MSGCorep: A package for corepresentations of magnetic space groups

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Abstract
Motivated by easy access to complete corepresentation (corep) data of all the 1651 magnetic space groups (MSGs) in three-dimensional space, we have developed a Mathematica package MSGCorep to provide an offline database of coreps and various functions to manipulate them, based on our previous package SpaceGroupIrep. One can use the package MSGCorep to obtain the elements of any MSG and magnetic little group, to calculate the multiplication of group elements, to obtain the small coreps at any k-point and full coreps of any magnetic k-star for any MSG and show them in a user-friendly table form, to calculate and show the decomposition of direct products of full coreps between any two specified magnetic k-stars, and to determine the small coreps of energy bands. Both single-valued and double-valued coreps are supported. In addition, the 122 magnetic point groups (MPGs) and their coreps are also supported by this package. To the best of our knowledge, MSGCorep is the first package that is able to calculate the direct product of full coreps for any MSG and able to determine small coreps of energy bands for general purpose. In a word, the MSGCorep package is an offline database and tool set for MSGs, MPGs, and their coreps, and it is very useful to study the symmetries in magnetic and nonmagnetic materials.

Keywords: corepresentation, magnetic space group, magnetic little group, direct product, Mathematica

Program summary

Program title: MSGCorep
Developer's repository link: https://github.com/goodluck1982/MSGCorep
Licensing provisions: GNU General Public Licence 3.0
Distribution format: tar.gz
Programming language: Wolfram
External routines/libraries used: SpaceGroupIrep (https://github.com/goodluck1982/SpaceGroupIrep)

Nature of problem: The package MSGCorep provides offline database and tools for easy access to 1651 magnetic space groups, 122 magnetic point groups, and their corepresentations. MSGCorep is the first package that is able to calculate the direct product of full corepresentations for any magnetic space group and able to determine small corepresentations of energy bands for general purpose.

Solution method: Corepresentations of a magnetic group are constructed from the representations of the maximal unitary subgroup of the magnetic group. Based on the complete representation data of 230 space groups provided by SpaceGroupIrep package, complete corepresentation data of 1651 magnetic space groups are derived in MSGCorep package.

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1. Introduction

It’s well known that group theory and symmetries play important roles in physics, especially in the booming topological physics in the recent decade [1–6]. An typical example is the application of space groups (SGs) and their representation theory in symmetry indicator method or topological quantum chemistry method to classify and search symmetry-protected band topology in nonmagnetic materials [7–18], and these two methods have been extended to magnetic space groups (MSGs) which are needed to describe the symmetries in magnetic materials [19–21]. Consequently, more and more interests are focused on MSGs and their applications in magnetic topological materials [22–28].

The term “magnetic (space) group” is also known as “Shubnikov (space) group” originating from A. V. Shubnikov who introduced the concept of anti-symmetry operation [29]. The anti-symmetry operation commutes with all spacial operations and can be defined as the change of an extra two-valued property. The change of color (black or white) is usually such an anti-symmetry operation in most general discussions about Shubnikov groups. While in the certain case of describing magnetic structures, time reversal operation $\mathcal{T}$ is the anti-symmetry operation which can reverse the direction (or sign) of magnetic moments. Accordingly, it can be said that MSG is a certain realization of Shubnikov group. In the case of MSG, $\mathcal{T}$ is an anti-unitary operation, but it should be emphasized that the anti-symmetry operation is not necessarily anti-unitary for general Shubnikov groups [29] and the color-changing operation is not always the same with $\mathcal{T}$ [30]. Nevertheless, MSGs are often described in terms of changing color due to historical reasons.

There are in total 1651 MSGs in three-dimensional space which can be divided into four types. The ordinary 230 SGs (also called Fedorov groups), which are all unitary, constitute the type-I MSGs, i.e. $M_I = G$ where $M_I$ and $G$ stand for type-I MSG and ordinary SG respectively. It is noteworthy that type-I MSGs can describe the magnetic structures of ferromagnetic (including ferrimagnetic, the same below) and antiferromagnetic, but not nonmagnetic (or paramagnetic) materials [31]. Type-II MSGs (230 in total, also called gray SGs) are of the form $M_{II} = G + \mathcal{T}G$ and can only describe nonmagnetic materials. Type-III MSGs (674 in total) are of the form $M_{III} = H + \mathcal{T}(G - H)$ in which the equi-translational subgroup $H$ consists of half the elements in $G$ and is also the maximal unitary subgroup of $M_{III}$. Similar to type-I MSGs, type-III MSGs can describe both ferromagnetic and antiferromagnetic materials. Type-IV MSGs (517 in total) are of the form $M_{IV} = G + \mathcal{T}\{E|t_0\}G$ in which $\{E|t_0\}$ is a pure translation in Seitz notation with $t_0$ half a lattice vector. Type-IV MSGs can only describe antiferromagnetic materials. Both type-III and type-IV MSGs are also called black-white SGs but only type-IV MSGs have black-white Bravais lattice due to the existence of $\mathcal{T}\{E|t_0\}$. Alternatively, type-III and type-IV are called $M_T$ and $M_R$ respectively by Litvin [32, 33] and called BW1 and BW2 respectively by Grimmer [34].

The tabulation of the irreducible representations (ireps) for the 230 SGs have been given in serveral monographs [29, 35–38], and the electronic data of them are also available in the ISOTROPY software suit [39, 40], on the Bilbao Crystallographic Server (BCS) [41–43], or in the SpaceGroupIrep package [44]. Introducing anti-unitary operations to MSGs makes it necessary to apply corepresentations (coreps), instead of ireps, to analyze the symmetries in most physics problems. However, to the best of our knowledge, the tabulation of irreducible coreps (irreducible is omitted for simplicity hereinafter) for all MSGs exists only in one book by Miller and Love [36], and the tabulation there is not complete and also difficult to read, as pointed out in Ref. [21]. Required by the study of magnetic topological quantum chemistry, it was not until recent two years that the first complete tabulation of the coreps for all MSGs were calculated and made publicly available on BCS [20, 21]. BCS is an excellent website for showing crystallographic data. It’s convenient to lookup small coreps of any specified k-point (i.e. wave vector) for any specified MSG on BCS. However, it’s not convenient to process all coreps of all MSGs ergodically because BCS does not provide offline tool to do this. Motivated by solving this problem, we have developed the package MSGCorep to provide offline database and functions for all coreps of MSGs, based on our homemade SpaceGroupIrep package for SGs as well as their irreps [44].

Generally speaking, the first step of applying the theory of MSG coreps to analyze energy bands is to determine the coreps of the bands, or more specifically, the irreducible coreps of the magnetic little group (MLG), also called “small coreps” here, at any required wave vector $k$ of the bands. Similarly, for ordinary SGs this step is to determine the small representations (reps) of the little groups (LGs) of the bands. There
have been several tools capable of doing this, e.g. irvsp [45], qeirreps [46], IrRep [47], and SpaceGroupRep [44]. However, there is still missing such a tool which can determine the MLG small cores for bands. Nevertheless, there is a precursor tool MagVasp2trace [20, 48] which is used to calculate the characters (i.e. the trace data) of the unitary operations of the MLGs for bands. In fact, MagVasp2trace was developed to assist the study of magnetic topological quantum chemistry, i.e. to prepare the trace data for the “Check Topological Magnetic Mat.” (CTMM) function on BCS [20, 49]. Although the CTMM has to determine first the small cores based on the input trace data, it is designed to analyze the topological properties using the determined cores, not to give the small cores directly. As a result, the CTMM is not a general tool to determine small cores at any k-points. To meet this requirement, we developed the getBandCorep function in our MSGCorep package which can determine small cores at any k-points based on the trace data from MagVasp2trace. This is the first tool to do this as we know.

2. Theory

2.1. Basis for corep

It’s well known that a group rep is defined by a homomorphism mapping to a matrix group. However, the corep of a nonunitary group, say a magnetic group $M$, is not defined by homomorphism any more. The corep matrices $D(M)$ obey the following algebra

$$\forall m_1, m_2 \in M \begin{cases} D(m_1)D(m_2) = D(m_1m_2), & m_1 \text{ is unitary} \\ D(m_1)D(m_2)^* = D(m_1m_2), & m_1 \text{ is anti-unitary} \end{cases}$$

and the set of matrices $D(M)$ is not necessarily a group. The corep of $M$ can be induced from an irep (a corep) $\Gamma$ of its unitary (nonunitary) subgroup $S$. However, this induction procedure is different from that of ordinary induced rep. To reflect this difference, here we use the symbol $\rightharpoonup$ instead of the ordinary $\rightrightarrows$ to describe the induced corep. Supposing that the (left) coset representatives of $S$ are $c_1, c_2, \cdots, c_r$ with $r = [M]/[S]$ being the index of the subgroup $S$ and $|M|$ being the size of the set $M$, then for $\forall m \in M$ the induced corep $\Gamma \rightharpoonup M$ of $M$ is defined as

$$(\Gamma \rightharpoonup M)_{\mu\nu}(m) = \begin{cases} \Gamma(c_\mu^{-1}mc_\nu), & c_\mu^{-1}mc_\nu \in S \text{ and } c_\mu \text{ is unitary} \\ \Gamma(c_\mu^{-1}mc_\nu)^*, & c_\mu^{-1}mc_\nu \in S \text{ and } c_\mu \text{ is anti-unitary} \\ 0, & \text{otherwise} \end{cases}$$

In fact, any nonunitary group $M$ can be written as $M = H + AH$, in which $H$ is the maximal unitary subgroup of $M$, $A$ is an anti-unitary coset representative, and the coset $AH$ contains all anti-unitary elements in $M$. In terms of Eq. (2), we have $S = H$, $\Gamma = \Delta$, $r = 2$, $e_1 = E$ (identity element), $e_2 = A$, and the obtained induced corep is

$$(\Delta \rightharpoonup M)(m) = \begin{bmatrix} \Delta(m) & 0 \\ 0 & \Delta(A^{-1}mA)^* \end{bmatrix}, \quad (\Delta \rightharpoonup M)(m') = \begin{bmatrix} 0 & \Delta(m'A)^* \\ \Delta(A^{-1}m') & 0 \end{bmatrix}$$

for $\forall m \in H$ and $\forall m' \in AH$. However, although $\Delta$ is irreducible for $H$, the induced corep $\Delta \rightharpoonup M$ is not necessarily irreducible in general. Corep theory shows that only one irreducible corep (up to equivalence) remains after the reduction of $\Delta \rightharpoonup M$ and there are only three cases (a), (b), and (c) [29]. In both cases (a) and (b), $\Delta(m)$ is equivalent to $\Delta(A^{-1}mA)^*$, i.e. there existing a matrix $N$ satisfying $\Delta(m) = N\Delta(A^{-1}mA)^*N^{-1}$ for $\forall m \in H$, while in case (c) $\Delta(m)$ is not equivalent to $\Delta(A^{-1}mA)^*$. Denoting the irreducible corep derived from $\Delta$ as $D\Delta$, then for $\forall m \in H$ and $\forall m' \in AH$ the results are

\begin{align*}
(a) & \quad D\Delta(m) = \Delta(m), \quad D\Delta(m') = \Delta'(m'), \quad NN^* = \Delta(A^2) \\
(b) & \quad D\Delta(m) = \begin{bmatrix} \Delta(m) & 0 \\ 0 & -\Delta(m) \end{bmatrix}, \quad D\Delta(m') = \begin{bmatrix} 0 & -\Delta'(m') \\ \Delta'(m') & 0 \end{bmatrix}, \quad NN^* = -\Delta(A^2) \\
(c) & \quad D\Delta(m) = (\Delta \rightharpoonup M)(m) 
\end{align*}

\footnote{All cosets refer to left cosets unless otherwise stated.}
where $\Delta'(m') \equiv \Delta(m'A^{-1})N$. For the matrix $N$ refer to Appendix A for details. The case of a corep $D\Delta$ can be determined simply by the following equation [29]

$$
\sum_{m' \in \Delta H} \chi(m'^2) = \begin{cases} 
+|H| & \text{: case (a)} \\
-|H| & \text{: case (b)} \\
0 & \text{: case (c)} 
\end{cases} 
$$

(7)
in which $\chi$ is the character of $\Delta$. This is related to the additional degeneracy of a system when its symmetry group changes from $H$ to $M$. In case (a), no additional degeneracy exists, i.e. the degeneracy keeps unchanged from $H$ to $M$. While in both cases (b) and (c) additional degeneracy appears, i.e. the degeneracy doubles from $H$ to $M$. The difference is that in case (b) two copies of the same irep of $H$ form a corep of $M$ but in case (c) two different irreps of $H$ form a corep of $M$.

2.2. Coreps for the 1651 MSGs

All the 1651 MSGs consist of both unitary groups (type-I) and nonunitary groups (type-II, -III, and -IV). Although corep is defined for nonunitary groups, it is still meaningful for unitary groups. Because Eq. (1) becomes $D(m_1)D(m_2) = D(m_1m_2)$ for all $m_1, m_2 \in M$ when no anti-unitary element exists in $M$, in which case the corep is just an ordinary rep. Accordingly, for the sake of concise and unified description, we use the term “corep” for all MSGs and MLGs no matter they are unitary groups or not.

Suppose $M$ is an MSG and $M_k$ is one of its MLGs. $M_k$ is defined at a certain wave vector $k$ and consists of all the elements in $M$ whose point parts transform $k$ to its equivalent wave vectors, i.e. $M_k = \{ Q | Q \in M & P(Q)k = k \}$. This is similar to the LG concept for SG. The point part of the element $Q$ in $M$ is defined as $P(Q) = R$ if $Q = \{ R|v \}$ and $P(Q) = TR$ if $Q = \{ TR|v \}$, in which $R$ is a rotation and $v$ is a translation vector (not necessarily a lattice vector). The symbol $\cong$ means the equivalence between two $k$-points, i.e. differing by a reciprocal lattice vector. And we use the convention $T\mathbf{k} = -k$ here. $M_k$ is a subgroup of $M$, and hence $M$ can be written as $M = c_1M_k + c_2M_k + \cdots + c_rM_k$ in which the first coset representative $c_1$ is usually set to $(E|0)$. Then, the magnetic (wave vector) star of $k$ can be defined as $\mathbf{k} = \{ k_{\mu} | \mu = 1, 2, \cdots, r \}$ with $k_{\mu} \equiv P(c_{\mu})k$ and $k_1 = k$.

For a certain MLG $M_k$, not all its irreducible coreps are useful. Only those compatible with the irreps of the translation group are important in physics. They, denoted as $D_k^p$ (p = 1, 2, …), satisfy the following relation

$$
D_k^p(\{|\alpha|v + t\}) = e^{-ik^p} \cdot D_k^p(\{|\alpha|v\}) \text{ for } \forall t \in \mathbb{L}.
$$

(8)
in which $\alpha$ can be $R$ or $TR$ and $\mathbb{L}$ is the set of all lattice vectors. These coreps are called “allowed” irreducible coreps of $M_k$ and are also termed “small coreps”. As for the own irreducible coreps of the MSG $M$, they can be obtained through the induction from the small coreps. That is to say, $D_k^p \uparrow M$ is an irreducible corep of $M$. For each $k_{\mu}$ in the magnetic star $*\mathbf{k}$, all coreps $D_k^{\mu p} \uparrow M$ ($\mu = 1, \cdots, r$) are equivalent to each other.

Therefore, the MSG corep $D_k^p \uparrow M$ is said to belong to the whole magnetic star $*\mathbf{k}$. It’s worth mentioning that two different concepts are involved here: “MLG corep” such as $D_k^p$ and “MSG corep” such as $D_k^p \uparrow M$. Despite this, when “corep of/for MSG” is generally mentioned, its meaning may cover both MLG corep and MSG corep, because the MLG corep $D_k^p$ of $M_k$ can also be said to be the small corep of the MSG $M$ at $k$. To differentiate from “small corep” (e.g. $D_k^p$) explicitly, MSG corep (e.g. $D_k^p \uparrow M$) can also be called the “full corep” of MSG.

The key to the corep theory of MSG is to obtain the small coreps of MLG. Suppose $G$ is the maximal unitary subgroup of $M$. Then $G$ has to be one of the 230 SGs. And the LG of $G$ at $k$, denoted as $G_k$, is also the maximal unitary subgroup of the MLG $M_k$. If $M_k$ is unitary, then $M_k = G_k$ and the small coreps of $M_k$ are just the small reps of $G_k$. But if $M_k$ is nonunitary, the small coreps of $M_k$ can be calculated from the small reps of $G_k$ via Eqs. (4)–(6). In either case, all the small reps of $G_k$ are known thanks to the SpaceGroupIrep package, and the small coreps of $M_k$ can be obtained subsequently.

For the full coreps of nonunitary MSGs (type-II, -III, and -IV), we extend the three cases (a), (b), and (c) to four types (a), (b), (c), and (x). Both (a) and (b) keep unchanged. But the case (c) is further divided
Table 1: The possible types and cases of both the small corep $D_{k}^{p}$ and the full corep $D_{k}^{p} \uparrow M$ for the MSG $M$. The symbol $-$ means undefined. The last two columns show whether the additional degeneracy will appear when the symmetry group changes from $G$ to $M$ in which $G$ is the maximal unitary subgroup of $M$.

| MSG type | $D_{k}^{p}$ type | $D_{k}^{p} \uparrow M$ type | doubled at $k$ in BZ |
|----------|------------------|-----------------------------|----------------------|
|          | case             | case                        |                      |
| non-unary| a                | a                           | no                   |
|          | b                | b                           | yes                  |
|          | c                | c                           | yes                  |
|          | x                | –                           | no                   |
| unitary  | a                | a                           | no                   |
|          | b                | b                           | yes                  |
|          | c                | c                           | yes                  |
|          | x                | –                           | yes                  |
|          | x                | –                           | no                   |

The type (x) in Eq. (9) implies that $M_k$ can be unitary even if $M$ is nonunitary, and for this type additional degeneracy does not exist at the $k$ point but does appear in the whole Brillouin zone (BZ) when the symmetry group changes from $G$ to $M$. According to Eq. (9), all the small coreps and full coreps of type-I MSGs belong to type (x). Here, we conclude that the four types are defined for both unitary and nonunitary groups but the three cases are only defined for nonunitary groups. The possible types and cases, together with their relations to the additional degeneracy, are listed in Table 1.

3. Files and installation

The MSGCorep package is developed in Wolfram language and can be used in the Mathematica software with version $\geq 11.2$. This package is dependent on the SpaceGroupIrep package, so users have to make sure SpaceGroupIrep (at best the latest version) properly installed prior to the installation of MSGCorep. The MSGCorep package mainly contains the files MSGCorep.wl, MSGData.wl, Usage.wl, and libMLGCorep.mx. The first three are core files and the fourth one contains the data of MLG coreps which are used only by the getBandCorep function. We also supply a file libMLGCorep.mx_RaspberryPi as an alternative version of libMLGCorep.mx working for raspberry pi platform, because Mathematica can be used free of charge on raspberry pi for non-commercial usage [50]. To install the package, just put the MSGCorep folder containing the above-mentioned files to the path $\$UserBaseDirectory/Applications/ or other available paths [44]. After installation, users can use the following statement to load the MSGCorep package and start using it.

```mathematica
<<"MSGCorep.wl" (* or just: <<MSGCorep.wl*)
```

Here we provide several useful tips for users [cf. Sec. 1 in the supplementary material (SM)]:

- Use `?MSGCorep` to browse all available functions in the package or `?MSGCorep`MLG for all functions containing MLG in their names such as `getMLGElem`.
- Use `getBandCorep` to see the information about a specific function such as `getBandCorep`.
- Many functions have options which can enrich their functionalities. Use `Options[fun]` to see the available options and their default values of a function `fun`.
4. Conventions

In both SpaceGrouprep and MSGCorep packages, we follow the convention used in the classic book written by C. J. Bradley and A. P. Cracknell (the BC book) [29] and call it “BC convention”. This convention is composed of various definitions and tables in the BC book, such as the basic vectors of primitive cells (defined in the Tab. 3.1 in the BC book, hereafter referred to as “BC-Tab. 3.1”), the names and operations of rotations (BC-Tabs. 1.4, 3.2, 3.4, and 6.7*), the elements of SGs (BC-Tab. 3.7* and MSGs (BC-Tabs. 7.2* and 7.3*), the high-symmetry k-points (BC-Tab. 3.6*), small reps (BC-Tabs. 5.7*, 5.11, 6.13*, and 6.15) and their labels (BC-Tabs. 5.8* and 6.14*). Note that the tables with * have corrections or adaptions given in this paper or the SM of Ref. [44].

As is well known, there are mainly two types of MSG notations (including numbers and symbols) which have been widely used for tens of years, namely the Belov-Neronova-Smirnova (BNS) notations [51, 52] and the Opechowski-Guccione (OG) notations [53]. Here we use the BNS MSG notations listed in BC-Tab. 7.4* with some corrections and adaptions (details are given in Appendix B and Table B.2). We made the adoptions to keep the BNS symbols the same as those in the latest and systematic MSG monograph written by Litvin in 2013 [32]. We regard these BNS symbols as the standard MSG symbols. It should be pointed out that the orientation of conventional cell in BC convention, shortened as BC orientation, is not always the same as the default orientation in “International Tables for Crystallography, Volume A” (hereafter referred to as ITA [54]), shortened as ITA orientation. The differences exist mainly in monoclinic and orthorhombic crystal systems. In principle, a self-consistent MSG symbol should reflect the cell orientation. But note that the standard BNS symbols that we use are not always self-consistent, because they correspond to the ITA orientation but not always to the BC orientation. For comparison purpose, we list all the symbols in BC-Tab. 3.1, the names and operations given in BC-Tab. 7.2 are mistaken for many MSGs, mainly involving orthorhombic and hexagonal rotations (BC-Tabs. 1.4, 3.2, 3.4, and 6.7*), the elements of SGs (BC-Tab. 3.7*) and MSGs (BC-Tabs. 5.8*). It should be pointed out that the tables with * have corrections or adaptions given in this paper or the SM of Ref. [44].

Users can use the following functions to get the MSG symbols,

\[
\text{MSGSymStd}[[28,92]] \quad (* \text{gives standard BNS symbol of } 28.92: \ P_{mna2} *)
\]
\[
\text{MSGSymBC}[[28,92]] \quad (* \text{gives the BNS symbol in BC orientation: } \ P_{nmb2} *)
\]
\[
\text{MSGSymOG}[[25,12,166]] \quad (* \text{gives the OG symbol of } 25.12.166: \ P_{2amnm2} *)
\]

in which we use a list of two (three) integers \( \{28,92\} \ (\{25,12,166\}) \) to describe the BNS (OG) MSG number 28.92 (25.12.166). The OG number \( \{25,12,166\} \) can be obtained by \( \text{BNSstoOG}[[28,92]] \), and reversely \( \text{OGtoBNS}[[25,12,166]] \) returns \( \{28,92\} \). If only the family number of an MSG is given as the argument, \( \text{MSGSymStd} \) (\( \text{MSGSymOG} \)) will return all possible MSGs in this family. For example, \( \text{MSGSymStd}[[119]] \) (\( \text{MSGSymOG}[[119]] \)) gives all the MSG symbols whose BNS (OG) numbers begin with 119, together with the correspondence to the OG (BNS) notations, as shown in the left (right) panel of Fig. 1. From Fig. 1 one can see that the BNS family of MSGs are different from the OG family of MSGs with the same family number. In addition, one can also use \( \text{showMSGSym}[[119]] \) to show the symbols of BNS family 119 in a formatted table form, or use \( \text{showMSGSym}[[110;;120]] \) to show a range of families from 110 to 120.

When we construct type-III MSGs according to BC-Tab. 7.2, we find that the “colored” generating elements given in BC-Tab. 7.2 are mistaken for many MSGs, mainly involving orthorhombic and hexagonal...
systems. Here, a colored element, also called a primed element, means that it’s an anti-unitary element and the multiplied \( T \) is usually represented by a ‘. For example, after being colored, \( \{ R[v] \} \) becomes \( \{ R[v]' \} \) which is equivalent to \( \{ R[v]T \} \) and \( \{ R[v]' \} \) is usually shown in red color as \( \{ R[v]' \} \) to attract attention. Taking the orthorhombic MSG 28.89 (Pm\( \alpha \)a\( \beta \)) for example, the \( \sigma_x \) given in BC-Tab. 7.2 means that the generating elements of Pm\( \alpha \)a\( \beta \) can be obtained by first getting the generating elements of SG 28 (Pm\( \alpha \)2), i.e. \( \{ \sigma_x, \frac{1}{2}00 \} \) and \( \{ \sigma_y [000] \} \) from BC-Tab. 3.7 (or run \textsc{SGGenElem}([28,11]) to get them) and then making the specified one, i.e. \( \{ \sigma_x, \frac{1}{2}00 \} \) which is specified by its rotation part \( \sigma_x \), colored. However, thus obtained generating elements, i.e. \( \{ \sigma_x, \frac{1}{2}00 \}' \) and \( \{ \sigma_y[000] \} \), are not consistent with the symbol Pm\( \alpha \)a\( \beta \). The symbol Pm\( \alpha \)a\( \beta \)' tells us that it has a primed mirror (i.e. \( m' \)) and an unprimed mirror plane (i.e. \( a \)), but \( \{ \sigma_x, \frac{1}{2}00 \}' \) and \( \{ \sigma_y[000] \} \) are a primed glide reflection and an unprimed mirror plane respectively. More specifically, \( \{ \sigma_x, \frac{1}{2}00 \}' \) ((\( \sigma_y[000] \)) gives a primed glide plane \( b^2 \) (unprimed mirror \( m' \)) with normal direction along \( x \) (y), and it should correspond to the first (second) place holder \( \square \) in the MSG symbol \( P\square\square \). So, the MSG with generating elements \( \{ \sigma_x, \frac{1}{2}00 \}' \) and \( \{ \sigma_y[000] \} \) should be Pm\( \alpha \)m'2\( \beta \). Recalling that in BC convention the actual orientation of SG 28 is \( \text{bac} \) (refer to the Table 5 in [44] or run \textsc{BCOrientation}[28] to get it), the symbol Pm\( \alpha \)m'2\( \beta \) is actually in BC orientation, and becomes Pm\( \alpha \)a\( \beta \) after converting to ITA orientation (i.e. abc). However, Pm\( \alpha \)a\( \beta \) is MSG 28.90, not 29.89! If the MSG generating elements are \( \{ \sigma_x, \frac{1}{2}00 \} \) and \( \{ \sigma_y[000] \} \), similar analyses directly give the MSG symbol Pm\( \alpha \)a\( \beta \)', corresponding to Pm\( \alpha \)a\( \beta \) (MSG 28.89) in ITA orientation. To this point, one can see that BC-Tab. 7.2 gives mistaken colored generating elements for MSGs 28.89 and 29.80. We think the reason of this mistake may be that Bradley and Cracknell simply copied the data in the original BNS table in [52] without essential adaptations to make them consistent with BC-Tab. 3.7. In Table B.3 we list the corrections to all the mistaken colored generating elements in BC-Tab. 7.2. And in the Table S2 of SM elements for each MSG are listed.

When we construct type-IV MSGs, we find that BC-Tab. 7.3 should also be adapted. Firstly, BC-Tab. 7.3 is not complete, lacking six black-white lattices (see Table B.4 for details), such as the \( P_c \) black-white lattice of MSG 7.28 (\( P(C) \)). Secondly, for all MSGs of orthorhombic crystal system, we should use the BNS symbols in BC orientation to obtain their black-white lattices. For example, MSG 51.300 should be constructed through the black-white lattice \( P_c \) in its symbol in BC orientation, namely P\( \alpha \)cm, not the \( P_c \) in the standard symbol P\( \alpha \)cm. Only thus can we obtain the correct elements of M\( 51,300 \) (MSG 51.300) based on \( G_{51} \) (SG 51) whose elements are consistent with BC-Tab. 3.7, and the equation is M\( 51,300 = G_{51} + T(E; t_0)G_{51} \) with \( t_0 \) taking the value \( \frac{1}{2}00 \) of the orthorhombic \( P_c \) in BC-Tab. 7.3. Accordingly, the \( A_{\alpha}, A_{\beta}, \) and \( A_{\gamma} \) in BC-Tab. 7.3 are of no use because the actual black-white lattices are \( C_{\alpha}, C_{\beta}, \) and \( C_{\gamma} \) respectively for corresponding symbols in BC orientation\(^3\).

In short, in order to construct MSGs from BC-Tab. 7.2 and 7.3 correctly, the actual BC orientation has to be considered and the two tables have to be corrected or adapted accordingly, or else the obtained MSG elements may not match the MSG numbers and symbols. The SM of Ref. [25] mentions that there are 126 MSGs whose numbers in the BC book are different from those on BCS and it also gives the correspondence between them. In fact, those 126 MSGs are merely constructed from the original BC-Tab. 7.2 and 7.3 literally in Ref. [25], which leads to the seeming differences between the BC book and BCS. However, the BNS numbers in both the BC book and on BCS should not be different from the original definitions by Belov, Neronova, and Smirnova, even if the BNS symbols may be different according to the cell orientation.

5. Functionalities of MSGCorep

5.1. Group elements and multiplication

In \textsc{SpaceGrouprep} an SG element \{\( R[v] \)\} is described as \{\( \text{Rname}, \{v1, v2, v3\} \)\} in the code, while in \textsc{MSGCorep} an MSG element is described as \{\( \text{Rname}, \{v1, v2, v3\}, au \)\} in which \( au \) describes whether this

\(^2\)Note that in BC convention, the basic vectors of orthorhombic primitive lattice are \( t_1 = (0,-b,0) = -b \), \( t_2 = (a,0,0) = a \), and \( t_3 = (0,c,0) = c \), and the translation part \( \{ \frac{1}{2}00 \} \) in \( \{ \sigma_x, \frac{1}{2}00 \} \) represents the translation vector \( \frac{1}{2}t_1 = -\frac{1}{2}b \). Therefore, \( \{ \sigma_x, \frac{1}{2}00 \} \) is a glide operation with glide direction \( b \) and it should be denoted as \( b \) in the SG symbol. Furthermore, \( \{ \sigma_x, \frac{1}{2}00 \}' \) gives a primed glide plane \( b' \) in the MSG symbol.

\(^3\)Taking MSG 40.208 for example, one can verify this by running \textsc{MSGSymStd}([40,208]) and \textsc{MSGSymBC}([40,208]) which returns \( A_{\alpha} \text{ma2} \) and \( C_{\gamma}e2m \) respectively.
element is anti-unitary whose value can only be 0 (no) or 1 (yes). For example, as MSG elements, \( \{e_2, \{0, 0, 1/2\}\} \) and \( \{e_2, \{0, 0, 1/2\}\}' \) are described as \( \{e_{C2z}, \{0, 0, 1/2\}, 0\} \) and \( \{e_{C2z}, \{0, 0, 1/2\}, 1\} \) respectively in the code. To get the list of the elements in an MSG with BNS number \( n,m \), one can use `getMSGElem[{n,m}]`, and similarly one can use `getMLGElem[{n,m},k]` to get the elements in the MLG of \( k \) in which \( k \) can be either the name string of a BC standard k-point\(^4\) or the fractional coordinates of any k-point. We have to point out that what returns by `getMSGElem` and `getMLGElem` are actually \( M/T \) and \( M_k/T \) respectively, namely the coset representatives with respect to the translation group \( T \). If the option "double"->True is used for the two functions, the elements of the corresponding double MSG (or MLG) are returned. For example,

\[
\text{In}[1]:= \text{getMSGElem}[[28,89]]
\]

\[
\text{getMLGv}[{28,89},"A"], (* \text{the coordinates of "A" is } \{0,u,1/2\} *)
\]

\[
\text{getMLGv}[[28,89],"A"("double"->True]
\]

\[
\text{showMSGSeitz/\%}
\]

\[
\text{Out}[1]= \{\{e_{E}, \{0,0,0\},0\},\{e_{C2z}, \{1/2,0,0\},1\},\{e_{sigma}, \{1/2,0,0\},0\},\{e_{sigma}, \{0,0,0\},1\}\}
\]

\[
\text{Out}[2]= \{\{e_{E}, \{0,0,0\},0\},\{e_{C2z}, \{1/2,0,0\},1\}\}
\]

\[
\text{Out}[3]= \{\{e_{E}, \{0,0,0\},0\},\{\text{bar}\_E, \{0,0,0\},0\},\{e_{C2z}, \{1/2,0,0\},1\},\{\text{bar}\_C2z, \{1/2,0,0\},1\}\}
\]

\[
\text{Out}[4]= \{\{E[000], \{7/000\},\{28,89\}\\{0,0,1/2\}\\{0,0,1/2\},0\},\{e_{MLGCorep}, \text{MSGinvSeitz}, \text{MSGpowerSeitz} \}
\]

in which `showMSGSeitz` shows an MSG element in the mathematical form and highlights anti-unitary element in red color.

The multiplication of two MSG elements \( \{R_1,v\}\text{au1}\{R_2,w\}\text{au2}\) = \( \{R_1R_2[R_1w+v]\text{au1}\text{au2}\}\), the inversion of an MSG element \( \{(R|v)\text{au}\}^{-1} = \{R^{-1} - R^{-1}v\text{au}\} \), and the n-th power of an MSG element \( \{(R|v)\text{au}\}^n \) can be calculated by `MSGSeitzTimes`, `MSGinvSeitz`, and `MSGpowerSeitz` in the code respectively. Here \( \{R|v\text{au}\} \) represents \( \{R|v\} \) if \( au = 0 \) or \( \{R|v\}' \) if \( au = 1 \), and the symbol \( \oplus \) means “exclusive or”. All the three functions have versions for double MSGs with a DMSG prefix because double MSGs have different multiplication as follows:

\[
\left\{ \begin{array}{l}
\{R_1|v\}\{R_2|w\} = \{R_1R_2|R_1w+v\}
\\
\{R_1|v\}'\{R_2|w\} = \{R_1|v\}\{R_2|w\}' = \{R_1R_2|R_1w+v\}'
\\
\{R_1|v\}'\{R_2|w\}' = \{R_1R_2|R_1w+v\}'.
\end{array} \right.
\]

Note the difference of \( T^2 \) between MSG and double MSG: for MSG \( \{(E|0)\}'^2 = \{E|0\} \) means \( T^2 = E \), while for double MSG \( \{(E|0)\}'^2 = \{E|0\} \) means \( T^2 = E' \). Finally the functions operating on (double) MSG elements are listed below.

\[
\text{MSGSeitzTimes}[\text{brav}][\{R_1,\{v_1,v_2,v_3\},\text{au1}\}, \{R_2,\{w_1,w_2,w_3\},\text{au2}\}, ...]
\]

\[
\text{MSGinvSeitz}[\text{brav}][\{R,\{v_1,v_2,v_3\},\text{au}\}]
\]

\[
\text{MSGpowerSeitz}[\text{brav}][\{R,\{v_1,v_2,v_3\},\text{au}\}, n]
\]

\[
\text{DMSGSeitzTimes}[\text{brav}][\{R_1,\{v_1,v_2,v_3\},\text{au1}\}, \{R_2,\{w_1,w_2,w_3\},\text{au2}\}, ...]
\]

\[
\text{DMSGinvSeitz}[\text{brav}][\{R,\{v_1,v_2,v_3\},\text{au}\}]
\]

\[
\text{DMSGpowerSeitz}[\text{brav}][\{R,\{v_1,v_2,v_3\},\text{au}\}, n]
\]

In the above code, “...” implies that `MSGSeitzTimes` and `DMSGSeitzTimes` can calculate not only the multiplication of two MSG elements, but also the continuous multiplication of three or more MSG elements.

5.2. Small Coreps

The small coreps of any MLG can be obtained by `getMLGCorep[{n,m},k]` and shown in table form by `showMLGCorep[{n,m},k]` in which \( {n,m} \) specifies the MSG number \( n,m \) and \( k \) can be either the name string of a BC standard k-point or the numerical fractional coordinates of any k-point. For using the corep data in the code one can use `getMLGCorep`, but if only for display purpose one can just use `showMLGCorep`. One example for the small coreps of the \( P \) point for MSG 97.155 (\( I4/2\)'2) is shown in Fig. 2, which is

---

\(^4\)A “BC standard k-point”, denoted as \( k_{BC} \), is a k-point whose coordinates are defined in BC-Tab. 3.6a.
MSG 97.155 (I422): k-point name is P, for TetrBody(a), TetrBody(b)

The unitary subgroup is SG 22(F222), whose standard BC basic vectors are \((a_1 a_2 a_3) = R(\vec{a}_1 \vec{a}_2 \vec{a}_3) T\) with origin shift \(\vec{O} = (0, 0, 0)\) and

\[
\begin{pmatrix}
0 & 0 & -1 \\
1 & 0 & 0 \\
0 & -1 & -1
\end{pmatrix}
\]

and rotation matrix

\[
R =
\begin{pmatrix}
\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

Transformation matrix

\[
\begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

k-point name is P, for TetrBody(a), TetrBody(b)

\(k = \left( \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \right)\) standard

k = \[TC, k = \left( \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \right)\]

\(H_{97.155} = \left( I_4 \right)

\section*{Figure 2: The result of showMLGCorep[(97, 155), "P"] which shows the small coreps of the P point for MSG 97.155 (I4'2'2').}

Part ① shows the MSG notation, the k-point information such as name and coordinates, and the types of BZs. Part ② shows that SG 22 (F222) is the maximal unitary subgroup of MSG 97.155 and it also shows the relations between the basic vectors of MSG 97.155 and the standard BC basic vectors of SG 22. Part ③ shows the converted k-point information from MSG 97.155 to SG 22. Parts ① and ② exist only for type-III MSGs. Part ③ is the table which shows the small coreps. Light green background shows single-valued coreps and light blue background shows double-valued coreps. The first, second, and third columns are the indexes, labels, and types of the small coreps respectively.

obtained by showMLGCorep[(97, 155), "P"] there are four parts ①-④ in Fig. 2. Part ① shows the basic information, including the MSG number 97.155 and symbol I4'2'2, the k-point name P and coordinates \((\frac{1}{4}, \frac{1}{4}, \frac{1}{4})\), and the available types of BZs TetrBody(a) and TetrBody(b). Strictly speaking, the k-point name shown here is only for the BC standard k-point \(k_{BC}\), and for a type-II or -III k-point (see the Sec. 2.3 in Ref. [44] for details) this name is merely borrowed from \(k_{BC}\) to name it. For example, if one calculate showMLGCorep[(97, 155),{-1/4,-1/4,-1/4}]], the part ③ of the result is shown below.

MSG 97.155 (I422): k-point name is P, for TetrBody(a), TetrBody(b)

\(k = \left( \frac{1}{4}, -\frac{1}{4}, -\frac{1}{4} \right)\) non-standard, \(k_{BC} = \left( \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \right)\) \([C_{2b}] k_{BC} \equiv k\)

which implies that the input k-point \(k = \left( \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \right)\) is not standard and can borrow the name P from \(k_{BC}\) = \([C_{2b}] k_{BC} \equiv k\).

Parts ② and ③ exist only for type-III MSGs. This is because for type-I, -II, and -IV MSGs, the Bravais lattice of an MSG \(M\) is the same with that of its maximal unitary subgroup \(G\) and their basic vectors are also the same, while for type-III MSGs, both Bravais lattice and basic vectors may be different between \(M\) and \(G\). In order to utilize the existing irep data of SGs to construct the coreps of MSGs, one has to find

Note that there are totally 22 types of BZs in BC convention and see details in BC-Figs. 3.2-3.15 and the Table 1 in [44].
the relations between the primitive cell of $M$ and the standard “BC cell$^6$” of $G$ for type-III MSGs. In the example of Fig. 2, $M$ (MSG 97.155) has body-centered tetragonal Bravais lattice whose basic vectors $t_1$, $t_2$, and $t_3$ form a basic-vector matrix

$$\begin{bmatrix} t_1 & t_2 & t_3 \end{bmatrix} = \begin{bmatrix} -a/2 & a/2 & a/2 \\ a/2 & -a/2 & a/2 \\ c/2 & c/2 & -c/2 \end{bmatrix}$$

in which $a$ and $c$ are lattice constants, while the BC cell of $G$ (SG 22) has face-centered orthorhombic Bravais lattice whose basic vectors $t'_1$, $t'_2$, and $t'_3$ are

$$\begin{bmatrix} t'_1 & t'_2 & t'_3 \end{bmatrix} = \begin{bmatrix} a'/2 & 0 & a'/2 \\ 0 & -b'/2 & -b'/2 \\ c'/2 & c'/2 & 0 \end{bmatrix}$$

in which $a'$, $b'$, and $c'$ are also lattice constants. Part $\S$ of Fig. 2 shows the relationship between the primitive cells of $M$ and $G$ in terms of transformation matrix $T$, rotation matrix $R$, and the origin shift $O_s$ as follows

$$R[t_1 \ t_2 \ t_3]T = \begin{bmatrix} a/\sqrt{2} & 0 & a/\sqrt{2} \\ 0 & -a/\sqrt{2} & -a/\sqrt{2} \\ c/\sqrt{2} & c/\sqrt{2} & 0 \end{bmatrix} = [t'_1 \ t'_2 \ t'_3] \quad \Rightarrow \quad a' = b' = \sqrt{2}a, \ c' = \sqrt{2}c.$$  

Here $O_s = (s_1, s_2, s_3)$ gives the shift vector $s_1t'_1 + s_2t'_2 + s_3t'_3$ from the origin of the cell of $G$ to the origin of the cell of $M$. According to the relation $k' = T^T k$, Part $\S$ of Fig. 2 gives the k-point name $H$ and coordinates $k' = (1\ 1\ 1)$ of $G$ which correspond to the input k-point $P$ of $M$ with coordinates $k = (\frac{1}{2} \frac{1}{2} \frac{1}{2})$.

Part $\S$ of Fig. 2 is the table of small coreps for the $P$ point of MSG 97.155. Both single-valued small coreps (light green background) and double-valued small coreps (light blue background) are shown, together with their labels (the second column) and types (the third column). The row “Element” lists the elements in the MLG. In fact only the coset representatives with respect to $T$ are listed in the table and the elements whose rotation parts have bars such as $\{E\}000$ are not shown because their coreps can be simply obtained from the coreps of their counterparts without bars. The simple relationship between them is

$$D^p_k(\{R|v\}^{|i}) = D^p_k(\{|R|v\}^{|i}) \quad \text{for single-valued coreps}$$
$$D^p_k(\{R|v\}^{|i}) = -D^p_k(\{|R|v\}^{|i}) \quad \text{for double-valued coreps}$$

in which $|i|$ means whether primed or not. And the coreps of the elements whose translation parts differ from those given in the table by a lattice vector can be obtained using Eq. (8).

The labels of small coreps are constructed from the labels of the corresponding small reps from which the small coreps are derived. (i) **Type-I, -II, and -IV MSGs.** A small corep, say $D$, of type (a) or (x) is derived from only one small rep, say $\Gamma$, and then $D$ just uses the label of $\Gamma$. For example, the small corep $P_3$ of MSG 97.152 (I4221)’ is of type (a) and it’s derived from the small rep $P_3$ of SG 97 (I422). One can check this by running `showMLGCorep[97,152], "P"]` and `showLGrepTab[97,"P"]`. If $D$ is of type (b), it contains two copies of $\Gamma$ for unitary elements, and then the label of $D$ is two copies of the label of $\Gamma$. For example, the small corep $A_5A_5$ of MSG 65.488 ($C_{mmm}$) is of type (b) and it’s derived from two copies of the small rep $A_5$ of SG 65 (mmm). If $D$ is of type (c), it contains two different small reps $\Gamma_i$ and $\Gamma_j$ for unitary elements, and then the label of $D$ is the combination of the labels of $\Gamma_i$ and $\Gamma_j$. For example, the small corep $P_2P_2$ of MSG 97.152 is of type (c) and it’s the combination of the small reps $P_2$ and $P_2$ of SG 97. (ii) **Type-III MSGs.** First, an elementary label is constructed according to the above-mentioned rules in case (i). Then an additional k-point name within parentheses has to be prefixed to the elementary label

---

$^6$Refer to the Sec. 8 in Ref. [44] for more details.
MSG 96.144 (P432121): k-point name of \( k_1 \) is \( X \), for TetrPrim

\( k_1 = (\frac{1}{2}, 0, \frac{1}{2}) \) standard

- The magnetic k-star \( \ast X \) (input k-point \( k_{\text{in}} = k_1 \)) contains:
  - \( k_1 = (\frac{1}{2}, 0, \frac{1}{2}) \); \( k_2 = (-\frac{1}{2}, 0, \frac{1}{2}) \)

The unitary subgroup is SG 96 (P43212), k-point coordinates unchanged

- The k-star of the unitary subgroup: \( \ast \{X(k_1, k_2)\} \)

| Index | Element | \( E \times t_1 t_2 t_3 \) | \( C_{2x}(1,1,0) \) | \( E \{000\} \) | \( C_{2x}(1,1,0) \) |
|-------|---------|----------------|----------------|----------------|----------------|
| 1 \( \ast X_1 \) a | \( e^{-i\pi t_3} \) | 1 0 0 0 | 0 -1 0 0 | 0 0 0 -1 | 0 0 1 0 |
| \( \ast X_2 X_3 \) c | \( e^{-i\pi t_3} \) | 0 0 0 0 | 0 0 1 0 | 0 0 0 -1 | 0 0 1 0 |
| \( \ast X_4 X_5 \) c | \( e^{-i\pi t_3} \) | 0 0 0 0 | 0 0 1 0 | 0 0 0 -1 | 0 0 1 0 |

Figure 3: The result of \( \text{showMSGCorep}\{\{96,144\}, \"X\", \"elem\"->\{1,2,9,10\}, \"rotmat\"->\text{False}\} \) shows the full coreps of the \( \ast X \) magnetic star for a type-II MSG 96.144 (P432121'). The coreps for only 4 elements are shown due to the space limitation. Above the table, related information is shown, including the notations of the MSG and its maximal unitary subgroup, the name and coordinates of the magnetic k-star and the input k-point, and so on. In the table of full coreps, light green background shows single-valued coreps and light blue background shows double-valued coreps. The first, second, and third columns are the indexes, labels, and types of the full coreps respectively.

5.3. Full Coreps

The full coreps of any MSG can be induced from the small coreps of its MLG according to Eq. (2). The calculated results can be obtained by \( \text{getMSGCorep}\{\{n,m\}, k\} \) and shown in table form by \( \text{showMSGCorep}\{\{n,m\}, k\} \) in which \( \{n,m\} \) specifies the MSG number \( n.m \) and \( k \) which is either the name string or the numerical fractional coordinates of a k-point specifies the magnetic star.\(^7\) Examples for the full coreps of the magnetic star \( \ast X \) for MSG 96.144 (P432121') and MSG 79.27 (I4') are shown in Fig. 3 and Fig. 4 respectively. The result of \( \text{showMSGCorep} \), similar to that of \( \text{showMLGCorep} \), is mainly composed of a text part and a table part. The text part gives the information about the MSG, the maximal unitary subgroup, the input k-point, the magnetic k-star, and so on. By default, the table part gives the full coreps of the elements in \( T \) (see the \( \{E|t_1 t_2 t_3\} \) column in the table part) and in the coset representatives with respect to \( T \) but not including those whose rotation parts have bars. For the elements whose rotation parts have bars, Eq. (14) is also available if \( D_k^p \) is substituted by a full corep. To save space, rotation matrices are not shown in Figs. 3 and 4 by using the option "rotmat"->\text{False}, and only

\(^7\) The magnetic star of a k-point can be obtained by \( \text{getMagKStar}\{\{n,m\}, k\} \).
**MSG 79.27 (I4?):** k-point name of \( k_1 \) is \( X \), for TetrBody(a), TetrBody(b)  
\( k_1 = (0, 0, \frac{1}{2}) \) standard  
- The magnetic k-star \( \ast X \) (input k-point \( k_{in} = k_1 \)) contains:  
  \( k_1 = (0, 0, \frac{1}{2}) \); \( k_2 = (-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \)  
The unitary subgroup is \( SG(2) \), whose standard BC basic vectors are \( t_1 t_2 t_3 = R(t_1 t_2 t_3) T \) with origin shift \( Os = (0, 0, 0) \) and  
- The k-point of the unitary subgroup: \( \ast M(k'_1) \) and \( \ast A(k'_2) \) (\( k'_1 = T \cdot k_i \))  
  \[ M: \; k'_1 = (-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \]  
  \[ A: \; k'_2 = (\frac{1}{2}, 0, 0) \]  
\( k'_1 = (-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \) standard for MonoBase  
\( k'_2 = (\frac{1}{2}, 0, 0) \) standard for MonoBase

| Index | Element | 2 | \( C_{2z} \) | 3 | \( C_{4x} \) | 4 | \( C_{4z} \) |
|-------|---------|---|-------------|---|-------------|---|-------------|
| 1 | \( * \langle X \rangle M_A \) in \( E_{t_1 t_2 t_3} \) | \( e^{-i \pi t_3} \) | \( 0 \) | \( 0 \) | \( 0 \) | \( 0 \) | \( 0 \) | \( 0 \) |
| 2 | \( * \langle X \rangle M_A \) in \( E_{t_1 t_2 t_3} \) | \( e^{i \pi t_3} \) | \( 0 \) | \( 0 \) | \( 0 \) | \( 0 \) | \( 0 \) | \( 0 \) |
| 3 | \( * \langle X \rangle M_A \) in \( E_{t_1 t_2 t_3} \) | \( e^{-i \pi t_3} \) | \( 0 \) | \( 0 \) | \( 0 \) | \( 0 \) | \( 0 \) | \( 0 \) |
| 4 | \( * \langle X \rangle M_A \) in \( E_{t_1 t_2 t_3} \) | \( e^{i \pi t_3} \) | \( 0 \) | \( 0 \) | \( 0 \) | \( 0 \) | \( 0 \) | \( 0 \) |

Figure 4: The result of showMSGCorep\((\{79,27\}, "X", "rotmat"->False\) which shows the full cores of the \( \ast X \) magnetic star for a type-III MSG 79.27 (I4?). Above the table, related information is shown, including the notations of the MSG and its maximal unitary subgroup, the name and coordinates of the magnetic k-star and the input k-point, the conversion relations between the MSG and its maximal unitary subgroup similar to those in the parts \( \mathcal{E} \) and \( \mathcal{O} \) of Fig. 2, and so on. In the table of full cores, light green background shows single-valued cores and light blue background shows double-valued cores. The first, second, and third columns are the indexes, labels, and types of the full cores respectively.

coreps of four elements, i.e. the 1st, 2nd, 9th, and 10th ones, are shown in Fig. 3 by using the option "elem"\( \rightarrow \{1, 2, 9, 10\} \).

In order to make the full cores independent of which k-point is selected from a given magnetic star as the input of showMSGCorep, the k-points in a given magnetic star have to be sorted in a fixed order before the full cores are constructed using Eq. (2). The input k-point of Fig. 3 is \( \ast X \) whose coordinates are \( k_{in} = (0, \frac{1}{2}, 0) \). Its magnetic star \( \ast X \) includes two k-points, namely \( k_1 = (0, 0, 0) \) and \( k_2 = (\frac{1}{2}, 0, 0) \). If one substitutes \( \{-1/2, 0, 0\} \) for \( \ast X \) as the input k-point, i.e. \( k_{in} = (\frac{1}{2}, 0, 0) \), the obtained magnetic star keeps unchanged in the sense of equivalence and the full cores also keep the same.\(^8\) Note that one may find that the matrix elements of the cores in the \( \{E_{t_1 t_2 t_3}\} \) column change seemingly from \( e^{-i \pi t_1} \) to \( e^{i \pi t_1} \) after the change of input k-point from \( \ast X \) to \( \{-1/2, 0, 0\} \), but they are indeed equal because \( t_1 (i = 1, 2, 3) \) is always an integer here.

The labels of full cores are constructed based on the labels of the small cores that induce the full cores and all the labels of full cores have an asterisk superscript on the left to indicate that full cores are defined according to magnetic k-stars. (1) For full cores of type (x) in type-I MSGs and full cores of types \( (a), (b), \) or \( (c) \) in all MSGs, the label of a full core is constructed by just putting an asterisk superscript on the left of the label of the corresponding small core. For example, the labels of small cores for the X point of MSG 96.144 are \( X_1, X_2 X_3 \), and \( X_4 X_5 \), and the labels of full cores for the \( \ast X \) magnetic

---

\(^8\)The result is not given here. One can run showMSGCorep\([\{96,144\}, \{-1/2, 0, 0\}, "elem"\( \rightarrow \{1, 2, 9, 10\}, "rotmat"\rightarrow False\)\] to check this.
**Direct products of coreps of magnetic space group** $P_{4}4$ (No. 75.4):

For Brillouin zone type: TetrPrim

$\mathbf{k} \otimes \mathbf{k}' = \langle 0, 0.5, 0 \rangle [X_{2}, 2], \quad \mathbf{k} = \langle 0, 0.5, 0.5 \rangle [R, 2]$

The results contain magnetic stars $\mathbf{k}_1 - \mathbf{k}_2$:

$k_1 = \langle 0, 0.5 \rangle [Z, 1] \quad k_2 = \langle 0.5, 0.5, 0.5 \rangle [A, 1]$

| Direct Product | Results |
|----------------|---------|
| $\mathbf{X}_1 (k_2) \otimes \mathbf{R}_1 \mathbf{R}_1 (k_4)$ | $Z_1 Z_4 (k_{1,2}) + \ast Z_3 Z_3 (k_{1,2}) + \ast A_1 A_1 (k_{2,2}) + \ast A_2 A_3 (k_{2,2})$ |
| $\mathbf{X}_1 (k_2) \otimes \mathbf{R}_2 \mathbf{R}_2 (k_4)$ | $2 Z_2 Z_4 (k_{1,2}) + 2 A_1 A_4 (k_{2,2})$ |
| $\mathbf{X}_2 (k_2) \otimes \mathbf{R}_1 \mathbf{R}_1 (k_4)$ | $2 Z_2 Z_4 (k_{1,2}) + 2 A_1 A_4 (k_{2,2})$ |
| $\mathbf{X}_2 (k_2) \otimes \mathbf{R}_2 \mathbf{R}_2 (k_4)$ | $Z_2 Z_3 (k_{1,2}) + \ast Z_3 Z_3 (k_{1,2}) + \ast A_1 A_1 (k_{2,2}) + \ast A_2 A_3 (k_{2,2})$ |
| $\mathbf{X}_3 \mathbf{X}_4 (k_4) \otimes \mathbf{R}_1 \mathbf{R}_1 (k_4)$ | $Z_2 Z_3 (k_{1,2}) + \ast Z_3 Z_3 (k_{1,2}) + \ast A_1 A_1 (k_{2,2}) + \ast A_2 A_3 (k_{2,2})$ |
| $\mathbf{X}_3 \mathbf{X}_4 (k_4) \otimes \mathbf{R}_2 \mathbf{R}_2 (k_4)$ | $2 Z_2 Z_4 (k_{1,2}) + 2 Z_2 Z_4 (k_{1,2}) + 2 A_1 A_4 (k_{2,2}) + 2 A_4 A_4 (k_{2,2})$ |

**Figure 5:** The result of `showMSGCorepDirectProduct[{75,4}, " X", " R"]` which shows the direct products of full coreps between two magnetic stars $\ast X$ and $\ast R$ for MSG 75.4 ($P_{4}$). In the text part above the table, the notation such as $\{X, 2\}$ after a k-point indicates the k-point name (X) and the number of k-points (2) in its magnetic star. The notation such as $\langle k_1, 2 \rangle$ in the table indicates that the full corep in front of it, e.g. $\ast_2 Z_{24}$, is for the magnetic star of $k_1$ and the dimension of this full corep is 2.

Light green (light blue) background stands for direct products between two single-valued (double-valued) full coreps, and light yellow background for direct products between a single-valued full corep and a double-valued full corep.

star of MSG 96.144 are $\ast X_1$, $\ast X_2 X_3$, and $\ast X_4 X_5$ respectively. (ii) For full coreps of type (x) in type-II, -III, and -IV MSGs, one magnetic k-star of an MSG corresponds to two different k-stars of the maximal unitary subgroup of the MSG. The label of such a full corep should combine the labels of two small reps of the maximal unitary subgroup from each of the two k-stars. To differentiate the two k-stars, two different labels have to be used for them. There are three cases: 1) The two k-stars have different labels of BC convention. For example, the $\ast X$ magnetic star corresponds to two different k-stars $\ast M$ and $\ast A$ of SG 5, and hence its labels of full coreps are $\{ (X) M_1 A_1, (X) M_2 A_2, (X) M_3 A_4, \}$ and $\{ (X) M_4 A_3, \}$, as shown in Fig. 4. This case only occurs for type-III MSGs. 2) The two k-stars are negative of each other. In such a case, the label of the second k-star is obtained by underlining the label of the first one. For example, the $\ast P$ magnetic star of MSG 44.230 corresponds to the k-stars $\ast P$ and $\ast P$ of SG 44, and its full coreps have labels $\{ P_1 P_1, P_1 P_2, P_3 P_4, P_3 P_4 \}$. All full coreps of type (x) for type-II and -IV MSGs are in this case, but this case also occurs for type-III MSGs. 3) The k-points in both the k-stars can be identified as the same k-point name, but the two k-stars are not negative of each other. In this case, one k-star uses the BC k-point name, and the other k-star uses a k-point name constructed by adding a letter “A” after the BC k-point name. For example, the $\ast W$ magnetic star of MSG 79.27 corresponds to the k-stars $\ast U$ and $\ast U A$ of SG 5, and its full coreps have labels $\{ (W) U_1 U A_1, (W) U_2 U A_2, (W) U_3 U A_4, \}$ and $\{ (W) U_4 U A_3, \}$. This case also occurs only for type-III MSGs.

### 5.4. Direct product of full coreps

The decomposition (or reduction) of the direct product (Kronecker product) of two full coreps is useful to analyze the selection rules of the quantum transition processes of electron, phonon, magnon and so on in a crystal belonging to a certain MSG. Although the basic calculation rules are all known, it’s cumbersome and prone to error to calculate the direct product manually. Accordingly, we have developed the functions to calculate and show the decomposition of direct product of full coreps for MSGs in the MSGCorep package, namely `MSGCorepDirectProduct` and `showMSGCorepDirectProduct` respectively, because there is no such a tool available to do this so far as we know. Suppose $M$ is MSG n.m and $G$ (an ordinary SG) is its maximal
unitary subgroup. \( \Gamma^i \) and \( \Gamma^j \) are two full irreps of \( G \), and \( \mathcal{D}\Gamma_i \) and \( \mathcal{D}\Gamma_j \) are the corresponding two full coreps of \( M \) derived from \( \Gamma_i \) and \( \Gamma_j \) respectively. The direct product of \( \mathcal{D}\Gamma_i \) and \( \mathcal{D}\Gamma_j \) can be reduced to the direct sum of a series of full coreps \( \mathcal{D}\Gamma^k \) of \( M \)

\[
\mathcal{D}\Gamma_i \otimes \mathcal{D}\Gamma_j = \bigoplus_k d_{ij,k} \mathcal{D}\Gamma^k,
\]

and the task is to find the occurrence number (reduction coefficient) \( d_{ij,k} \) of the full corep \( \mathcal{D}\Gamma^k \) in the decomposition for each \( k \). To calculate \( d_{ij,k} \), one can first calculate the reduction coefficient \( c_{ij,k} \) in the direct product \( \Gamma^i \otimes \Gamma^j = \bigoplus_k c_{ij,k} \Gamma^k \) for \( G \), which can be done via the \text{SGIrepDirectProduct} function in the \text{SpaceGroupRep} package. Then, \( d_{ij,k} \)'s can be calculated through their relations to \( c_{ij,k} \)'s which are given in BC-Tab. 7.8, and in the package one can use the following codes to get the results.

```latex
\text{MSGCorepDirectProduct}([n,m], k, kp)
\text{showMSGCorepDirectProduct}([n,m], k, kp)
```

In fact, the above codes calculate all the direct products between two magnetic stars \( 'k \) and \( 'k' \) which are specified via one k-point in each of them by \( k \) and \( kp \) respectively. An example is shown in Fig. 5 for the direct products between the full coreps of the magnetic stars \( 'X \) and \( 'R \) of MSG 75.4 (\( P_\text{m}1 \)). There are three full coreps for the magnetic star \( 'X \), namely \( 'X_1 \), \( 'X_2 \), and \( 'X_3X_4 \), and three full coreps for \( 'R \), namely \( 'R_1R_1 \), \( 'R_2R_2 \), and \( 'R_3R_4 \). Fig. 5 shows all the nine direct products between these two sets of full coreps, which are decomposed into the full coreps of the magnetic stars \( 'Z \) and \( 'A \).

### 5.5. Determine the small coreps of energy bands

The small coreps of energy bands are very useful to construct the \( \mathbf{k} \cdot \mathbf{p} \) models via symmetry systematically and to determine the type of band crossings, just as done in Refs. [5, 23–25]. These references directly tell one which small corep corresponds to which \( \mathbf{k} \cdot \mathbf{p} \) model and what type of band crossing, but they do not tell what is the small corep of a degenerate energy level for a given band structure. To obtain the small coreps, two main steps are needed: the first step is to calculate the characters of the elements of the MLG at a desired k-point for each degenerate energy level, and the second step is to determine small coreps by looking up the character table of the MLG. In fact the characters of only unitary elements need to be calculated because the equivalence of coreps only need the characters of unitary elements. The first step can be done by the tool \text{MagVasp2trace} [20, 48] which is capable of post-processing the results of the first-principles code VASP [56], and the second step can be done by the \text{readMagTrace} and \text{getBandCorep} functions in \text{MSGCorep}.

To successfully go through the procedure of determining small coreps, there are three points needing attention. (1) The cell used for band calculation has to conform to the BC convention, i.e. the rotation matrices and translation components of the MSG elements determined from the cell have to be compatible\(^9\) with those from \text{getMSGElem}. (2) The \text{msg.txt} file which contains the MSG elements used by \text{MagVasp2trace} also has to conform to the BC convention. Accordingly, do not use the \text{msg.txt} file provided in the original \text{MagVasp2trace} package, but use the files in the BC MSG elements directory provided by \text{MSGCorep}. (3) For the VASP calculations which turn on non-collinear spin but do not turn on spin-orbit coupling, the wavefunctions are in fact spinors. In this case, \text{MagVasp2trace} has to be modified a little as follows to output correct results.

```latex
! read (nfst ,"( A90 )") chaps ! line 111 of init.f90: comment it
read (nfst ,"( A20L5 )") chtp15 ,FL (2) ! line 112 of init.f90: change A15 to A20
```

Then, one can first use \text{MagVasp2trace} to generate a \text{trace.txt} file from the VASP outputs and then use the following functions in \text{MSGCorep} to obtain the small coreps.

\(^9\)Here “compatible” means the translation components can differ by any integers.
Figure 6: Examples of the bands and their small cores determined by \texttt{getBandCorep} for (a) Mn$_3$NiN (MSG 166.101, \(R\bar{3}m\)) and (b) 2Q phase of \(\gamma\)-Fe$_2$Mn$_{1-x}\) with \(x = 1\) (MSG 134.481, \(P2_1/4_2/nnm\)). The right panels of (a) and (b) show the results of \texttt{showBandCorep} which give the small cores at (a) \(F\) and (b) \(X\) k-points respectively. The integer in the parentheses following the label of each small core is the dimension of the small core. The dashed red boxes indicate the states displayed in the band diagrams.

(* put the trace.txt to the working directory (check this by Directory[]) *)

\texttt{tr1=\text{readMagTrace}["trace.txt"];} (* read the trace.txt file from MagVasp2trace *)
\texttt{cr1=\text{getBandCorep}[(n,m), tr1);} (* determine the small cores of the bands *)
\texttt{showBandCorep[cr1, ik, ibs]} (* show the small cores of the ik-th k-point for bands ibs *)

Two examples are shown in Fig. 6. Fig. 6(a) shows the bands and determined small cores of Mn$_3$NiN with MSG 166.101 (\(R\bar{3}m\)), a non-collinear antiferromagnetic material with anomalous Hall effect, magnetooptical effect, and giant anomalous Nernst effect [57, 58]. Another example is \(\gamma\)-Fe$_2$Mn$_{1-x}\) which is a topological magneto-optical antiferromagnet when \(0.4 < x < 0.8\) [59]. For simplicity, here the 2Q phase for \(x = 1\) with MSG 134.481 (\(P2_1/4_2/nnm\)) is taken for example and its bands and determined small cores are shown in Fig. 6(b). The function \texttt{showBandCorep} can be used to extract the results for specified k-point and bands. For example, the right panel of 6(a) lists the small cores of the 201st k-point, which is the k-point \(F\) in the data of \texttt{cr1}, for the bands from 32nd to 40th, and the red dashed box indicates the three bands displayed in the band diagram, namely the 37th, 38th, and 39th bands with small cores \((F)F_0^{-}, (F)F_0^{+}\), and \((F)F_2^{\pm}\) respectively.

The identification of small cores can help one to judge whether two bands are crossed or anticrossed. For example, the positions marked by \(\star\) along the \(\Delta\) and \(\Sigma\) paths in Fig. 6(b) are seemingly band crossings, but they are actually anticrossings because the related bands have the same small cores and the MSG symmetry does not protect the crossings along these two paths. However, the positions marked by \(\bullet\) along the \(Y\) path in Fig. 6(b) are true band crossings, because the related bands have different small cores. And one can also lookup the encyclopedia of emergent particles for type-IV MSGs [24] to find that each of these crossings along \(Y\) path are in fact of the type P-DNL, i.e. a point residing on a Dirac nodal line.
### 5.6. Support for magnetic point group

As the finite subgroups of MSGs, magnetic point groups (MPGs) are also supported by the MSGCorep package, including group multiplication, cores, and direct product of cores for MPGs. There are in total 122 MPGs in three-dimensional space, including 32 type-I MPGs (i.e. the 32 ordinary point groups), 32 type-II MPGs (also called gray point groups), and 58 type-III MPGs (also called black-white point groups). One can use `showMPGInfo[]` to show the information of the full list of the 122 MPGs, including their numbers, symbols, unitary subgroups, types, etc. One can also specify the sequence numbers to be shown. For example, `showMPGInfo[17;;28]` gives the MPGs with sequence numbers from 17 to 28, i.e. all the orthorhombic MPGs, as shown in Fig. 7(b). In order to simplify the relationship between MPGs and MSGs, the symbol of an MPG is determined by the BNS symbol of the first MSG whose point operations compose the MPG and keep the BNS order of the MSG. For example, MSG 47.252 ($Pn'm'm'$) is the first MSG with the MPG $m'm'm'$ in BNS order, and MPG 5.3 ($2'/m'$) precedes MPG 5.4 ($2'/m'$) because MSG 10.44 ($P2'/m'$) precedes MSG 10.45 ($P2/m'$). Accordingly, the MPG symbols and order are not always the same with those in BC-Tab. 7.1, but they happen to be the same with those used by BCS.

An element of MPG is described as $\{Rname, au\}$ in the code where $Rname$ is the name string of the rotation and $au$ specifies the unitarity (0 for unitary and 1 for anti-unitary), such as $\{C2x, 0\}$ for $C_{2x}$ and $\{"C2z", 1\}$ for $C_{2z}$ ($\equiv C_{2z}.\Gamma$). Similar to getMSGElement, one can use getMPGElement to obtain the elements of an MPG. For example, either `getMPGElement["2'2'2"]` or `getMPGElement["e.3"]` gives the result of $\{"E", 0, \{"C2z", 0\}, \{"C2x", 1\}, \{"C2y", 1\}\}$. The multiplication, inversion, and power of (double) MPG elements can be calculated by the following functions:

```plaintext```
MagRotTimes[{R1, au1}, {R2, au2}] (* the multiplication of two MPG elements *)
invMagRot[{R, au}] (* the inverse of an MPG element *)
```

![Figure 7: Examples of MPG-related functions. (a) The cores of the MPG 8.5 ($m'm'm'$) given by showMPGCorep. Similar to the result of showMLGCorep, single-valued (double-valued) cores are shown in light green (light blue) background. The second and third columns are the extended Mulliken labels and the $\Gamma$ labels of the cores respectively, and the fourth column is the corep type. (b) The information of the MPGs with sequence numbers from 17 to 28 given by showMPGInfo[17;;28]. (c,d) showMPGCorepDirectProduct gives the direct products (c) between all the cores or (d) between two sets of specified cores ((3,5) and 1,5) with the third corep emphasized in red color ("emph"->3).](image-url)
In fact, as an argument of the above six functions, an MPG element can also be expressed simply in a string form with a ' representing \( T \), such as "C2x'" which is equivalent to {"C2x",1}. Furthermore, MagRotTimes and DMagRotTimes can also calculate the continuous multiplication of three MPG elements or more. For example, MagRotTimes ["C2x", "C2a", "C31+'"] returns {"C4x+'",1}.

The cores of an MPG can be obtained by getMPGCorep[mpg] and shown by showMPGCorep[mpg] in which mpg is the symbol (or number) string of the MPG. One example is Fig. 7(a) which shows the cores of the MPG \( m'm'm' \): single-valued cores in light green background and double-valued cores in light blue background, similar to the result of showMLGCorep. The decomposition of direct product of MPG cores can be calculated by MPGCorepDirectProduct[mpg] and shown by showMPGCorepDirectProduct[mpg]. For example, the direct products for the cores of MPG 8.5 (\( m'm'm' \)) are shown in Fig. 7(c). Furthermore, one can specify the input cores by their indexes and even emphasize certain corep(s) in the results via the "emph" option. For example, Fig. 7(d) shows the direct products between two sets of cores, one set is the 3rd and 5th corep and the other set is all the cores from the 1st to the 5th, with emphasizing the 3rd corep (i.e. \( B_2 \)) in red color.

6. Applications

The MSGCorep package has been successfully applied in the systematic classification of emergent particles, namely the quasiparticles emerging from various band crossings [23, 24, 60]. The properties of a type of emergent particle are determined by the \( k \cdot p \) model around the band crossing, and the \( k \cdot p \) model can be constructed according to the symmetry constraints imposed by the small cores of the degeneracy at the band crossing. In order to interface with the systematic full data of small cores provided by MSGCorep for all k-points and all MSGs, a package called MagneticKP is developed to construct \( k \cdot p \) models based on an efficient iterative simplification algorithm [61]. Accordingly, we have systematically investigated the classification of emergent particles in all the 674 type-III MSGs [23] and 517 type-IV MSGs [24] by means of analyzing the \( k \cdot p \) models obtained from MagneticKP plus MSGCorep. Furthermore, we have also proposed a method of calculating the small cores of magnetic subperiodic groups, specifically all the 528 magnetic layer groups and 394 magnetic rod groups, using the small cores data from MSGCorep, and have systematically classified the possible emergent particles existing in these magnetic subperiodic groups [60].

7. Conclusions

We have developed a package named MSGCorep to provide convenient offline access to the complete corep data of all 1651 MSGs in three-dimensional space. In addition, access to the cores of 122 MPGs is also supported by this package. The functionalities of this package include: obtaining the elements of any MSG, MLG, MPG, and their double groups; calculating the multiplication, inverse, and power of group elements; obtaining the small cores at any k-point and full cores of any magnetic k-star for any MSG and showing them in a user-friendly table form; calculating and showing the decomposition of direct products of full cores between any two specified magnetic k-stars; supporting both single-valued and double-valued cores; and determining the small cores of energy bands. To the best of our knowledge, MSGCorep is the first package that provides tools to calculate the direct product of full cores for any MSG and to determine small cores of energy bands for general purpose. In a word, the MSGCorep package is a useful database and tool set for the MSGs, MPGs, and their cores, it has been successfully applied in systematic studies on emergent particles, and it can play an important role in future studies on the symmetries in magnetic and nonmagnetic materials.
then substitute \( \bar{\Delta} = \Delta_p \) as we get in which the orthogonality theorem of irreps, namely \( \Delta \times \Delta = \Delta^0 \). For simplicity, denote \( \Delta(A^{-1}mA)^* \) as \( \Delta(m) \) and the task becomes to find a matrix \( N \) satisfying \( \Delta(m) = N^{-1}\Delta^0(m)N \) for \( \forall m \in H \), i.e.

\[
\bar{\Delta}_{ij}(m) = \sum_{k,l}(N^{-1})_{ik}\Delta_k^0(m)N_{lj} = \sum_{k,l}N^*_{ki}\Delta^0_k(m)N_{lj}.
\]  \( \text{(A.1)} \)

Multiply two sides of the above equation by \( \Delta^0_{k'l'}(m)^* \) and then sum over \( m \) to get

\[
\sum_{m \in H} \Delta^0_{k'l'}(m)^*\bar{\Delta}_{ij}(m) = \sum_{k,l}N^*_{ki}N_{lj}\sum_{m \in H} \Delta^0_{k'l'}(m)^*\Delta_k^0(m)
\]

\[
= \sum_{k,l}N^*_{ki}N_{lj}\frac{|H|}{d_q}\delta_{pq}\delta_{kk}\delta_{ll'} = N^*_{ki}N_{lj}\frac{|H|}{d_q}\delta_{pq}.
\]  \( \text{(A.2)} \)

in which the orthogonality theorem of irreps matrices is used and \( d_q \) is the dimension of \( \Delta^0 \). Letting \( p = q \), we get

\[
N^*_{ki}N_{lj} = \frac{d_q}{|H|}\sum_{m \in H} \Delta^0_k(m)^*\bar{\Delta}_{ij}(m).
\]  \( \text{(A.3)} \)

Further letting \( l = k \) and \( j = i \), we get

\[
|N_{ki}|^2 = \frac{d_q}{|H|}\sum_{m \in H} \Delta^0_k(m)^*\bar{\Delta}_{ii}(m).
\]  \( \text{(A.4)} \)

Using the above equation to find a nonzero element of the matrix \( N \), e.g. \( N_{it} = \sqrt{|N_{11}|^2} \neq 0 \) \( (k = 1, i = t) \), then substitute \( k = 1 \) and \( i = t \) into Eq. (A.3) and obtain every matrix element of \( N \) by

\[
N_{ij} = \frac{1}{N^*_{it}}\frac{d_q}{|H|}\sum_{m \in H} \Delta^0_k(m)^*\bar{\Delta}_{ij}(m).
\]  \( \text{(A.5)} \)

Appendix B. Corrections and adaptions to the tables in the BC book

**BC-Tab. 7.4:** As stated in the BC book, BC-Tab. 7.4 is basically the same as the original table given by Belov, Neronova, and Smirnova in 1957 [52]. To be consistent with the BNS symbols given in the latest monograph about MSGs by Litvin [32], we have made some adaptions to BC-Tab. 7.4. Firstly, we make all the symbols of type-II MSGs be the corresponding ones of type-I MSGs followed by \( 1 \). Not all the original type-II symbols in BC-Tab. 7.4 obey this rule, such as some trigonal MSGs (e.g. 149.22 P31'2) and all cubic MSGs (e.g. 207.41 P43'2). New symbols of this type are shown in green color in Table B.2. Secondly, all the MSG symbols derived from the PG symbols \( m3 \) (\( T_h \)) and \( m3m \) (\( O_h \)) should be updated, because \( m3 \) and \( m3m \) have been changed to \( m3 \) and \( m3m \) respectively for tens of years. This change from 3 to \( \bar{3} \) involves all the MSGs with numbers \( n,m,n \in [200,206] \cup [221,230] \). Especially, there are 27 type-III MSGs for which \( \bar{3} \) should be further primed after the change, which are shown in blue color in Table B.2. Finally, there are two typos and the corrections are shown in red color in Table B.2.

**BC-Tab. 7.2:** See Table B.3 for the corrections to BC-Tab. 7.2.

**BC-Tab. 7.3:** See Table B.4 for the supplement to BC-Tab. 7.3.
| BNS No. | Old       | New       | BNS No. | Old       | New       |
|--------|-----------|-----------|---------|-----------|-----------|
| 1.2    | $P_1'$    | $P_11'$   | 1.2     | $P_1$     | $P_1$     |
| 33.155 | $P_{na2}$ | $P_{na2}$ | 33.155  | $P_3$     | $P_3$     |
| 114.276| $P_{2c}$  | $P_{2c1}$ | 114.276 | $P_3$     | $P_3$     |
| 149.22 | $P_{31/2}$| $P_{31/2}$| 149.22  | $P_3$     | $P_3$     |
| 150.26 | $P_{31}$  | $P_{31}$  | 150.26  | $P_3$     | $P_3$     |
| 151.30 | $P_{31}'$ | $P_{31}'$ | 151.30  | $P_3$     | $P_3$     |
| 152.34 | $P_{31}'$ | $P_{31}'$ | 152.34  | $P_3$     | $P_3$     |
| 153.38 | $P_{31}'$ | $P_{31}'$ | 153.38  | $P_3$     | $P_3$     |
| 154.42 | $P_{31}'$ | $P_{31}'$ | 154.42  | $P_3$     | $P_3$     |
| 156.50 | $P_{31}'$ | $P_{31}'$ | 156.50  | $P_3$     | $P_3$     |
| 157.54 | $P_{31}'$ | $P_{31}'$ | 157.54  | $P_3$     | $P_3$     |
| 158.58 | $P_{31}'$ | $P_{31}'$ | 158.58  | $P_3$     | $P_3$     |
| 159.62 | $P_{31}'$ | $P_{31}'$ | 159.62  | $P_3$     | $P_3$     |
| 162.74 | $P_{31}'$ | $P_{31}'$ | 162.74  | $P_3$     | $P_3$     |
| 163.80 | $P_{31}'$ | $P_{31}'$ | 163.80  | $P_3$     | $P_3$     |
| 164.86 | $P_{31}'$ | $P_{31}'$ | 164.86  | $P_3$     | $P_3$     |
| 165.92 | $P_{31}'$ | $P_{31}'$ | 165.92  | $P_3$     | $P_3$     |
| 195.2  | $P_{31}'$ | $P_{31}'$ | 195.2   | $P_3$     | $P_3$     |
| 198.10 | $P_{31}'$ | $P_{31}'$ | 198.10  | $P_3$     | $P_3$     |
| 199.13 | $P_{31}'$ | $P_{31}'$ | 199.13  | $P_3$     | $P_3$     |
| 200.14 | $P_{31}'$ | $P_{31}'$ | 200.14  | $P_3$     | $P_3$     |
| 200.15 | $P_{31}'$ | $P_{31}'$ | 200.15  | $P_3$     | $P_3$     |
| 200.16 | $P_{31}'$ | $P_{31}'$ | 200.16  | $P_3$     | $P_3$     |
| 201.17 | $P_{31}'$ | $P_{31}'$ | 201.17  | $P_3$     | $P_3$     |
| 201.18 | $P_{31}'$ | $P_{31}'$ | 201.18  | $P_3$     | $P_3$     |
| 201.19 | $P_{31}'$ | $P_{31}'$ | 201.19  | $P_3$     | $P_3$     |
| 201.20 | $P_{31}'$ | $P_{31}'$ | 201.20  | $P_3$     | $P_3$     |
| 201.21 | $P_{31}'$ | $P_{31}'$ | 201.21  | $P_3$     | $P_3$     |
| 202.22 | $P_{31}'$ | $P_{31}'$ | 202.22  | $P_3$     | $P_3$     |
| 202.23 | $P_{31}'$ | $P_{31}'$ | 202.23  | $P_3$     | $P_3$     |
| 202.24 | $P_{31}'$ | $P_{31}'$ | 202.24  | $P_3$     | $P_3$     |
| 202.25 | $P_{31}'$ | $P_{31}'$ | 202.25  | $P_3$     | $P_3$     |
| 203.26 | $P_{31}'$ | $P_{31}'$ | 203.26  | $P_3$     | $P_3$     |
| 203.27 | $P_{31}'$ | $P_{31}'$ | 203.27  | $P_3$     | $P_3$     |
| 203.28 | $P_{31}'$ | $P_{31}'$ | 203.28  | $P_3$     | $P_3$     |
| 203.29 | $P_{31}'$ | $P_{31}'$ | 203.29  | $P_3$     | $P_3$     |
| 204.30 | $P_{31}'$ | $P_{31}'$ | 204.30  | $P_3$     | $P_3$     |
| 204.31 | $P_{31}'$ | $P_{31}'$ | 204.31  | $P_3$     | $P_3$     |
Table B.3: Corrections to the “colored generating elements (CGE)” in BC-Tab. 7.2. The column “SymStd” lists the standard BNS symbols. Here we also list the BNS symbols conforming to the BC orientation for comparison, if they are different from the standard symbols.

| BNS No. | SymStd  | SymBC  | CGE   | BNS No. | SymStd  | SymBC  | CGE   |
|---------|---------|--------|-------|---------|---------|--------|-------|
| 28.89   | Pn’a2’ | Pbm’2’ | σ_y   | 57.380  | Pbc’m  | Pb’ma  | C_{2y}, I |
| 28.90   | Pm’a2’ | Pb’m2’ | σ_x   | 57.381  | Pbcn’  | Pbm’a  | C_{2x}, I |
| 29.101  | P’c’a2’ | Pb’c’2’ | σ_y   | 57.382  | Pbc’e’m | Pb’’ma’ | C_{2x} |
| 29.102  | P’c’a2’ | Pb’c’2’ | σ_x   | 57.383  | Pb’c’m’ | Pb’’m’a’ | C_{2x}, C_{2y} |
| 31.125  | Pnm’n’2’ | Pmn’2’ | σ_y   | 57.384  | Pbc’n’ | Pbm’a’ | C_{2y} |
| 31.126  | Pnm’n’2’ | Pmn’2’ | σ_x   | 60.420  | Pbc’n’ | Pcn’b’ | C_{2x}, C_{2y}, I |
| 33.146  | P’na’2’ | Pbn’2’ | σ_y   | 60.421  | Pbc’n’ | Pcn’b’ | C_{2x}, I |
| 33.147  | P’na’2’ | Pbn’2’ | σ_x   | 60.422  | Pbc’’n’ | Pc’’n’b’ | C_{2x} |
| 36.174  | Cm’c’2’ | Ccm’2’ | σ_y   | 60.424  | Pbc’n’ | Pc’’n’b’ | C_{2x}, C_{2y} |
| 36.175  | Cmc’2’ | Cc’m’2’ | σ_x   | 160.67  | R3m’c’ | σ_{d1} |
| 38.189  | Am’2’ | Cm’2’ | σ_z   | 161.71  | R3c’ | σ_{d1} |
| 38.190  | Am’m’2’ | Cm’2’ | σ_x   | 166.100 | R3m’l’ | S_{d1}^+ |
| 38.191  | Am’m’2’ | Cm’d’2m’ | σ_x, σ_x | 166.101 | R3m’l’ | σ_{d1} |
| 39.197  | Ab’m’2’ | Cm’2’a’ | σ_z   | 167.106 | R3c’ | S_{d1}^+ |
| 39.198  | Ab’m’2’ | Cm’2’a’ | σ_x   | 167.107 | R3c’ | σ_{d1} |
| 39.199  | Ab’m’2’ | Cm’2’a’ | σ_z, σ_x | 177.151 | P6’22’ | C_{6}^+ |
| 40.205  | Am’a2’ | Cc’2’m’ | σ_z   | 177.152 | P6’22’ | C_{6}^+ C_{21} |
| 40.206  | Ama’2’ | Cc’2’m’ | σ_x   | 178.157 | P6’22’ | C_{6} |
| 40.207  | Am’2’ | Cc’2’m’ | σ_z, σ_x | 178.158 | P6’22’ | C_{6}^+ C_{21} |
| 41.213  | Ab’2’ | Cc’2’a’ | σ_z   | 179.163 | P6’22’ | C_{6} |
| 41.214  | Abc’2’ | Cc’2’a’ | σ_x   | 179.164 | P6’22’ | C_{6}^+ C_{21} |
| 41.215  | Abc’2’ | Cc’2’a’ | σ_z, σ_x | 180.169 | P6’22’ | C_{6} |
| 46.243  | I’a2’ | Ibm’2’ | σ_y   | 180.170 | P6’22’ | C_{6}^+ C_{21} |
| 46.244  | I’m’a2’ | Ibm’2’ | σ_x   | 181.175 | P6’22’ | C_{6} |
| 51.291  | Pn’ma | Pcmn’ | C_{2x}, C_{2y}, I | 181.176 | P6’22’ | C_{6}^+ C_{21} |
| 51.293  | Pnma’ | Pcmn’ | C_{2y}, I | 182.181 | P6’22’ | C_{6}^+ C_{21} |
| 51.294  | Pnm’a | Pcmn’ | C_{2y} | 182.182 | P6’22’ | C_{6}^+ C_{21} |
| 51.295  | Pnm’a | Pcmn’ | C_{2x}, C_{2y} | 183.187 | P6’6’m’ | C_{6}^+ σ_{e1} |
| 52.308  | Pn’ma | Pmn’ | C_{2x}, C_{2y}, I | 183.188 | P6’6’m’ | C_{6}^+ σ_{e1} |
| 52.309  | Pnma’ | Pmn’ | C_{2x}, I | 184.193 | P6’6’c’ | C_{6}^+ σ_{e1} |
| 52.310  | Pn’n’a | Pmn’ | C_{2x} | 184.194 | P6’6’c’ | C_{6}^+ σ_{e1} |
| 52.312  | Pn’na’ | Pn’a’n’ | C_{2x}, C_{2y} | 185.199 | P6’6’c’ | C_{6}^+ σ_{e1} |
| 53.323  | Pnn’a | Pmm’b | C_{2x}, I | 185.200 | P6’6’m’ | C_{6}^+ σ_{e1} |
| 53.324  | Pnn’m’a | Pmm’b | C_{2y}, I | 186.205 | P6’6’m’ | C_{6}^+ σ_{e1} |
| 53.327  | Pnm’a | Pmm’b | C_{2x} | 186.206 | P6’6’m’ | C_{6}^+ σ_{e1} |
| 53.328  | Pnm’nd | Pmm’b’ | C_{2y} | 191.236 | P6’6’6’m’m’ | C_{6}^+ C_{21}, I |
| 54.339  | P’c’a | Pca’ | C_{2x}, C_{2y}, I | 191.237 | P6’6’6’m’m’ | C_{6}^+ I |
| 54.341  | Peca’ | Pca’ | C_{2x}, C_{2y}, I | 191.238 | P6’6’6’m’m’ | C_{6}^+ I |
| 54.342  | P’c’a | Pca’ | C_{2y} | 191.239 | P6’6’6’m’m’ | C_{6}^+ C_{21}, I |
| 54.343  | P’c’a | Pca’ | C_{2x}, C_{2y} | 192.246 | P6’6’6’m’m’ | C_{6}^+ C_{21}, I |
| 57.379  | Pb’cm | Pbma’ | C_{2x}, C_{2y}, I | 192.247 | P6’6’6’m’m’ | C_{6}^+ I |
Table B.4: Black-white lattices which should be added to BC-Tab. 7.3 to make it complete.

| Crystal system | Ordinary lattice | Black-white lattice | \( t_0 \) |
|----------------|------------------|---------------------|----------|
| Monoclinic     | \( P(\Gamma_m) \) | \( P_c \)           | \( \frac{1}{2}t_1 \) |
|                |                  | \( P_A \)           | \( \frac{1}{2}(t_1 + t_3) \) |
| Orthorhombic   | \( P(\Gamma_o) \) | \( P_b \)           | \( \frac{1}{2}t_1 \) |
|                |                  | \( P_B \)           | \( \frac{1}{2}(t_2 + t_3) \) |
| Orthorhombic   | \( I(\Gamma_o^v) \) | \( I_a \)           | \( \frac{1}{2}(t_1 + t_3) \) |
|                |                  | \( I_b \)           | \( \frac{1}{2}(t_2 + t_3) \) |

Appendix C. Differences of MSG symbols between Litvin and ISO-MAG

The standard MSG symbols of both BNS and OG types here we use are consistent with those used by Litvin [32]. But they are different from those used by ISO-MAG [55] and BCS [41] for some MSGs. We list these differences in Tables C.5 and C.6 for reference so as not to result in misunderstanding in certain cases. The version 1.3 (Jan 2022) of ISO-MAG is consistent with BCS, and both Tables C.5 and C.6 show their differences from Litvin. After our communication to one author of ISO-MAG about the differences, the version 1.4 (May 2022) of ISO-MAG changed the seven OG symbols in Table C.5 to those of Litvin. However, the twenty-one BNS symbols of ISO-MAG in Table C.6 keep the same from version 1.3 to 1.4 because the authors want to keep them consistent with BCS.

Table C.5: Differences of OG symbols between Litvin and ISO-MAG of version 1.3 as well as BCS. These symbols of ISO-MAG have been changed to be the same with those of Litvin in version 1.4.

| OG No. | Litvin | ISO-MAG (v1.3) |
|--------|--------|----------------|
| 16.6.104 | \( P_F222 \) | \( P_I222 \) |
| 25.9.163 | \( P_Fmm2 \) | \( P_Imm2 \) |
| 34.5.235 | \( P_Fnn2 \) | \( P_Inn2 \) |
| 47.8.354 | \( P_Fmmm \) | \( P_Immm \) |
| 48.6.363 | \( P_Fmmm \) | \( P_Immn \) |
| 153.4.1270 | \( P_{2c31}12' \) | \( P_{2c31}12 \) |
| 154.4.1274 | \( P_{2c31}2'1 \) | \( P_{2c31}21 \) |

Table C.6: Differences of BNS symbols between Litvin and ISO-MAG as well as BCS. These symbols of ISO-MAG did not change from version 1.3 to 1.4.

| BNS No. | Litvin | ISO-MAG | BNS No. | Litvin | ISO-MAG | BNS No. | Litvin | ISO-MAG |
|---------|--------|---------|---------|--------|---------|---------|--------|---------|
| 17.13   | \( P_A222_1 \) | \( P_B222_1 \) | 39.201  | \( A_{b}bm2 \) | \( A_{b}bm2 \) | 49.274  | \( P_{Accm} \) | \( P_{Bccm} \) |
| 18.20   | \( P_{2c21}12 \) | \( P_{b}2c2_1 \) | 39.202  | \( A_{c}bm2 \) | \( A_{g}bm2 \) | 56.372  | \( P_{ec}ccn \) | \( P_{e}ccn \) |
| 18.22   | \( P_{2c21}12 \) | \( P_{B}2c2_1 \) | 40.209  | \( A_{c}ma2 \) | \( A_{g}ma2 \) | 58.402  | \( P_{Ammn} \) | \( P_{Bmmn} \) |
| 19.28   | \( P_{2c21}12_1 \) | \( P_{c}2c2_1 \) | 40.210  | \( A_{c}ma2 \) | \( A_{B}ma2 \) | 59.412  | \( P_{c}mmn \) | \( P_{Bmm} \) |
| 32.140  | \( P_{bc}2a \) | \( P_{b}ba2 \) | 41.217  | \( A_{c}ba2 \) | \( A_{g}ba2 \) | 59.414  | \( P_{Ammn} \) | \( P_{Bmm} \) |
| 38.193  | \( A_{mm}2 \) | \( A_{bb}mm2 \) | 41.218  | \( A_{c}ba2 \) | \( A_{g}ba2 \) | 72.547  | \( I_{b}bam \) | \( I_{sb}am \) |
| 38.194  | \( A_{c}mm2 \) | \( A_{B}mm2 \) | 48.262  | \( P_{c}nnn \) | \( P_{s}nnn \) | 74.562  | \( I_{c}mma \) | \( I_{sym} \) |

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