and $\mathbf{H}_{(3|3)}$ and the harmonics they produce. With this normalization, Eq. (46) agrees with the Cartesian harmonic tensor of Ref. 22, and Sec. S9 of the supplementary material gives the conversion between the two conventions. Although mathematically equivalent, the two differ in form. The classical result is an expression for the harmonic of a given direction, with $\hat{\mathbf{a}}$ written inside it, whereas $\mathbf{H}_{(n|n)}$ depends only on n and meets the vector only through a contraction. Bond directions, surface normals, gradients, and other vector descriptors are the elementary building blocks of orientational order parameters in materials modeling and of equivariant machine learning models built on irreducible Cartesian tensors,[15–17] and the construction applies to all of them directly.

VII. COUPLING OF IRREDUCIBLE CARTESIAN TENSORS

Given two ICTs $\mathbf{X}_{\ell_1}$ and $\mathbf{Y}_{\ell_2}$, their product $\mathbf{P}_n = \mathbf{X}_{\ell_1} \otimes \mathbf{Y}_{\ell_2}$ is a tensor of rank $n = \ell_1 + \ell_2$, symmetric within its first ℓ_1 indices and within its last ℓ_2 but not across the two groups. That is an intrinsic symmetry in the sense of Sec. IV, so the reduction developed there applies to $\mathbf{P}_n$ unchanged. Its irreducible parts $\mathbf{Z}_{\ell_3}$ have weights $|\ell_1 - \ell_2| \le \ell_3 \le \ell_1 + \ell_2$, following the same selection rule as Clebsch–Gordan coupling in the spherical formalism.[20] For each weight triple, the reduction yields a single operator that produces $\mathbf{Z}_{\ell_3}$ from the pair by contraction.

As in Sec. VI, two properties simplify the reduction, here narrowing the choices within its steps rather than removing steps outright: being ICTs, $\mathbf{X}_{\ell_1}$ and $\mathbf{Y}_{\ell_2}$ are traceless, and each is symmetric. A contraction taken inside either of them vanishes, so only contractions between the two survive, and since each is symmetric, all such contractions give the same result. Step (i) of Procedure 1 is therefore left with a single candidate instead of the N_ℓ^c of Sec. II C, and step (iii) with a single series. Step (ii) is not free, since $\mathbf{P}$ is symmetric only within each group, and it is carried out by $\mathbf{E}_{(\ell_3|\ell_3)}$ along with the trace removal.

Write α for the indices of $\mathbf{X}_{\ell_1}$, β for those of $\mathbf{Y}_{\ell_2}$, and γ for the free indices of $\mathbf{Z}_{\ell_3}$. Write $L = \ell_1 + \ell_2 + \ell_3$, and let $L_i = \lfloor L/2 \rfloor - \ell_i$ be the *triangle numbers* of the weight triple. Each L_i counts the contractions between the two groups other than i: L_1 those between $\mathbf{Y}_{\ell_2}$ and $\mathbf{Z}_{\ell_3}$, L_2 those between $\mathbf{X}_{\ell_1}$ and $\mathbf{Z}_{\ell_3}$, and L_3 those between $\mathbf{X}_{\ell_1}$ and $\mathbf{Y}_{\ell_2}$. By the two properties above, rank lowering keeps only the L_3 contractions between $\mathbf{X}_{\ell_1}$ and $\mathbf{Y}_{\ell_2}$, so the rank-lowering tensors $\mathbf{F}^{p}_{n\to\ell_3}$ of Sec. II C reduce to a single candidate. It takes one of the two forms of Sec. II C, $\boldsymbol{\epsilon}$ entering exactly when the rank drop $n - \ell_3$ is odd, which is the parity of $L = n + \ell_3$,

$$F_{n\to\ell_3} = \begin{cases} \delta_{\alpha\beta}^{\,L_3}, & L \text{ even}, \\ \epsilon_{\gamma\alpha\beta}\, \delta_{\alpha\beta}^{\,L_3}, & L \text{ odd}, \end{cases} \tag{48}$$

every $\boldsymbol{\delta}$, and the $\boldsymbol{\epsilon}$ of the odd case, taking one index from each group.

The natural projector $\mathbf{E}_{(\ell_3|\ell_3)}$ of Eq. (7) simplifies for the same reason. The symmetrization of step (ii) collapses, every surviving permutation of the Roman indices returning the same tensor. For the trace removal of step (iii), the projector's factor δ_{ii}^t takes t traces of $\mathbf{P}$, of which only the cross traces survive, each contracting $\mathbf{X}_{\ell_1}$ with $\mathbf{Y}_{\ell_2}$ once more, so the series is indexed by the number t of these. As in Eq. (45), δ_{ii}^t then comes outside the average, leaving the average over the free γ indices alone.

Composing the two through Eq. (13) gives a single mapping tensor $\mathbf{G}_{(\ell_3|n)} = \mathbf{E}_{(\ell_3|\ell_3)}\, \mathbf{F}_{n\to\ell_3}$, which reduces $\mathbf{P}$ to $\mathbf{Z}_{\ell_3}$. The composition carries c_t of Eq. (8) into

$$k_t = (-1)^t \, \frac{(2\ell_3 - 2t - 1)!!}{(2\ell_3 - 1)!!} \, \frac{L_2!\, L_1!}{(L_2 - t)!\, (L_1 - t)!\, t!}, \tag{49}$$

the counterpart of c_t for the coupling, derived in Sec. S9.1 of the supplementary material. With the weight-ℓ_3 mapping space one-dimensional, the selection and orthonormalization of Sec. III are not needed, and extraction and embedding differ only by the single Gram-matrix element g_{11}.

Rescaling $\mathbf{G}_{(\ell_3|n)}$ by a scalar C gives the *coupling operator* $\mathbf{K}_{(\ell_3|\ell_1,\ell_2)} = C\, \mathbf{G}_{(\ell_3|n)}$ for the weights (ℓ_1, ℓ_2, ℓ_3). When L is even,

$$K_{(\ell_3|\ell_1,\ell_2)} = C \sum_{t=0}^{\min(L_2,L_1)} k_t \left\langle \delta_{\alpha\gamma}^{\,L_2-t} \delta_{\beta\gamma}^{\,L_1-t} \delta_{\gamma\gamma}^{\,t} \right\rangle \delta_{\alpha\beta}^{\,L_3+t}, \tag{50}$$

and when L is odd,

$$K_{(\ell_3|\ell_1,\ell_2)} = C \sum_{t=0}^{\min(L_2,L_1)} k_t \left\langle \epsilon_{\alpha\beta\gamma}\, \delta_{\alpha\gamma}^{\,L_2-t} \delta_{\beta\gamma}^{\,L_1-t} \delta_{\gamma\gamma}^{\,t} \right\rangle \delta_{\alpha\beta}^{\,L_3+t}, \tag{51}$$

where the averages are those of Eq. (7), read as in Eq. (45): only the average over γ survives, and the factors $\delta_{\alpha\beta}$, which carry the contractions between $\mathbf{X}_{\ell_1}$ and $\mathbf{Y}_{\ell_2}$, stand outside it. Applied to the pair, it returns the weight-ℓ_3 ICT,

$$\mathbf{Z}_{\ell_3} = \left(\mathbf{K}_{(\ell_3|\ell_1,\ell_2)} \odot^{\ell_2} \mathbf{Y}_{\ell_2} \right) \odot^{\ell_1} \mathbf{X}_{\ell_1}. \tag{52}$$

The two contractions are independent, so the rank-$(\ell_1 + \ell_2)$ product $\mathbf{P}$ is never formed.

Here, C is a scaling factor, as in Sec. VI, and the one thing the construction leaves open. Its value depends on the three weights and differs between the even and odd cases. We fix it by the two conditions of Ref. 22: for even L, that two harmonics of the same direction couple to the harmonic of weight ℓ_3 of that direction; for odd L, where that coupling vanishes as the directions merge, that its rate of vanishing is unity. See Appendix G for the conditions in full, which give, for even L,

$$C = \frac{\ell_1!\, \ell_2!\, (2\ell_3 - 1)!!}{(2L_2 - 1)!!\, (2L_1 - 1)!!\, (2L_3 - 1)!!\, (L/2)!} \tag{53}$$

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and, for odd L,

$$C = \frac{2\,\ell_3\,\ell_1!\,\ell_2!\,(2\ell_3-1)!!}{(2L_2+1)!!\,(2L_1+1)!!\,(2L_3+1)!!\,\left(\frac{L+1}{2}\right)!}, \tag{54}$$

with $(-1)!! = 1$.

The two operators in Eqs. (50) and (51) agree with the coupling obtained previously, normalization included.[22] The coupling of two irreducible tensors into a given weight is unique up to a factor, so they also agree, up to normalization, with the fixed Cartesian coupling tensors of Ref. 7. What the derivation here adds is the route and the form. The coupling follows from Eq. (7), the operator that reduces an arbitrary tensor, rather than from a derivation specific to this problem. It is also delivered as a tensor that depends only on the three weights and meets $\mathbf{X}_{\ell_1}$ and $\mathbf{Y}_{\ell_2}$ only through contractions: the sum that produces it is carried out once, before $\mathbf{X}_{\ell_1}$ and $\mathbf{Y}_{\ell_2}$ are given, and the operator is reused for every pair at those weights. In the expression of Ref. 22, in contrast, $\mathbf{X}_{\ell_1}$ and $\mathbf{Y}_{\ell_2}$ appear inside every term of the sum, so it is carried out after they are given for each pair. The form used in Ref. 22 and its relation to ours are discussed in Sec. S9 of the supplementary material. The same coupling appears in the spherical formalism as the Clebsch–Gordan coefficients and, in the form symmetric in the three weights, as the 3j symbols; Sec. S10 of the supplementary material gives the Cartesian counterpart of the latter, and Sec. S11 of the supplementary material compares the two formalisms.

The cost of building and applying the coupling operators is given in Sec. S12 of the supplementary material.

VIII. CONCLUSION

We have presented a constructive Cartesian reduction of high-rank tensors with prescribed intrinsic symmetry into ICTs. The construction separates three tasks that are often entangled in hand-derived decompositions: constructing all symmetry-free candidate mappings from invariant tensors, resolving repeated weights by QR selection and Gram orthonormalization, and reinstating intrinsic symmetry through symmetry-adapted mapping tensors that reconstruct the original Cartesian tensor. This gives an explicit reduction–reconstruction pair rather than only a representation-theoretic spectrum.

The same construction also gives Cartesian operators for two further operations. The harmonic operators build the Cartesian harmonics from repeated products of a vector, and the coupling operators couple two ICTs into a third. These are the Cartesian counterparts of the spherical harmonics and of the Clebsch–Gordan coefficients, and both are operations at which a Cartesian treatment would otherwise convert to the spherical formalism. Keeping them in Cartesian form removes the conversion along with the phase and normalization conventions that come with it.

The elastic tensor puts the construction to work both where the answer is already known and where it is not. At rank four, it recovers the decomposition established in the elasticity literature,[4,13,25] with no elasticity-specific input. At rank six, it gives a systematic treatment of the third-order elastic tensor, previously handled case by case.[47–49] The same operators also make anisotropy measurable rather than merely classifiable. Distinct weights carry distinct angular dependence, so a material's departure from isotropy separates into parts that a single scalar index cannot tell apart. Nothing in this is specific to elasticity, with the same weight fractions resolving the angular content of any property tensor that the construction reduces, among them the piezoelectric and photoelastic tensors.

More broadly, the weight-resolved decomposition provides a design principle for equivariant machine learning. Predicting a tensor through its ICTs and embedding them back makes the output equivariant by construction and enforces its intrinsic symmetry exactly. The partition of the norm across weights also gives a weight-wise normalization of the learning targets. Part of the scheme developed here is already in use in Ref. 19.

Everything the construction produces shares one character. The natural projector, the rank-lowering and mapping tensors, and the harmonic and coupling operators are all constant isotropic arrays: built from $\boldsymbol{\delta}$ and $\boldsymbol{\epsilon}$ alone, and fixed by the ranks, weights, and intrinsic symmetry at hand rather than by the data they act on. Each can therefore be pre-evaluated once, in exact symbolic or in numerical form, stored as an array, and then reused for every tensor of that rank and symmetry. Applying it is a single tensor contraction, the operation an array library provides through, for example, matrix multiplication or `einsum`. The operators are fast to build, and the reduction and the tensor product that apply them are fast to evaluate (supplementary material, Sec. S12). Reduction, reconstruction, formation of harmonics, and coupling are then the same operation with different stored arrays, which makes the construction straightforward to implement and use. They are what the open-source package `natto`[31] builds, stores, and applies.

SUPPLEMENTARY MATERIAL

The supplementary material provides additional mathematical details and worked examples supporting the construction presented in the main text. It includes (1) the number of independent components of an irreducible Cartesian tensor, (2) the isotropic tensor identities used throughout, (3) the counts of distinct symmetrized products, (4) an explicit form of the natural projector, (5) the conventions that fix the channels of a repeated weight, (6) worked examples of the reduction for generic tensors and (7) for tensors with intrinsic symmetry, (8) the character counts behind the multiplicities and the crystal-system content, (9) the conversion between operator conventions, (10) the relation between the coupling operator and the Cartesian 3j tensor, and (11) a comparison of the Cartesian and spherical formalisms.

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AUTHOR DECLARATIONS

Conflict of Interest

The author has no conflicts to disclose.

Author Contributions

Mingjian Wen: Conceptualization (lead); Formal analysis (lead); Methodology (lead); Software (lead); Visualization (lead); Writing – original draft (lead); Writing – review & editing (lead).

DATA AVAILABILITY

The data that support the findings of this study are available within the article and its supplementary material. The `natto` package implementing the irreducible Cartesian tensor algorithms described in this work is openly available at https://github.com/wengroup/natto.[31]

APPENDIX A: NOTATION

Table V lists the symbols used throughout, and Table VI lists the tensor operations.

APPENDIX B: COUNTING RANK-LOWERING TENSORS

The distinct rank-lowering tensors $\mathbf{F}^{p}_{n\to\ell}$ correspond to the distinct ways of assigning the indices of $\mathbf{T}_n$ to the $\boldsymbol{\delta}$ and $\boldsymbol{\epsilon}$ factors in Eqs. (3) and (5), and counting those assignments gives N^{c}_{ℓ}. It is also the number of candidate mapping tensors, as summarized in Sec. III A.

The number of ways to form k disjoint unordered pairs from N labeled indices is

$$P(N,k) = \frac{1}{k!}\prod_{s=0}^{k-1}\binom{N-2s}{2} = \frac{N!}{(N-2k)!\;k!\;2^{k}}. \tag{B1}$$

TABLE V. Symbols.

Symbol	Indicial notation	Explanation
$\boldsymbol{\delta}$	δ_{ij}	Kronecker delta
$\boldsymbol{\epsilon}$	ϵ_{ijk}	Levi–Civita symbol
$\mathcal{T}^n$		Rank-n Cartesian tensor space
$\mathcal{X}^\ell$		Weight-ℓ ICT space
$\mathbf{a}$ and $\hat{\mathbf{a}}$	a_i and $\hat{a}_i$	Vector and the corresponding unit vector
$\mathbf{T}$ or $\mathbf{T}_n$	$T_{i_1 i_2 \ldots i_n}$	Rank-n tensor in $\mathcal{T}^n$
$\mathbf{U}$ or $\mathbf{U}_n$	$U_{i_1 i_2 \ldots i_n}$	Rank-n symmetric tensor in $\mathcal{T}^n$
$\mathbf{X}$ or $\mathbf{X}_\ell$	$X_{\alpha_1\alpha_2\ldots\alpha_\ell}$	Weight-ℓ ICT in $\mathcal{X}^\ell$
$\mathbf{X}^p_\ell$	$X^p_{\alpha_1\alpha_2\ldots\alpha_\ell}$	Weight-ℓ ICT in $\mathcal{X}^\ell$ with multiplicity index p
$\mathbf{S}^{\ell,p}_n$	$S^{\ell,p}_{i_1 i_2 \ldots i_n}$	Embedding of $\mathbf{X}^p_\ell$ in $\mathcal{T}^n$
$\mathbf{E}_{(\ell\|\ell)}$	$E_{(\alpha_1\ldots\alpha_\ell\|i_1\ldots i_\ell)}$	Natural projector, $\mathcal{T}^\ell \to \mathcal{X}^\ell$
$\mathbf{F}^p_{n\to\ell}$		Rank-lowering tensor, $\mathcal{T}^n \to \mathcal{T}^\ell$
$\mathbf{G}^p_{(\ell\|n)}$	$G^p_{(\alpha_1\ldots\alpha_\ell\|i_1\ldots i_n)}$	Mapping tensor, embeds $\mathcal{X}^\ell \to \mathcal{T}^n$
$\widetilde{\mathbf{G}}^p_{(\ell\|n)}$	$\widetilde{G}^p_{(\alpha_1\ldots\alpha_\ell\|i_1\ldots i_n)}$	Dual mapping tensor, extracts $\mathcal{T}^n \to \mathcal{X}^\ell$
$\widehat{\mathbf{G}}^p_{(\ell\|n)}$	$\widehat{G}^p_{(\alpha_1\ldots\alpha_\ell\|i_1\ldots i_n)}$	Orthonormal mapping tensor, self-dual, $\mathcal{T}^n \leftrightarrow \mathcal{X}^\ell$
$\mathbf{Q}^p_{(\ell\|n)}$	$Q^p_{(\alpha_1\ldots\alpha_\ell\|i_1\ldots i_n)}$	Symmetry-adapted mapping tensor, embeds $\mathcal{X}^\ell \to \mathcal{T}^n$
$\widetilde{\mathbf{Q}}^p_{(\ell\|n)}$	$\widetilde{Q}^p_{(\alpha_1\ldots\alpha_\ell\|i_1\ldots i_n)}$	Dual symmetry-adapted mapping tensor, extracts $\mathcal{T}^n \to \mathcal{X}^\ell$
$\widehat{\mathbf{Q}}^p_{(\ell\|n)}$	$\widehat{Q}^p_{(\alpha_1\ldots\alpha_\ell\|i_1\ldots i_n)}$	Orthonormal symmetry-adapted mapping tensor, self-dual, $\mathcal{T}^n \leftrightarrow \mathcal{X}^\ell$
$\mathbf{H}_{(n\|n)}$	$H_{(\alpha_1\ldots\alpha_n\|i_1\ldots i_n)}$	Harmonic operator
$\mathbf{V}_n$	$V_{i_1 i_2 \ldots i_n}$	Cartesian harmonic of weight n
$\mathbf{K}_{(\ell_3\|\ell_1,\ell_2)}$	$K_{(\gamma\ldots\|\alpha\ldots,\beta\ldots)}$	Cartesian coupling operator
$\mathbf{g}$	g_{pq}	Gram matrix of the $\mathbf{G}^p_{(\ell\|n)}$
$\mathcal{S}$		Intrinsic symmetry class of $\mathbf{T}_n$
Π_a, η_a		Index-permutation operator and sign of generator a
N^{c}_ℓ		Number of candidate mappings at weight ℓ, for a rank-n tensor
N_ℓ		Multiplicity at weight ℓ: The number of independent ICTs or channels
$N^{\mathcal{S}}_\ell$		Multiplicity at weight ℓ restricted to the symmetry class $\mathcal{S}$

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TABLE VI. Operations and relations.

Operation	Example	Explanation
$\otimes$	$\mathbf{T}\otimes\mathbf{S}\to T_{i_1\ldots i_n}S_{j_1\ldots j_n}$	Tensor product
$\otimes^n$	$\mathbf{a}^{\otimes n}\to a_{i_1}\cdots a_{i_n}$	n-fold tensor product
$\odot^n$	$\mathbf{T}\odot^n\mathbf{S}\to T_{i_1\ldots i_n}S_{i_1\ldots i_n}$	n-fold contraction
$\cong$		Equality under the specified conditions
$\langle\cdot\rangle$		Average over index permutations
$\lfloor\cdot\rfloor$		Floor function

The product chooses the pairs successively, and the factor $1/k!$ removes the ordering of the k pairs.

For even $n-\ell$, the $\boldsymbol{\delta}$ factors of Eq. (3), $k=(n-\ell)/2$ of them, draw their pairs from all n indices, so

$$N_\ell^{\mathrm{c}} = P(n,k) = \frac{n!}{\ell!\,\left(\frac{n-\ell}{2}\right)!\,2^{(n-\ell)/2}}. \tag{B2}$$

Read as two choices, in turn, the same count is $N_\ell^{\mathrm{c}}=\binom{n}{\ell}(n-\ell-1)!!$: which ℓ indices are left unpaired, these being the ones the rank-ℓ result keeps, and how the remaining $n-\ell$ are paired among themselves. For $\mathbf{F}^p_{3\to1}$ of Eq. (4), this is $3\times1=3$, the three choices of the contracted pair. As another example, for $n=5$ and $\ell=1$, it is $5\times3=15$, and leaving i_5 unpaired gives the three,

$$\delta_{i_1i_2}\delta_{i_3i_4},\ \delta_{i_1i_3}\delta_{i_2i_4},\ \delta_{i_1i_4}\delta_{i_2i_3}, \tag{B3}$$

with the other twelve following from the four other choices of unpaired index.

For odd $n-\ell$ and $\ell>0$, $\mathbf{F}^p_{n\to\ell}$ of Eq. (5) contains one $\boldsymbol{\epsilon}$ and $k=(n-\ell-1)/2$ of $\boldsymbol{\delta}$ factors. The two indices of $\mathbf{T}_n$ contracted with $\boldsymbol{\epsilon}$ can be chosen in $\binom{n}{2}$ ways; exchanging them changes only the sign and does not produce a distinct candidate. The k unordered $\boldsymbol{\delta}$ pairs are then selected from the remaining $n-2$ indices in $P(n-2,k)$ ways. Therefore,

$$N_\ell^{\mathrm{c}} = \binom{n}{2}P(n-2,k) = \frac{n!}{(\ell-1)!\,\left(\frac{n-\ell-1}{2}\right)!\,2^{(n-\ell+1)/2}}. \tag{B4}$$

After these contractions, $\ell-1$ indices of $\mathbf{T}_n$ remain; together with the free index of $\boldsymbol{\epsilon}$, they form the ℓ indices of the rank-lowered tensor.

The $\boldsymbol{\epsilon}$ and $\boldsymbol{\delta}$ factors are not interchangeable. For example, at $n=4$ and $\ell=1$, the candidates $F^p_{4\to1}=\epsilon_{ji_3i_4}\delta_{i_1i_2}$ and $F^q_{4\to1}=\epsilon_{ji_1i_2}\delta_{i_3i_4}$ use the same two pairs but assign them to different isotropic tensors and are therefore distinct candidates.

The remaining case is $\ell=0$ with n odd, where $\boldsymbol{\epsilon}$ contracts all three of its indices with $\mathbf{T}_n$ rather than supplying a free index,

$$F^p_{n\to0} = \epsilon_{i_wi_ui_v}\prod_{(a,b)\,\in\,\mathcal{D}_p}\delta_{i_ai_b}, \tag{B5}$$

where $k=(n-3)/2$ is the number of $\boldsymbol{\delta}$ factors. The rank of $\mathbf{F}^p_{n\to0}$ is $3+2k=n$, and all n indices are contracted with $\mathbf{T}_n$ in Eq. (2), leaving a scalar.

There are $\binom{n}{3}$ choices for the indices contracted with $\boldsymbol{\epsilon}$ and $P(n-3,k)$ pairings of the remaining indices. Permuting the three $\boldsymbol{\epsilon}$ indices changes at most the sign and does not produce a distinct candidate. Thus,

$$N_0^{\mathrm{c}} = \binom{n}{3}P(n-3,k) = \frac{n!}{6\cdot\left(\frac{n-3}{2}\right)!\,2^{(n-3)/2}}. \tag{B6}$$

For $n=3$, there is a single such tensor, the rank-3 $F^1_{3\to0}=\epsilon_{i_1i_2i_3}$. For $n=5$, $k=1$, and $N_0^{\mathrm{c}}=\binom{5}{3}=10$,

$$\begin{aligned}
F^1_{5\to0}&=\epsilon_{i_3i_4i_5}\delta_{i_1i_2},\ F^2_{5\to0}=\epsilon_{i_2i_4i_5}\delta_{i_1i_3},\\
F^3_{5\to0}&=\epsilon_{i_2i_3i_5}\delta_{i_1i_4},\ F^4_{5\to0}=\epsilon_{i_2i_3i_4}\delta_{i_1i_5},\\
F^5_{5\to0}&=\epsilon_{i_1i_4i_5}\delta_{i_2i_3},\ F^6_{5\to0}=\epsilon_{i_1i_3i_5}\delta_{i_2i_4},\\
F^7_{5\to0}&=\epsilon_{i_1i_3i_4}\delta_{i_2i_5},\ F^8_{5\to0}=\epsilon_{i_1i_2i_5}\delta_{i_3i_4},\\
F^9_{5\to0}&=\epsilon_{i_1i_2i_4}\delta_{i_3i_5},\ F^{10}_{5\to0}=\epsilon_{i_1i_2i_3}\delta_{i_4i_5},
\end{aligned} \tag{B7}$$

one for each choice of the three indices taken by $\boldsymbol{\epsilon}$, the remaining pair going to $\boldsymbol{\delta}$.

APPENDIX C: EXPLICIT FORM OF THE MAPPING TENSORS

Equation (13) writes the mapping tensor compactly as $\mathbf{G}^p_{(\ell|n)}=\mathbf{E}_{(\ell|\ell)}\mathbf{F}^p_{n\to\ell}$, leaving implicit which index of $\mathbf{T}_n$ meets which slot of the projector. This appendix writes that out in the two cases, the rank drop allows even and odd $n-\ell$.

When $n-\ell$ is even, let $i_{s_1},\ldots,i_{s_\ell}$ be the indices of $\mathbf{T}_n$ that do not occur in the pairs $\mathcal{D}_p$ of Eq. (3). These ℓ indices occupy the i-index slots of $\mathbf{E}_{(\ell|\ell)}$, giving

$$G^p_{(\ell|n)} = E_{(\alpha_1\ldots\alpha_\ell|i_{s_1}\ldots i_{s_\ell})}\prod_{(a,b)\,\in\,\mathcal{D}_p}\delta_{i_ai_b}. \tag{C1}$$

For example, take $n=3$ and $\ell=1$, where each $\mathcal{D}_p$ of Eq. (4) is a single pair and the one remaining index goes to the projector, $E_{(\alpha_1|i)}=\delta_{\alpha_1 i}$. The three choices give

$$\begin{aligned}
G^1_{(1|3)}&=E_{(\alpha_1|i_3)}\delta_{i_1i_2}=\delta_{\alpha_1i_3}\delta_{i_1i_2},\\
G^2_{(1|3)}&=E_{(\alpha_1|i_2)}\delta_{i_1i_3}=\delta_{\alpha_1i_2}\delta_{i_1i_3},\\
G^3_{(1|3)}&=E_{(\alpha_1|i_1)}\delta_{i_2i_3}=\delta_{\alpha_1i_1}\delta_{i_2i_3}.
\end{aligned} \tag{C2}$$

When $n-\ell$ is odd and $\ell>0$, let $i_{s_1},\ldots,i_{s_{\ell-1}}$ be the indices of $\mathbf{T}_n$ that occur in neither the pairs $\mathcal{D}_p$ nor the $\boldsymbol{\epsilon}$ pair (i_u,i_v) of Eq. (5).

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These $\ell-1$ indices occupy $\ell-1$ of the i-index slots of $\mathbf{E}_{(\ell|\ell)}$, while its remaining i-index slot is contracted with the free index j of $\boldsymbol{\epsilon}$,

$$G^{p}_{(\ell|n)} = E_{(\alpha_1\ldots\alpha_\ell|i_{s_1}\ldots i_{s_{\ell-1}}j)}\epsilon_{j\ i_u i_v}\prod_{(a,b)\,\in\,\mathcal{D}_p}\delta_{i_a i_b}, \tag{C3}$$

where j is summed. The three mapping tensors of Eq. (14), for $n=3$ and $\ell=2$, are the three choices of the index retained by $\mathbf{E}_{(2|2)}$ in this form. Substituting $\mathbf{E}_{(2|2)}$ from Table I expands them into $\boldsymbol{\delta}$ and $\boldsymbol{\epsilon}$ alone,

$$\begin{aligned}
G^{1}_{(2|3)} &= \frac{1}{2}\left(\delta_{\alpha_1 i_3}\epsilon_{\alpha_2 i_1 i_2} + \delta_{\alpha_2 i_3}\epsilon_{\alpha_1 i_1 i_2}\right) - \frac{1}{3}\delta_{\alpha_1\alpha_2}\epsilon_{i_1 i_2 i_3},\\
G^{2}_{(2|3)} &= \frac{1}{2}\left(\delta_{\alpha_1 i_2}\epsilon_{\alpha_2 i_1 i_3} + \delta_{\alpha_2 i_2}\epsilon_{\alpha_1 i_1 i_3}\right) + \frac{1}{3}\delta_{\alpha_1\alpha_2}\epsilon_{i_1 i_2 i_3},\\
G^{3}_{(2|3)} &= \frac{1}{2}\left(\delta_{\alpha_1 i_1}\epsilon_{\alpha_2 i_2 i_3} + \delta_{\alpha_2 i_1}\epsilon_{\alpha_1 i_2 i_3}\right) - \frac{1}{3}\delta_{\alpha_1\alpha_2}\epsilon_{i_1 i_2 i_3},
\end{aligned} \tag{C4}$$

with the middle sign differing because $\epsilon_{i_2 i_1 i_3} = -\epsilon_{i_1 i_2 i_3}$ while $\epsilon_{i_3 i_1 i_2} = \epsilon_{i_1 i_2 i_3}$. By construction in Eq. (7), $\mathbf{E}_{(\ell|\ell)}$ is symmetric under every permutation of its i indices, so the order in which its i-index slots receive the remaining indices and j does not affect the mapping tensor.

In the remaining case, $n-\ell$ odd with $\ell=0$, the projector is $E_{(0|0)}=1$, and the mapping tensor is the rank-lowering tensor itself, $G^{p}_{(0|n)} = F^{p}_{n\to 0}$, which Appendix B writes out.

At rank two, each weight has a single mapping tensor, and the two cases above reproduce the $G_{(\ell|n)}$ row of Table I, the $\ell=2$ entry because a zero rank drop leaves $\mathcal{D}_p$ empty and Eq. (C1) returns the projector alone.

APPENDIX D: GRAM MATRIX, DUALITY, AND ORTHONORMALITY

This appendix evaluates the Gram coefficient g_{pq} of Eq. (15), derives the duality relation Eq. (17) and the orthonormality relation Eq. (22), and gives the eigendecomposition used to compute $\mathbf{g}^{-1/2}$.

Taking the trace of both sides of Eq. (15) and rearranging gives

$$g_{pq} = \frac{\operatorname{tr}\left(\mathbf{G}^{p}_{(\ell|n)}\odot^{n}\mathbf{G}^{q}_{(\ell|n)}\right)}{\operatorname{tr}\,\mathbf{E}_{(\ell|\ell)}} = \frac{\mathbf{G}^{p}_{(\ell|n)}\odot^{\ell+n}\mathbf{G}^{q}_{(\ell|n)}}{2\ell+1}. \tag{D1}$$

In the second equality, the trace of a tensor carrying two groups of ℓ ICT-space indices is the contraction of the first group with the second, which adds ℓ contractions to the n of Eq. (15) and closes all $\ell+n$ indices of the two mapping tensors. The value $\operatorname{tr}\mathbf{E}_{(\ell|\ell)} = 2\ell+1$ comes from Sec. II D. Exchanging p and q leaves the numerator unchanged, so $g_{pq}=g_{qp}$ and $\mathbf{g}=[g_{pq}]$ is symmetric.

The duality relation Eq. (17) follows directly. Using Eqs. (15) and (16),

$$\begin{aligned}
\widetilde{\mathbf{G}}^{p}_{(\ell|n)}\odot^{n}\mathbf{G}^{q}_{(\ell|n)} &= \sum_{r}\left(\mathbf{g}^{-1}\right)_{pr}\left(\mathbf{G}^{r}_{(\ell|n)}\odot^{n}\mathbf{G}^{q}_{(\ell|n)}\right)\\
&= \sum_{r}\left(\mathbf{g}^{-1}\right)_{pr}g_{rq}\mathbf{E}_{(\ell|\ell)}\\
&= \left(\mathbf{g}^{-1}\mathbf{g}\right)_{pq}\mathbf{E}_{(\ell|\ell)}\\
&= \delta_{pq}\mathbf{E}_{(\ell|\ell)}.
\end{aligned} \tag{D2}$$

The inverse square root used in Eq. (21) is obtained from the eigendecomposition,

$$\mathbf{g} = \mathbf{W}\boldsymbol{\Lambda}\mathbf{W}^{\mathsf{T}}, \quad \boldsymbol{\Lambda} = \operatorname{diag}\,(\lambda_1,\ldots,\lambda_{N_\ell}), \tag{D3}$$

where $\mathbf{W}$ is orthogonal and all eigenvalues λ_p are positive. The symmetric positive-definite inverse square root is then

$$\begin{aligned}
\mathbf{g}^{-1/2} &= \mathbf{W}\boldsymbol{\Lambda}^{-1/2}\mathbf{W}^{\mathsf{T}},\\
\boldsymbol{\Lambda}^{-1/2} &= \operatorname{diag}\,(\lambda_1^{-1/2},\ldots,\lambda_{N_\ell}^{-1/2}).
\end{aligned} \tag{D4}$$

The orthonormality relation Eq. (22) follows by substituting Eq. (21) and applying Eq. (15),

$$\begin{aligned}
\widehat{\mathbf{G}}^{p}_{(\ell|n)}\odot^{n}\widehat{\mathbf{G}}^{q}_{(\ell|n)} &= \sum_{r,s}\left(\mathbf{g}^{-1/2}\right)_{pr}\left(\mathbf{g}^{-1/2}\right)_{qs}\left(\mathbf{G}^{r}_{(\ell|n)}\odot^{n}\mathbf{G}^{s}_{(\ell|n)}\right)\\
&= \sum_{r,s}\left(\mathbf{g}^{-1/2}\right)_{pr}g_{rs}\left(\mathbf{g}^{-1/2}\right)_{qs}\mathbf{E}_{(\ell|\ell)}\\
&= \left(\mathbf{g}^{-1/2}\mathbf{g}\mathbf{g}^{-1/2}\right)_{pq}\mathbf{E}_{(\ell|\ell)}\\
&= \delta_{pq}\mathbf{E}_{(\ell|\ell)}.
\end{aligned} \tag{D5}$$

Here, the third equality uses the symmetry of $\mathbf{g}^{-1/2}$, and the last uses $\mathbf{g}^{-1/2}\mathbf{g}\mathbf{g}^{-1/2}=\mathbf{I}$.

APPENDIX E: MIXING MATRICES AND SYMMETRY CONSTRAINTS

This appendix derives Eq. (30) for the mixing coefficients M^{a}_{pq} of Sec. IV, the constraint [Eq. (31)] that one generator imposes, and the stacked system for all N_Π generators. As in the main text, a fixed weight ℓ is understood throughout and is suppressed in the notation for $\mathbf{M}^{a}$.

To extract the M^{a}_{pq} of Eq. (29), contract that equation over the n Cartesian indices with the dual mapping tensor $\widetilde{\mathbf{G}}^{p}_{(\ell|n)}$ and use the duality relation [Eq. (17)],

$$\widetilde{\mathbf{G}}^{p}_{(\ell|n)}\odot^{n}\left(\Pi_a\mathbf{G}^{q}_{(\ell|n)}\right) = \sum_{r=1}^{N_\ell}M^{a}_{rq}\,\delta_{pr}\mathbf{E}_{(\ell|\ell)} = M^{a}_{pq}\mathbf{E}_{(\ell|\ell)}. \tag{E1}$$

The δ_{pr} that Eq. (17) supplies collapses the sum to its $r=p$ term. Taking the trace of both sides as in Eq. (D1) and dividing by $\operatorname{tr}\mathbf{E}_{(\ell|\ell)} = 2\ell+1$ gives Eq. (30).

Write $\mathbf{Q}=\sum_q c_q\mathbf{G}^{q}_{(\ell|n)}$ for a general combination of the mapping tensors, as in Eq. (27), and impose on it the requirement $\Pi_a\mathbf{Q}=\eta_a\mathbf{Q}$ that $\mathbf{Q}$ transforms as $\mathbf{T}_n$ does in Eq. (25). On the left-hand side, Π_a acts term by term, and Eq. (29) replaces each $\Pi_a\mathbf{G}^{q}_{(\ell|n)}$ by $\sum_p M^{a}_{pq}\mathbf{G}^{p}_{(\ell|n)}$, so

$$\Pi_a\left(\sum_{q=1}^{N_\ell}c_q\mathbf{G}^{q}_{(\ell|n)}\right) = \sum_{p=1}^{N_\ell}\left(\mathbf{M}^{a}\mathbf{c}\right)_p\,\mathbf{G}^{p}_{(\ell|n)}, \tag{E2}$$

while the right-hand side is simply $\eta_a\sum_p c_p\mathbf{G}^{p}_{(\ell|n)}$. Equating the two and collecting the coefficient of each $\mathbf{G}^{p}_{(\ell|n)}$ gives

$$\sum_{p=1}^{N_\ell}\left[\left(\mathbf{M}^{a}\mathbf{c}\right)_p - \eta_a c_p\right]\mathbf{G}^{p}_{(\ell|n)} = \mathbf{0}. \tag{E3}$$

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The $\mathbf{G}^{p}_{(\ell|n)}$ are independent as mappings on a general tensor, by the selection of Sec. III, so each bracket must vanish separately. Thus, $(\mathbf{M}^{a} - \eta_{a}\mathbf{I})\mathbf{c} = \mathbf{0}$; taking $\mathbf{c} = \mathbf{c}^{p}$ gives Eq. (31) for each symmetry-adapted mapping.

Imposing all N_Π generators at once gives the stacked system,

$$\mathbf{A}^{(\ell)}\mathbf{c} = \mathbf{0}, \quad \mathbf{A}^{(\ell)} = \begin{bmatrix} \mathbf{M}^{1} - \eta_{1}\mathbf{I} \\ \vdots \\ \mathbf{M}^{N_\Pi} - \eta_{N_\Pi}\mathbf{I} \end{bmatrix}. \tag{E4}$$

The admissible coefficient vectors are therefore the null space of $\mathbf{A}^{(\ell)}$, and the symmetry-restricted multiplicity is

$$N^{S}_{\ell} = N_{\ell} - \operatorname{rank}\mathbf{A}^{(\ell)}. \tag{E5}$$

The entries of $\mathbf{G}^{p}_{(\ell|n)}$, $\widetilde{\mathbf{G}}^{p}_{(\ell|n)}$, and hence $\mathbf{M}^{a}$ and $\mathbf{A}^{(\ell)}$ are rational, so the null space is obtained exactly by Gaussian elimination over the rationals. Its N^{S}_{ℓ} basis vectors define the symmetry-adapted mappings through Eq. (27); any other basis of the same null space gives the same mapping subspace.

If $\mathbf{A}^{(\ell)}$ has full column rank, the only solution is $\mathbf{c} = \mathbf{0}$ and weight ℓ is absent from the reduction spectrum of the symmetry class. If every $\mathbf{M}^{a} = \eta_{a}\mathbf{I}$, then $\mathbf{A}^{(\ell)} = \mathbf{0}$, and the symmetry imposes no restriction at that weight, so $N^{S}_{\ell} = N_{\ell}$.

APPENDIX F: PROJECTOR FOR A POLYADIC

This appendix gives the steps leading from Eq. (7) to Eq. (45) for a polyadic $\mathbf{a}^{\otimes n}$ and writes out the harmonic operators and the harmonics they give at low rank. Only full symmetry is used, so the result holds for any fully symmetric $\mathbf{U}_n$, and the length of $\mathbf{a}$ is left free; Sec. VI sets $a = 1$. Write Δ_t for the object inside the angle brackets of Eq. (7), taken at $\ell = n$, since the weight extracted here equals the rank, before either average is applied,

$$\begin{aligned} \Delta_t &= \delta_{\alpha i}^{\,n-2t}\,\delta^{t}_{\alpha\alpha}\,\delta^{t}_{ii} \\ &= \prod_{k=1}^{n-2t}\delta_{\alpha_k i_k}\prod_{k=1}^{t}\delta_{\alpha_{n-2k+1}\alpha_{n-2k+2}}\,\delta_{i_{n-2k+1}i_{n-2k+2}}. \end{aligned} \tag{F1}$$

The first product carries $n - 2t$ indices from Roman to Greek, and the second contracts the remaining $2t$ Greek indices in pairs and the remaining $2t$ Roman indices in the matching pairs. The average in Eq. (7) runs over the $(n!)^2$ pairs of Greek and Roman permutations of Δ_t.

Nothing so far restricts the argument, with Eq. (7) holding for any rank-n tensor. Contracting with $\mathbf{a}^{\otimes n}$ is what makes the Roman average redundant. Permuting the Roman indices of Δ_t only changes which index of $\mathbf{a}^{\otimes n}$ each $\boldsymbol{\delta}$ meets. Since $\mathbf{a}^{\otimes n}$ is unchanged by any permutation of its indices, all $n!$ Roman permutations contribute equally, and their average is any one of them. Fixing the Roman indices in the order written above leaves an average over the $n!$ Greek permutations alone, and the t factors δ_{ii} carry no Greek index and so stand outside it, giving Eq. (45). Rescaling it by $C = (2n-1)!!/n!$ forms the harmonic operator of Eq. (46).

Examples at low rank make the operator explicit. The coefficients c_t are those of Eq. (8), which depend on n as well as t and give $c_0 = 1$ for every n. For $n = 0$ and $n = 1$, only the $t = 0$ term is present and $C = 1$, so $\mathbf{H}_{(0|0)} = 1$ and $\mathbf{H}_{(1|1)} = \delta_{\alpha_1 i_1}$. The first two nontrivial cases are

$$\begin{aligned} \mathbf{H}_{(2|2)} &= \frac{3}{2}\left(\langle\delta^{2}_{\alpha i}\rangle - \frac{1}{3}\delta_{\alpha_1\alpha_2}\delta_{i_1 i_2}\right) \\ &\cong \frac{3}{2}\left(\delta_{\alpha_1 i_1}\delta_{\alpha_2 i_2} - \frac{1}{3}\delta_{\alpha_1\alpha_2}\delta_{i_1 i_2}\right) \end{aligned} \tag{F2}$$

for $n = 2$, with $C = 3/2$ and $c_1 = -1/3$, and

$$\begin{aligned} \mathbf{H}_{(3|3)} &= \frac{5}{2}\left(\langle\delta^{3}_{\alpha i}\rangle - \frac{3}{5}\langle\delta_{\alpha i}\delta_{\alpha\alpha}\rangle\delta_{i_2 i_3}\right) \\ &\cong \frac{5}{2}\left(\delta_{\alpha_1 i_1}\delta_{\alpha_2 i_2}\delta_{\alpha_3 i_3} - \frac{1}{5}\left(\delta_{\alpha_1 i_1}\delta_{\alpha_2\alpha_3} + \delta_{\alpha_2 i_1}\delta_{\alpha_1\alpha_3} + \delta_{\alpha_3 i_1}\delta_{\alpha_1\alpha_2}\right)\delta_{i_2 i_3}\right) \end{aligned} \tag{F3}$$

for $n = 3$, with $C = 5/2$ and $c_1 = -3/5$, the $\frac{1}{3}$ of the three-term average combining with c_1 to give the $\frac{1}{5}$ shown. The second line of each drops the Greek average on the $t = 0$ term, which a single representative product replaces once the argument is symmetric, hence the $\cong$ of Eq. (45); the $t \geq 1$ terms keep theirs, the result being symmetric in α only after the average is taken.

Contracting these operators with $\mathbf{a}^{\otimes n}$ sends each $\delta_{\alpha i}$ to a_α and each δ_{ii} to $a^2 = \mathbf{a}\cdot\mathbf{a}$, so they return the Cartesian harmonics, which are $V(\mathbf{a}) = 1$ and $V_i(\mathbf{a}) = a_i$ at $n = 0$ and $n = 1$, and

$$\begin{aligned} V_{ij}(\mathbf{a}) &= \frac{3}{2}\left(a_i a_j - \frac{1}{3}a^2\delta_{ij}\right), \\ V_{ijk}(\mathbf{a}) &= \frac{5}{2}\left(a_i a_j a_k - \frac{1}{5}a^2\left(\delta_{ij}a_k + \delta_{jk}a_i + \delta_{ki}a_j\right)\right), \end{aligned} \tag{F4}$$

one factor of a^2 for each δ_{ii}. The entries are homogeneous polynomials of degree two and three, each satisfying Laplace's equation.

Writing $a_i = a\hat{a}_i$ pulls a factor a^n out of every term,

$$V_{ij}(\mathbf{a}) = \frac{3}{2}\left(a^2\,\hat{a}_i\hat{a}_j - \frac{1}{3}a^2\delta_{ij}\right) = a^2\,V_{ij}(\hat{\mathbf{a}}), \tag{F5}$$

and likewise for V_{ijk}, leaving the unit-vector harmonics of Sec. VI and the scaling $\mathbf{V}_n(\mathbf{a}) = a^n\mathbf{V}_n(\hat{\mathbf{a}})$ stated there.

APPENDIX G: NORMALIZATION OF THE HARMONIC AND COUPLING OPERATORS

Contracting Eq. (45) with $\hat{\mathbf{a}}^{\otimes n}$ sends each δ_{ii} to unity and each $\delta_{\alpha i}$ to $\hat{a}_\alpha$. Contracting the result with a second unit vector $\hat{\mathbf{b}}$ replaces each $\hat{a}_\alpha$ by $u = \hat{\mathbf{a}}\cdot\hat{\mathbf{b}}$ and each $\delta_{\alpha\alpha}$ by unity, so every term of the average reduces to u^{n-2t},

$$\mathbf{V}_n \odot^{n} \hat{\mathbf{b}}^{\otimes n} = C\sum_{t=0}^{\lfloor n/2\rfloor} c_t\,u^{\,n-2t} = C\,\frac{n!}{(2n-1)!!}\,P_n(u). \tag{G1}$$

The second equality follows by writing the coefficients c_t of Eq. (8) in double-factorial form,

$$c_t = (-1)^t\,\frac{(2n-2t-1)!!}{(2n-1)!!}\,\frac{n!}{2^t\,t!\,(n-2t)!}, \tag{G2}$$

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since $(-1)^t(2n-2t-1)!!/[2^t t!(n-2t)!]$ is the coefficient of u^{n-2t} in the Legendre polynomial P_n, leaving the common factor $n!/(2n-1)!!$. The projector therefore delivers P_n up to a single overall factor, and $C = (2n-1)!!/n!$ removes it, giving Eq. (47) and, at $\hat{\mathbf{b}} = \hat{\mathbf{a}}$, the unit normalization $\mathbf{V}_n \odot^n \hat{\mathbf{a}}^{\otimes n} = P_n(1) = 1$.

The coupling constants of Sec. VII likewise rest on the conditions of Ref. 22. The constants of Eqs. (53) and (54) are fixed by two conditions on the ICT $\mathbf{Z}_{\ell_3}$ that Eqs. (50) and (51) produce from $\mathbf{X}_{\ell_1}$ and $\mathbf{Y}_{\ell_2}$. C is fixed for even L by requiring that when $\mathbf{X}_{\ell_1}$ and $\mathbf{Y}_{\ell_2}$ are constructed from a unit vector $\hat{\mathbf{a}}$ as in Eq. (46), $\mathbf{Z}_{\ell_3}$ obtained from Eq. (50) is the same as the ICT constructed from the same unit vector $\hat{\mathbf{a}}$ using Eq. (46). The second condition fixes C for odd L: when $\mathbf{X}_{\ell_1}$ is constructed from a unit vector $\hat{\mathbf{a}}$ and $\mathbf{Y}_{\ell_2}$ from another unit vector $\hat{\mathbf{b}}$,

$$\lim_{\hat{\mathbf{b}}\to\hat{\mathbf{a}}} \frac{|\mathbf{Z}_{\ell_3} \odot^{\ell_3-1} \hat{\mathbf{a}}^{\otimes \ell_3-1}|}{|\hat{\mathbf{a}} \times \hat{\mathbf{b}}|} = 1, \tag{G3}$$

where $|\cdot|$ denotes the norm of a vector.

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