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Space Group Representations. Theory, Tables and Applications. By Nikolai B. Melnikov and Boris I. Reser. Springer Nature Switzerland AG, 2022. ISBN 978-3-031-13990-1.

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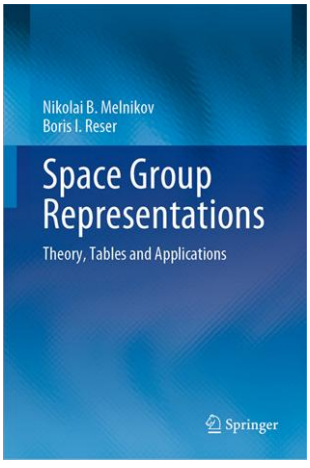

The book offers a clear explanation of space-group representation theory, focusing on the projective representations of crystallographic point groups and their practical applications in energy band calculations. Detailed tables are provided for constructing irreducible representations of all space groups. The authors aim to promote their approach by making each chapter standalone and accessible for purchase separately. The book targets researchers and graduate students in solid-state physics and chemistry, assuming only a basic understanding of linear algebra and quantum mechanics. However, it is less suitable for crystallographers for a number of reasons that are expanded on below.

The book consists of three parts: theory (chapters 2–5), tables (chapter 6) and applications (chapters 7–17). Within the appendices, the authors have assembled proofs of certain mathematical theorems, along with supplementary content on projective representations and double-valued representations.

The initial part of the book consists of an introductory chapter followed by three central chapters. Chapter 2 gives a concise overview of group theory, linear algebra and representation theory. Chapter 3 focuses on induced representations, while chapter 4 covers projective representations, which, according to the method developed in the book, are essential for the construction of space-group representations. To ensure self-sufficiency, chapters 3 and 4 provide proofs for most assertions and theorems in a constructive and concise manner. Practitioners seeking immediate applications may choose to defer or revisit these chapters later as they require some level of abstraction. In chapter 5 the theoretical results of the previous chapters are applied to the construction of irreducible representations of space groups. Specifically, the focus is on irreducible projective representations of the 32 crystallographic point groups, with a convenient approach for deriving them. As a next step, the matrices of all irreducible (single- and double-valued) representations of a space group are derived from the irreducible projective representations of the 32 crystallographic point groups. Additionally, the text discusses the role of spin and the consequences of time-reversal symmetry.

Part II features chapter 6, a crucial component of the book with comprehensive tables of irreducible representations for space groups. This chapter is substantial in both content and size and serves as a standalone reference. Section 6.1 gives a brief overview of the preceding theory and offers guidance on using the tables. Sections 6.2–6.19 contain condensed tables displaying irreducible projective representations of the 32 crystallographic point groups, which form the basis for deriving all irreducible representations, including double-valued ones, for all 230 space groups. Section 6.20 provides practical methods for using these tables.

Part III focuses on applying group theory in solid-state physics and energy band calculations, and is divided into four sections based on application areas. The first section (covering chapters 7–9) includes the exploration of symmetry in classifying quantum-mechanical eigenstates, followed by the analysis of its application to solid-state physics, considering also spin and time-reversal symmetry. Chapter 9 introduces electronic energy band calculations, emphasizing symmetry in the orthogonal plane wave (OPW) method. To illustrate representation theory practically, the second section (chapters 10–12) offers real-world examples, especially focusing on non-symmorphic space groups. The third section (chapters 13–15) explores the tight-binding method, also known as the linear

combination of atomic orbitals (LCAO) method, while the fourth section focuses on symmetrized functions crucial for energy band calculations. Chapters 16 and 17 detail methods for constructing symmetrized plane waves (SPW) and symmetrized Bloch sums (SBS), respectively, applicable to crystals with diverse symmetry properties.

Finally, chapter 18 compares the theories and tables presented in the book with existing literature and provides references for further exploration.

While some typographical errors persist in the text (see *e.g.* p. 184), the chapters maintain clarity and conciseness. The book features an index, likely to be highly beneficial. A notable strength of the book lies in the comprehensive list of cited references at the end of each chapter, despite occasional overlaps between chapters. Additionally, the authors provide a very helpful, albeit quite detailed, list of symbols. However, in the extensive listings, the abbreviations, for example like ARPES or TB-LMTO-ASA (*e.g.* p. 260) are not included, which may pose difficulties for readers.

According to the details provided, the book seems to offer significant value for solid-state physicists, especially those involved in energy band calculations. However, the treatment of symmetry and crystallography lacks the precision and clarity desired for a thorough understanding. I would advise against recommending it to the crystallographic community for the following reasons:

Terminology and notation. Unfortunately, the authors do not follow the rules, symbols and standards of the *International Tables for Crystallography*.

(i) Space-group symbolism. For crystallographic groups and their representations, the authors claim to adhere to the notation established by Schönflies (1923), Seitz (1936), Bouckaert *et al.* (1936), Koster (1957), Faddeev (1961, 1964) *etc*. Probably, this is a natural decision for the solid-state community but definitely not for the crystallographic community, especially when crystallographic space groups are discussed. The Schoenflies symbols describe the point-group type (known as the geometric crystal class), while different space groups of the same crystal class are distinguished by a superscript index appended to the point-group symbol. In this way, Schoenflies symbols display the space-group symmetry only partly. Therefore, they are nowadays rarely used for the description of the symmetry of crystal structures. In comparison with the Schoenflies symbols, the Hermann–Mauguin symbols are more indicative of the space-group symmetry and that of the crystal structures.

(ii) Seitz symbols for space-group operations. Following the traditions established in solid-state physics and chemistry, the authors use Seitz symbols for denoting the space-group symmetry operations. Unfortunately, the applied Seitz notation for symmetry operations differs from the notation adopted by the Commission on Crystallographic Nomenclature as the standard convention for Seitz symbolism of the International Union of Crystallography (Glazer *et al.*, 2014).

(iii) Examples of real structures. The book offers limited real-world structural examples. It appears that, in line with Bouckaert *et al.* (1936), the examples focus on structures exhibiting full point-group symmetry, such as the diamond structure (*cf.* ch. 10). Furthermore, in most instances, the authors restrict their analysis to applications in energy band calculations, sidestepping the use of crystallographic conventions. For example, following the tradition in solid-state physics: for the description of structural symmetry in direct space, the authors use the Wigner–Seitz unit cells instead of a crystallographic unit cell, see *e.g.* the description of the diamond crystal structure given in ch. 10. However, I really wonder about the necessity of using the Wigner–Seitz unit cell in direct space if the components of the special **k** vectors (listed in Table 10.2) are given with respect to the conventional coordinate system used in Vol. *A* of *International Tables for Crystallography* (Aroyo, 2016). The authors use the rectangular coordinate system in describing the symmetry operations of the group *D*6*h* (6/*mmm*) (p. 75).

(iv) Unclear terminology: 'helical axes and slip planes' (p. 56, before equation 5.5), probably meaning 'screw axes and glide planes'. It seems that the authors do not differentiate between point (and space) groups and types of point (and space) groups (pp. 56–57). There is an unclear term on p. 129 'conjugate points on the Wigner–Seitz cell boundary'; 'irreducible Brillouin zone' (*cf.* for example p. 60), probably referring to what is known as a 'representation domain'.

References to the tables of space-group representations:

(i) In the final chapter (ch. 18) of the book (pp. 293–297), the authors conduct a comparison between the theory and tables of irreducible representations of space groups found within their work and existing compilations available. It seems unusual that a notable reference such as the book authored by Cracknell *et al.* (1979), which contains what is believed to be the most comprehensive collection of character tables and matrix representatives of irreducible representations for classical space groups, is not included in the list of reference books on space-group representations [the book by Cracknell *et al.* (1979) is not even cited].

(ii) In the explanations of the compatibility relations (pp. 66–68) the authors mention that 'the compatibility tables for symmorphic space groups are presented in Bouckaert *et al.* (1936)'. However, if I remember correctly, compatibility tables of the irreducible representations of all space groups can be found in the book by Miller & Love (1967). In discussing the compatibility relations (p. 67), the authors mention just **k** vectors 'sitting' on symmetry lines or symmetry planes. What about symmetry points?

(iii) In many problems of solid-state physics, it is necessary to derive the correspondence between the electronic states in the crystal and in the free atoms that form the crystal. The authors discuss a method for the calculation of such a correspondence, *e.g. cf.* Sections 11.2.2 or 12.5. However, in their discussions the authors do not even mention the results of the site-symmetry approach discussed in detail by Evarestov & Smirnov (1997). Are the two methods related?

References to web resources and web servers. The emergence of online courses and novel teaching techniques incorporating multimedia, online tools and interactive resources has profoundly transformed the educational landscape. Gone are

the days when interactive resources were confined to traditional classrooms; now, students have the freedom to interact with learning materials at their own speed and convenience, thereby enriching their educational journey. Although the authors claim to have presented complete tables of irreducible representations of space groups, there are no references to web resources and web servers that provide complete compilations of space-group representations, including their matrices. For example, the determination, classification, labelling and tabulation of irreducible representations of space groups is based on the use of wavevectors **k**. The **k**-vector database available on the Bilbao Crystallographic Server (https://www.cryst.ehu.es/) contains figures of the Brillouin zones and tables which form the background of a classification of the irreducible representations of all 230 space groups. In addition, the matrices of single- and double-valued representations of space groups are also available on the same web site. Further, one can find programs for the derivation of the compatibility relations between the representations or for the correspondence between atomic and crystal states.

Unclear and wrong statements. Numerous unconventional or awkward phrases are scattered throughout the text, likely stemming from an imperfect translation from Russian. Some examples:

p. 26 'the set of indices $[i_g]$ is called the star of the representation d^{i}'. (I hope I understand the meaning of the statement although I find it a bit strange to define a star of a representation by a set of indices.)

p. 56 'The factor group of the space group over the translation subgroup G/T is isomorphic to the point group G_0 of the lattice'. (Probably what is meant is the point group of the space group?)

p. 57 'Nonsymmorphic space groups correspond to crystals that have more stationary positions of the atoms than the lattice sites'. (I really do not understand that statement.)

p. 163 'all interior points of the irreducible Brillouin zone are in a general position; *i.e.* they do not have symmetry'. (Of course, even general **k**-vector points have certain symmetry, although this could only be the trivial one.)

To sum up, this book may be valuable for solid-state physicists who are interested in irreducible representations of space groups and their applications, particularly in energy band calculations. Nonetheless, I would not suggest it to those in the crystallographic community, as it does not take into account their needs. Apart from the reasons described above, the book is not designed for self-study and does not offer a pedagogical introduction to the problem of irreducible representations of space groups. For example, the authors did not choose an example-driven approach that could have helped readers to apply the learned material.

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