Magnetic Groups and Their Corepresentations

C. J. BRADLEY, B. L. DAVIES
Department of Metallurgy, University of Oxford, Oxford, England

A review is given of the theory of magnetic groups and of their unitary corepresentations. Particular application is made to magnetic space groups, this part of the work being set in the framework of little-group theory. The symmetry problems in physics which lead to magnetic groups are analyzed and various applications of the theory to such problems are pointed out. Finally a method is given for obtaining the Kronecker products of corepresentations of magnetic groups, and an example is presented in which the unitary subgroup of the magnetic group is the point group $\mathbf{C}_{2v}$.

1. INTRODUCTION

A particularly famous work in the study of crystallography is the book by Shubnikov[1] on the symmetry and antisymmetry of finite figures. It opened the flood gates to a remarkable development in the theory of symmetry. For it was not long before it was realized that the ideas it contained were just those required to make an analysis of crystals which have a nonzero average magnetic moment. The next stage was, independently of each other, that Zamorzaev[2] first, and then Belov, Neronova, and Smirnova[3] derived the 1651 colored space groups. These masterly works by Shubnikov[1] and Belov,[3] together with other articles, are now combined in a book[4] which contains an extensive bibliography of 201 references to work on the symmetry of finite figures.

If the operation of color change in the colored groups is replaced by the antiunitary time-reversal operator one obtains the magnetic groups. Of the 1651 magnetic space groups, 230 correspond to the classical space groups, 230 to these groups together with time reversal, and the other 1191 to groups in which time reversal occurs only in combination with other operations and not by itself. Likewise there are 122 magnetic point groups which are partitioned into three types by the above classification, the number of groups in each type being 32, 32, and 58, respectively.

Tavger and Zaitzev[5] first classified the magnetic point groups and realized their significance in the study of the macroscopic properties of magnetic crystals. Since then there has been considerable interest in magnetic crystals and in the application of group theory to the study of their properties.

The main problems of physical interest which have received attention are the following. First of all there is the classification problem: given a spin ordered structure to what symmetry group does the crystal belong? A knowledge of what symmetry groups are possible will obviously assist the experimental worker in his quest for determining the spin order of a given material and will limit the amount of effort he has to put in to determine the structure uniquely. Work along these lines was initiated by Donnay, Corliss, Donnay, Elliott, and Hastings[6] who determined the magnetic structure of chalcopyrite by neutron diffraction experiments. Then there is the converse problem of whether a particular magnetic space group permits an invariant spin structure; that is, whether the abstract group has a physical realization. Opechowski and Guccione[7] have a good deal to say about this. Also bound up with this is the solved problem of determining those structures which can exhibit the various types of permanent magnetism.

Also at a macroscopic level there is the determination of those structures which can exhibit certain physical effects in the presence of applied fields such as the electric and magnetic fields. The general problem here is the determination of the symmetry properties of tensors and their invariant properties under transformations of the magnetic point groups. The books by Birss[8] and Bhagavantam[9] give the most comprehensive accounts of this subject.

There are, of course, a number of problems at the microscopic level which require analysis of the magnetic space groups for their solution. For example, the classification of the electron energy levels in magnetic crystals, and the study of second-order phase transitions. The solution of such problems as these depends on an analysis of the irreducible corepresentations of magnetic space groups and of their Kronecker products. The founding father of corepresentation theory was Wigner[10] and development of his work in the U.S.S.R. is due mainly to Kudryavsteva and Chaldyshev[11] and

[1] A. V. Shubnikov, *Symmetry and Antisymmetry of Finite Figures* (U.S.S.R. Academy of Sciences, Moscow, 1951).
[2] A. M. Zamorzaev, Generalization of the Space groups: Dissertation, Leningard University (1953).
[3] N. V. Belov, N. N. Neronova, and T. S. Smirnova, Trudy, Akad. Nauk SSSR, Inst. Kristall., **11**, 33 (1955).
[4] A. V. Shubnikov and N. V. Belov, *Coloured Symmetry* (Pergamon Press Ltd., London, 1964).
[5] B. A. Tavger and V. M. Zaitzev, Soviet Phys.—JETP **3**, 430 (1956).
[6] G. Donnay, L. M. Corliss, J. D. H. Donnay, N. Elliott, and J. M. Hastings, Phys. Rev. **112**, 1917 (1958).
[7] W. Opechowski and R. Guccione, in *Magnetism*, G. T. Rado and H. Suhl, Eds. (Academic Press Inc., New York, 1965), Vol. IIA.
[8] R. R. Birss, *Symmetry and Magnetism* (North-Holland Publ. Co., Amsterdam, 1964); also Rept. Progr. Phys. **26**, 307 (1963).
[9] S. Bhagavantam, *Crystal Symmetry and Physical Properties* (Academic Press Inc., New York, 1966).
[10] E. P. Wigner, *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra* (Academic Press Inc., New York, 1959).
[11] N. V. Kudryavsteva and V. A. Chaldyshev, Izv. Vysshikh Uchebn. Zavendenii Fiz. **2**, 104 (1962); **3**, 133 (1962); **4**, 98 (1962); **2**, 46 (1963); **3**, 3; (1965); **3**, 50; (1965); and **9**, 93 (1966).

in the U.S.A. to Dimmock and Wheeler,[12–14] though one must also mention the important papers by Dimmock,[15] and by Karavaev, Kudryavsteva, and Chaldyshev.[16]

The theory of second-order phase transitions goes back to Landau and Lifshitz[17] and is beautifully reviewed in its application to crystals belonging to the classical space groups by Lyubarskii.[18] This theory has been extended to cover the magnetic group case by Dimmock.[19] The analysis involves the Kronecker products of corepresentations. More recently problems in spin wave theory have been put in the setting of magnetic groups; the groups introduced by Brinkman and Elliott[20] for this purpose they term spin-space groups: these contain more elements than the magnetic space groups of the corresponding structures because the appropriate interaction Hamiltonians have greater symmetry than the structures themselves.

This article has three aims in view, first to give a review of the main group-theoretical points of interest in the applications that have occurred, secondly to present some new methods of proof which we have found helpful and which we hope will therefore prove helpful to others, and thirdly to give sight to certain ideas (for example, projective corepresentations) which are current in the Russian literature,[11,16] but which have so far received little attention elsewhere. Because the applications are so diverse the theory has been kept in an abstract form, particularization being made more easily when the general theory is adequately set out. Of course, particular physical problems are often dealt with more quickly by *ad hoc* methods, but these tend to obscure general procedures. Also many results which are physically obvious often need heavy mathematical machinery to give them conclusive support from a theoretical point of view: this is the reason for the rather elaborate discussion of the magnetic little group (or group of **k**) in Secs. 3 and 4. We also give an outline of the physical problems for which the theory is useful; there is no pretence to completeness in this respect—the fact that several books[4,8,9] and long reviews[7,12] have been written along these lines speaks for itself. What we hope to do is to show how the mathematical tools are used, why they are appropriate, and to compare different methods when more than one method can be used.

In Sec. 2 we show first of all how to classify and to obtain magnetic groups, with particular reference to the magnetic point groups. Then we review the basic theory of corepresentations. The results were derived a long time ago by Wigner and have appeared in English translation[10]; our treatment follows much the same line of approach as that given by Wigner: so in this part we give detailed proofs of results only where we have made simplifications. It may be remembered that corepresentations are of three types; a criterion for determining which of the three types arises out of a given representation of the unitary subgroup is presented. This result is also given by Dimmock and Wheeler.[12] The physical significance of corepresentation theory in classifying energy spectra is given along with various examples. Also the different methods available for treating the symmetry properties of tensors in magnetic groups are outlined and a new application is made of the group theoretical approach to this problem.

There follows in the first part of Sec. 3 a short account of the theory of little groups as applied to crystallographic space groups. No proofs are given here, for such proofs appear either in the paper by Bradley[21] or in earlier works such as the review article by Koster.[22] This part serves to introduce notation and to give the reader an idea of the previous knowledge he requires for an understanding of the later theory in Sec. 3. It will be recalled that the irreducible representations of space groups are those induced out of the small representations of the various little groups (or groups of **k**). It is shown in the second part of Sec. 3 how to define magnetic little groups which have a similar fundamental property, namely that the irreducible corepresentations of magnetic space groups are those induced out of the small corepresentations of the various magnetic little groups. Many authors, including Dimmock and Wheeler,[12–14] give a geometrical definition of the magnetic little group which is perfectly correct. But, although the extension from a little group to a magnetic little group is trivial to effect, the proof that the magnetic little group so defined has all the required properties is far from trivial. We prefer to hold the following point of view: that a little group has significance and is therefore defined only if the fundamental property stated above is shown to be satisfied, and that only then is a meaningful geometrical interpretation to be given in terms of the vectors in **k** space. This point may not have deserved such emphasis if it had not been for a recent paper by Cracknell[23] who defines geometrically (but incorrectly) a magnetic little group; his group only has the required fundamental property

[12] J. O. Dimmock and R. G. Wheeler, *The Mathematics of Physics and Chemistry* (D. Van Nostrand Co. Inc., New York, 1964), Vol. 2, Chap. 12.

[13] J. O. Dimmock and R. G. Wheeler, J. Phys. Chem. Solids **23**, 729 (1962).

[14] J. O. Dimmock and R. G. Wheeler, Phys. Rev. **127**, 391 (1962).

[15] J. O. Dimmock, J. Math. Phys. **4**, 1307 (1963).

[16] G. F. Karavaev, N. V. Kudryavsteva, and V. A. Chaldyshev, Soviet Phys.—Solid State **4**, 2540 (1963).

[17] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Gostekhizdat, Moscow, 1951 and Pergamon Press Ltd., Oxford, England, 1958).

[18] G. Ya. Lyubarskii, *The Application of Group Theory in Physics* (Pergamon Press Ltd., Oxford, England, 1960).

[19] J. O. Dimmock, Phys. Rev. **130**, 1337 (1963).

[20] W. F. Brinkman and R. J. Elliott, J. Appl. Phys. **37**, 1457 (1966); and Proc. Roy. Soc. (London) **A294**, 343 (1966).

[21] C. J. Bradley, J. Math. Phys. **7**, 1145 (1966).

[22] G. F. Koster, Solid State Physics **5**, 173, (1957).

[23] A. P. Cracknell, Progr. Theoret. Phys. **33**, 812 (1965).

for vectors **k** which are equivalent to $-\mathbf{k}$; fortunately most of the vectors he treats satisfy this condition so that his work is only invalidated in part and it has now been corrected.[24] The presentation here of the magnetic little group theorem fills a lacuna in the literature. Most treatments of corepresentation theory apart from that in the monumental series of papers by Kudryavsteva and Chaldyshev[11] (which is untranslated) omit a rigorous proof and it therefore seemed sensible to fill the gap, although we are conscious of the fact that by taking the problem in rather an abstract setting (one appropriate to any magnetic group with a unitary invariant Abelian subgroup) we might be thought over-elaborate. Actually the results here are more general than those obtained before and may well be of use in further developments of group theory to Physics, for example, in the development of the spin-space groups of Brinkman and Elliott.[20]

The work on magnetic space groups is continued in Sec. 4. The description and general form of the magnetic space groups and Bravais lattices is outlined and interpretation is made of some of the theory in Sec. 3. Certain further applications to physical problems are noted, in particular the spin classification problem and the effect of time-reversal on energy bands.

Section 5 is devoted to the theory involved in the reduction of inner Kronecker products of irreducible corepresentations of magnetic groups. It is shown that this problem is easily solved by formulae relevant to the unitary subgroup of the magnetic group. An example is given using a magnetic point group. Using the theorems of Bradley[21] this is also a useful method for magnetic space groups. In this connection see also the treatment given by Karavaev.[25] Finally the problems of second-order phase transitions and of the development of crystal field theory to situations involving a magnetic environment are mentioned as examples which require results of the analysis of these inner Kronecker products for their solution.

2. COREPRESENTATIONS OF MAGNETIC GROUPS

2.1. The Structure of Magnetic Groups

A finite magnetic group **M** is a finite group of operators half of which are unitary and half antiunitary. They occur in physics because the operator Θ of time reversal in quantum mechanics is antiunitary: we refer to the work of Wigner[10] and Bargmann[26] for proof of this fact. That exactly half the elements of **M** are unitary follows from the fact that the unitary elements form a subgroup **G**, which, since the product of two antiunitary operators is unitary, is an invariant subgroup of **M** of index 2.

We can therefore express **M** in terms of left cosets with respect to **G**:

$$\mathbf{M}=\mathbf{G}+A\mathbf{G}, \tag{2.1}$$

where all the elements of the coset $A\mathbf{G}$ are antiunitary. A can of course be any of the antiunitary elements but once chosen it remains fixed. (We prove later that the results themselves are independent, in a sense to be defined, of the particular choice made—it is simply for convenience of proof that one fixes on a particular coset representative.) Equation (2.1) can also be taken to characterize an infinite magnetic group in the case in which **G** is infinite, but we are dealing almost entirely with the case in which **G** is finite. (The theory we develop can be taken over immediately if **G** is a compact topological group—as, for example, when **G** is the rotation group.) As pointed out by Indenbom,[27] Eq. (2.1) gives immediately a method for determining all magnetic groups. There are, in effect, just two types of magnetic groups which contain antiunitary operators. Those in which Θ occurs in the coset $A\mathbf{G}$, and then it is convenient to choose $A=\Theta$. In this way we see that for every unitary group **G** there is just one corresponding magnetic group **M** of this type and we can write

$$\mathbf{M}=\mathbf{G}+\Theta\mathbf{G}. \tag{2.2}$$

And secondly there are those in which Θ does not appear in the coset $A\mathbf{G}$. To obtain magnetic groups of this second type it is sufficient to note that $A=\Theta R$, where R is some unitary operator and hence (since Θ commutes with all spatial unitary operators) that

$$\mathbf{M}'=\mathbf{G}+R\mathbf{G} \tag{2.3}$$

is a unitary group isomorphic with **M** and that **G** is a subgroup of **M** of index 2. Reversing the argument, for each unitary group of operators $\mathbf{M}'$ which has a subgroup **G** of index 2, and hence a decomposition of the form (2.3), there can be constructed a magnetic group **M**. Indenbom's contribution to the argument was to note that given a group $\mathbf{M}'$ of unitary operators then its subgroups of index 2 are in 1–1 correspondence with the kernels of those one dimensional representations of **M** which consist *entirely* of the numbers $+1$ and -1 (occurring of course in equal quantities). Hence to obtain all magnetic groups of this type all one needs to do is to search systematically through the character tables of the unitary groups picking out the appropriate one-dimensional representations, as described above. To each such representation there exists a magnetic group (not all of which may be distinguishable crystallographically).

Consider for example the crystallographic point group $\mathbf{C}_{4v}$ ($4mm$). Its character table is given in Table I.

[24] C. J. Bradley and A. P. Cracknell, Progr. Theoret. Phys. **36**, 648 (1966).
[25] G. F. Karavaev, Soviet Phys.—Solid State **6**, 2943 (1965).
[26] V. Bargmann, J. Math. Phys. **5**, 862 (1964).
[27] V. L. Indenbom, Soviet Phys.—Cryst. **4**, 578 (1959).

TABLE I. The character table of C_{4v} (4 *mm*). (*Note*: The notation used for the operators in Tables I, II, and III is the same as in Altmann and Cracknell, Ref. 31. As in that paper the active convention whereby the operators move the points of space and leave the axes fixed is also used here.

C_{4v}	E	C_{2z}	$C_{4z}^{\pm}$	σ_x, σ_y	σ_{da}, σ_{db}
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
B_1	1	1	−1	1	−1
B_2	1	1	−1	−1	1
E	2	−2	0	0	0

It has three representations of the appropriate type, namely, A_2, B_1, and B_2. The kernels corresponding to these representations, that is, the invariant subgroups of index 2, are the point groups $C_4(4)$, C_{2v} (2*mm*), and C_{2v}(2*mm*), respectively (the two C_{2v} groups having a different setting with respect to a set of fixed axes, but being crystallographically indistinguishable). There are therefore two distinguishable magnetic point groups **M** to be constructed by choosing $\mathbf{M}'=C_{4v}$ (4*mm*). These are named appropriately $C_{4v}(C_4)$ and $C_{4v}(C_{2v})$ using Schönflies notation, or $4\underline{mm}$ and $\underline{4}m\underline{m}$ using the International notation.

By letting $\mathbf{M}'$ run through the 32 crystallographic point groups one obtains altogether 58 distinguishable magnetic groups **M** of this second type. Taken together with the 32 of the previous type and the 32 point groups themselves this accounts for the 122 magnetic crystallographic point groups of Tavger and Zaitzev.[5] For a complete classification of these groups see, for example, Table 12–1 of Dimmock and Wheeler[12] or the book by Hammermesh[28] (in which the Schönflies and International notations are explained).

2.2. Corepresentations

We denote elements of **G** by R, S, T, etc., and elements of $A\mathbf{G}$ by A, B, C, etc. We often use the fact that products such as A^2 and AB belong to **G**. We suppose further that Δ is a unitary irreducible representation of **G** of dimension d, with basis

$$\langle\psi_1, \psi_2, \cdots, \psi_d| \equiv \langle\psi|,$$

so that, for all $R\in\mathbf{G}$,

$$R\psi_i=\sum_{j=1}^{d}\psi_j\Delta(R)_{ji}. \tag{2.4}$$

We write equations such as this in a shorthand form in which, for example, Eq. (2.4) reads as follows:

$$R\langle\psi| = \langle\psi|\Delta(R). \tag{2.5}$$

We now introduce the d functions ϕ_i ($i=1$ to d) which are produced by operating on ψ_i with A: that is

$$A\langle\psi| = \langle\phi|. \tag{2.6}$$

[28] M. Hammermesh, *Group Theory* (Addison-Wesley Publ. Co., Inc., Reading, Mass., 1962), pp. 63-67.

As well as acting on functions, A also acts on complex numbers and being antilinear it has the characteristic property of transforming them into their conjugates. Define

$$\langle\gamma| = \langle\psi, \phi| = \langle\psi_1, \psi_2, \cdots, \psi_d, \phi_1, \phi_2, \cdots \phi_d|. \tag{2.7}$$

Then, from Eq. (2.5),

$$\begin{aligned} R\langle\phi| &= RA\langle\psi| \\ &= A(A^{-1}RA)\langle\psi| \\ &= A\langle\psi|\Delta(A^{-1}RA) \qquad (2.8)\\ &= \langle\phi|\Delta^*(A^{-1}RA) \qquad (2.9)\end{aligned}$$

in which Eq. (2.8) holds because $A^{-1}RA\in\mathbf{G}$, and where in Eq. (2.9) the complex conjugate (denoted by an asterisk) appears because A is antilinear. It follows that for all $R\in G$

$$R\langle\gamma| = \langle\gamma|D(R), \tag{2.10}$$

where

$$D(R)=\begin{pmatrix}\Delta(R) & 0\\ 0 & \Delta^*(A^{-1}RA)\end{pmatrix}. \tag{2.11}$$

We often write $\Delta^*(A^{-1}RA)=\bar{\Delta}(R)$. The reason for this is that $\bar{\Delta}(R)$ is also a representation of **G**.

Similarly, for all $B\in A\mathbf{G}$,

$$B\langle\gamma| = \langle\gamma|D(B), \tag{2.12}$$

where

$$D(B)=\begin{pmatrix}0 & \Delta(BA)\\ \Delta^*(A^{-1}B) & 0\end{pmatrix}. \tag{2.13}$$

The set of unitary matrices D defined by Eqs. (2.11) and (2.13) forms what is called the corepresentation of **M** derived from Δ. From what has been said so far its properties may depend on the choice of A. Using multiplication and the fact that Δ is a representation of **G** it follows that

$$D(R)D(S)=D(RS), \tag{2.14a}$$

$$D(R)D(B)=D(RB), \tag{2.14b}$$

$$D(B)D^*(R)=D(BR), \tag{2.14c}$$

$$D(B)D^*(C)=\mathrm{D}(BC). \tag{2.14d}$$

The complex conjugates that appear in Eqs. (2.14c) and (2.14d) in general prevent D from being a homomorphism of **M**.

Also, looking at the matter the other way round, any set of unitary matrices D defined for all elements of **M** and which satisfy equations of the form (2.14) is called a corepresentation of **M**.

Let us now perform a unitary transformation U on the basis $\langle\gamma|$ such that $\langle\gamma'| = \langle\gamma|U$ and let the corepresentation of **M** that follows from using $\langle\gamma'|$ as basis be denoted by D'; then it soon follows that

$$D'(R)=U^{-1}D(R)U \tag{2.15}$$

and

$$D'(B) = U^{-1}D(B)U^*. \tag{2.16}$$

This enables us to define two corepresentations D' and D of $\mathbf{M}$ to be unitarily equivalent if there exists a unitary matrix U such that Eqs. (2.15) and (2.16) hold for all $R \in \mathbf{G}$ and all $B \in A\mathbf{G}$.

In particular, if we had chosen another antiunitary operator $A' = TA$, where $T \in \mathbf{G}$, instead of A as coset representative the resulting corepresentation D' would have had as basis $\langle \gamma' | = \langle \psi', \phi' |$, where $\langle \psi' | = \langle \psi |$, and

$$\langle \phi' | = A' \langle \psi | = TA \langle \psi | = T \langle \phi | = \langle \phi | \Delta^*(A^{-1}TA). \tag{2.17}$$

So, with the following choice for U:

$$U = \begin{pmatrix} 1 & 0 \\ 0 & \Delta^*(A^{-1}TA) \end{pmatrix} \tag{2.18}$$

we see that U is unitary, that $\langle \gamma' | = \langle \gamma | U$, and hence that D' would be unitarily equivalent to D. It is in this sense that the choice of A in defining the corepresentation of $\mathbf{M}$ derived from Δ is immaterial.

2.3. Reducibility of Corepresentations

Once the concept of equivalence is defined it is possible to define reducibility and irreducibility of corepresentations. This is done exactly as for ordinary representations. If the basis of a corepresentation D can be transformed by a unitary transformation so that the space it spans devolves into the direct sum of two spaces both invariant under $\mathbf{M}$ then D is said to be *reducible*; if not, then D is said to be *irreducible*. As in ordinary representation theory reducibility implies a transformation to matrices all of which are in the same block diagonal form. Theorems on complete reducibility hold exactly as in the ordinary representation theory of finite groups. We now discuss whether or not the corepresentation D defined by Eqs. (2.11) and (2.13) is reducible or not. The answer depends on the relationship between the two representations $\Delta(R)$ and $\bar{\Delta}(R) = \Delta^*(A^{-1}RA)$ of the subgroup $\mathbf{G}$.

First note that $\bar{\bar{\Delta}}(R) = \bar{\Delta}^*(A^{-1}RA) = \Delta(A^{-2}RA^2) = \Delta^{-1}(A^2)\Delta(R)\Delta(A^2)$ and so $\bar{\bar{\Delta}}(R)$ is equivalent to $\Delta(R)$. From this it follows easily that the corepresentation of $\mathbf{M}$ derived from $\bar{\Delta}(R)$ is equivalent to that derived from $\Delta(R)$. This means that when we consider the collection of all irreducible representations of $\mathbf{G}$ some of them fall into pairs $\Delta(R)$ and $\bar{\Delta}(R)$ which are mutually inequivalent and which come together to form a single corepresentation of $\mathbf{M}$ (which from what we have proved so far may be reducible, though we shall in fact prove shortly that such corepresentations are irreducible); and the remainder are such that $\Delta(R)$ and $\bar{\Delta}(R)$ are equivalent and then the corepresentation D contains Δ twice. (We prove shortly that such corepresentations may or may not be reducible according to a criterion that we establish.)

Take first the case in which $\Delta(R)$ and $\bar{\Delta}(R)$ are mutually inequivalent. Suppose there exists a unitary matrix U which reduces D. Since $D(R)$, $R \in \mathbf{G}$, is the direct sum of irreducibles $\Delta(R)$ and $\bar{\Delta}(R)$ the only reduced form of $D(R)$ is

$$\begin{pmatrix} X(R) & 0 \\ 0 & Y(R) \end{pmatrix},$$

where $X(R)$ is equivalent, say, to $\Delta(R)$ and $Y(R)$ to $\bar{\Delta}(R)$. Then if

$$U = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

Eq. (2.15) implies amongst other things that

$$\bar{\Delta}(R)c = cX(R). \tag{2.19}$$

But $\bar{\Delta}(R)$ and $X(R)$ are inequivalent, so by Schur's lemma $c=0$. Similarly $b=0$, and hence U is of the form

$$\begin{pmatrix} a & 0 \\ 0 & d \end{pmatrix}.$$

But no such diagonal block matrix is capable of reducing matrices $D(B)$ of the form given by Eq. (2.13), because $D'(B) = U^{-1}D(B)U^*$ will still be in off-diagonal block form. The conclusion is that when $\Delta(R)$ and $\bar{\Delta}(R)$ are inequivalent the corepresentation of $\mathbf{M}$ derived from Δ is irreducible.

Suppose next that $\Delta(R)$ and $\bar{\Delta}(R)$ are equivalent. Then there exists a unitary matrix P such that

$$\Delta(R) = P\Delta^*(A^{-1}RA)P^{-1}, \qquad \text{for all } R \in \mathbf{G} \tag{2.20}$$

so that, in particular

$$\Delta(A^2) = P\Delta^*(A^2)P^{-1}. \tag{2.21}$$

From Eqs. (2.20) and (2.21) it follows, after some manipulation, that $PP^*\Delta^{-1}(A^2)$ commutes with $\Delta(R)$ for all $R \in \mathbf{G}$. Hence, by Schur's lemma,

$$PP^* = \lambda\Delta(A^2), \tag{2.22}$$

where λ is a scalar. Substituting for $\Delta(A^2)$ and $\Delta^*(A^2)$ in Eq. (2.21) we obtain $\lambda = \lambda^* = \pm 1$, so that only two possibilities exist:

$$PP^* = \pm\Delta(A^2). \tag{2.23}$$

We now prove that the sign which holds in Eq. (2.23) governs whether or not D is irreducible.

Now $D(R)$, $R \in \mathbf{G}$, is already in reduced form but first it is convenient to apply the unitary transformation

$$U = \begin{pmatrix} 1 & 0 \\ 0 & P^{-1} \end{pmatrix}$$

so that, using Eqs. (2.15) and (2.16), D is transformed into the equivalent form

$$D'(R)=\begin{pmatrix}\Delta(R) & 0\\ 0 & \Delta(R)\end{pmatrix}, \quad (2.24)$$

and

$$D'(B)=\begin{pmatrix}0 & \Delta(BA)P^{*-1}\\ P\Delta^*(A^{-1}B) & 0\end{pmatrix}. \quad (2.25)$$

Suppose next that we try to find a unitary matrix V which will reduce $D'(B)$ to block diagonal form and, of course, leave $D'(R)$ unaltered. Since V must commute with $D'(R)$ it follows, using Schur's lemma, that

$$V=\begin{pmatrix}\lambda 1 & \mu 1\\ \nu 1 & \rho 1\end{pmatrix}, \quad (2.26)$$

where 1 is the unit matrix and where λ, μ, ν, ρ are scalars, which since V is unitary must satisfy

$$\lambda\lambda^*+\mu\mu^*=1,$$
$$\lambda\nu^*+\mu\rho^*=0,$$
$$\nu\nu^*+\rho\rho^*=1. \quad (2.27)$$

If we now demand that $D''(B)=VD'(B)V^{*-1}$ should be in block diagonal form we find the requirement to be

$$\rho\lambda P\Delta^*(A^{-1}B)+\mu\nu\Delta(BA)P^{*-1}=0$$
$$\mu\nu P\Delta^*(A^{-1}B)+\rho\lambda\Delta(BA)P^{*-1}=0. \quad (2.28)$$

Writing $B=AR$ in Eq. (2.28) and using Eq. (2.20) it follows after some algebra that

$$\mu\nu PP^*=-\rho\lambda\Delta(A^2). \quad (2.29)$$

Equations (2.29) and (2.23) impose the requirement $\mu\nu=\pm\rho\lambda$. Now if $PP^*=-\Delta(A^2)$ the requirement is $\mu\nu=\rho\lambda$ and this cannot be satisfied because it would imply that V was singular; so that in this case we cannot obtain a reduction. However if $\mu\nu=-\rho\lambda$ no such restriction holds; so that if $PP^*=\Delta(A^2)$ reduction is possible. We can then choose $\lambda=\mu=\rho=1/\sqrt{2}$ and $\nu=-1/\sqrt{2}$ and after some manipulation we find eventually that

$$D''(B)=\begin{pmatrix}\Delta(BA^{-1})P & 0\\ 0 & -\Delta(BA^{-1})P\end{pmatrix}. \quad (2.30)$$

In the other case when $PP^*=-\Delta(A^2)$ we have

$$\Delta(BA)P^{*-1}=\Delta(BA^{-1})\Delta(A^2)P^{*-1}=-\Delta(BA^{-1})P, \quad (2.31)$$

and, from Eq. (2.20), that

$$P\Delta^*(A^{-1}B)=\Delta(BA^{-1})P, \quad (2.32)$$

so that Eq. (2.25) becomes

$$D'(B)=\begin{pmatrix}0 & -\Delta(BA^{-1})P\\ \Delta(BA^{-1})P & 0\end{pmatrix}. \quad (2.33)$$

2.4. The Three Types of Irreducible Corepresentation

We can now summarize the three cases:

Case (a)

$$\Delta(R)=P\Delta^*(A^{-1}RA)P^{-1},$$
$$PP^*=\Delta(A^2),$$
$$D''(R)=\Delta(R),$$

and

$$D''(B)=\pm\Delta(BA^{-1})P. \quad (2.34)$$

Note: The corepresentation with the plus sign is equivalent to the corepresentation with the minus sign.

Case (b)

$$\Delta(R)=P\Delta^*(A^{-1}RA)P^{-1},$$
$$PP^*=-\Delta(A^2),$$
$$D'(R)=\begin{pmatrix}\Delta(R) & 0\\ 0 & \Delta(R)\end{pmatrix},$$

and

$$D'(B)=\begin{pmatrix}0 & -\Delta(BA^{-1})P\\ \Delta(BA^{-1})P & 0\end{pmatrix}. \quad (2.35)$$

Case (c)

$\Delta(R)$ not equivalent to $\bar{\Delta}(R)=\Delta^*(A^{-1}RA)$.

$$D(R)=\begin{pmatrix}\Delta(R) & 0\\ 0 & \bar{\Delta}(R)\end{pmatrix}$$

and

$$D(B)=\begin{pmatrix}0 & \Delta(BA)\\ \bar{\Delta}(BA^{-1}) & 0\end{pmatrix}. \quad (2.36)$$

Wigner[10] has shown that all unitary irreducible corepresentations of **M** are equivalent to one or other of these three types, where Δ is some unitary irreducible representation of **G**.

The important thing from our point of view is to know which of the three cases is appropriate for a given irreducible representation Δ of **G**. For this Dimmock and Wheeler[12] give a very simple test using the characters of Δ. We remember that if Δ^i and Δ^j are two unitary irreducible representations of **G** then

$$\sum_{R\in G}\Delta^i(R)_{rl}\Delta^{j*}(R)_{sm}=(|\,\mathbf{G}\,|/d_i)\delta_{ij}\delta_{rs}\delta_{lm}, \quad (2.37)$$

where $|\,\mathbf{G}\,|$ is the order of **G** and d_i the dimension of Δ^i.

Now, if $B\in A\mathbf{G}$, we have

$$\sum_{B\epsilon A\mathbf{G}} \Delta(B^2)_{rr} = \sum_{R\epsilon\mathbf{G}} \Delta(ARAR)_{rr}$$
$$= \sum_{R\epsilon\mathbf{G}} \Delta(A^2)_{rs}\Delta(A^{-1}RA)_{st}\Delta(R)_{tr}.$$

In cases (a) and (b) the sum is

$$\Delta(A^2)_{rs}\sum_{R\epsilon\mathbf{G}} P_{sp}{}^{*-1}\Delta^*(R)_{pq}P_{qt}{}^*\Delta(R)_{tr}$$
$$=\Delta(A^2)_{rs}P_{sp}{}^{*-1}P_{qt}{}^*(|\mathbf{G}|/d)\delta_{pt}\delta_{qr},$$
$$=(|\mathbf{G}|/d)\Delta(A^2)_{rs}P_{rt}{}^*P_{ts},$$
$$=\pm(|\mathbf{G}|/d)\Delta(A^2)_{rs}\Delta^*(A^2)_{rs},$$
$$=\pm(|\mathbf{G}|/d)\Delta(E)_{rr},$$
$$=\pm|\mathbf{G}|. \tag{2.38}$$

In the simplification we have used the fact that Δ and P are unitary and that since Δ is of dimension d the character of the identity E is d and we have also used Eqs. (2.20), (2.23), and (2.37). In case (c) the sum is

$$\Delta(A^2)_{rs}\sum_{R\epsilon\mathbf{G}} \bar{\Delta}^*(R)_{st}\Delta(R)_{tr}=0. \tag{2.39}$$

This follows from Eq. (2.37), Δ and $\bar{\Delta}$ being inequivalent. Collecting these results and writing χ for the character of Δ we have

$$\sum_{B\epsilon A\mathbf{G}} \chi(B^2) = |\mathbf{G}| \quad \text{in case (a)}$$
$$= -|\mathbf{G}| \quad \text{in case (b)}$$
$$= 0 \quad \text{in case (c)}. \tag{2.40}$$

When the group $\mathbf{M}$ contains the time reversal operator Θ itself we can choose $A=\Theta$, and Eq. (2.40) reduces to

$$\sum_{R\epsilon\mathbf{G}} \chi(R^2) = \omega|\mathbf{G}| \quad \text{in case (a)}$$
$$= -\omega|\mathbf{G}| \quad \text{in case (b)}$$
$$= 0 \quad \text{in case (c)}, \tag{2.41}$$

where, as Wigner[10] has shown,

$$\Theta^2=\omega=1 \quad \text{for an even number of fermions or when spin is not being taken into account,}$$
$$=-1 \quad \text{for an odd number of fermions.} \tag{2.42}$$

2.5. Examples

The physical significance of corepresentation theory is exactly the same for the classification of the energy spectra of systems whose Schrödinger group is a magnetic group as ordinary representation theory is for this classification when the Schrödinger group is a unitary group. That is to say, the labeling and the degeneracy of each level of a spectrum corresponds to the labeling and the dimension of one or other of the corepresentations of the magnetic group involved.

Because of the strong relationship that exists between the corepresentations of a magnetic group $\mathbf{M}$ and the representations of its unitary subgroup $\mathbf{G}$ of index 2 it follows that there is a neat relationship between the spectra of systems whose Schrödinger groups are, respectively, $\mathbf{M}$ and $\mathbf{G}$. Indeed the physical importance of the classification in Sec. 2.4 can now been seen. In cases (b) and (c) the existence of antiunitary operators in the Schrödinger group $\mathbf{M}$ implies a doubling of the degeneracy that would be expected from merely considering the operators of $\mathbf{G}$ alone. But in case (a) there is no doubling of the degeneracy. Conversely, the classification in Sec. 2.4 determines whether or not an energy level splits under a small perturbation which reduces the symmetry of the system from $\mathbf{M}$ to $\mathbf{G}$. In case (a) there is no splitting. In cases (b) and (c) splitting of the levels will occur and furthermore one will know which levels to expect close together, the ones that derive from a single level or corepresentation of $\mathbf{M}$.

As a first example consider the case of a quantum mechanical system with an odd number of electrons in which the Hamiltonian has no symmetry except that of time-reversal. $\mathbf{G}$ has no nontrivial elements and is therefore the double group of $\mathbf{C}_1$, consisting of the identity E and $\bar{E}$. The only representation of physical significance is one-dimensional and has $\Delta(E)=1$ and $\Delta(\bar{E})=-1$. Clearly $\chi(E^2)+\chi(\bar{E}^2)=2\chi(E)=2$. Also $\omega=-1$. From Eq. (2.41) we see that we are in case (b). Each level of the system, barring additional (accidental) degeneracy, is therefore doubly degenerate. This degeneracy, due entirely to time-reversal symmetry, is called Kramers'[29] degeneracy and has been known for nearly forty years.

As a second example consider the case in which $\mathbf{G}$ is the 3-dimensional rotation group $\mathbf{O}_3$. Let Δ^j be the irreducible representation of dimension $d_j=(2j+1)$ $(j=0, \frac{1}{2}, 1, \frac{3}{2}, \cdots)$. The character in Δ^j of an element R whose angle of rotation is θ is given by

$$\chi^j(R) = \sin(j+\tfrac{1}{2})\theta/\sin\tfrac{1}{2}\theta. \tag{2.43}$$

Now we have to replace the summation over group elements appropriate to finite groups by an integration over the group parameters and with a kernel appropriate to the double group of $\mathbf{O}_3$. For functions f depending only on the angle of rotation θ this means (see, for example, Lomont[30]) replacing

$$|\mathbf{G}|^{-1}\sum_R f(R) \quad \text{by} \quad (2\pi)^{-1}\int_0^{4\pi} f(\theta)\sin^2\tfrac{1}{2}\theta\, d\theta.$$

We are interested here in the case $f(R)=\chi^j(R^2)$ and

[29] H. Kramers, Koninkl. Ned. Akad. Wetenschap. Proc. **33**, 959 (1930).

[30] J. S. Lomont, *Applications of Finite Groups* (Academic Press Inc., New York, 1959), p. 149.

TABLE II. The character table of $\mathbf{C}_{2v}$ $(2m)$.

$\mathbf{C}_{2v}$	E	C_{2z}	σ_x	σ_y
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

since R^2 corresponds to an angle of rotation 2θ the integral for evaluation is

$$(2\pi)^{-1}\int_0^{4\pi}\frac{\sin(2j+1)\theta}{\sin\theta}\sin^2\tfrac{1}{2}\theta\, d\theta.$$

For j an integer the value of this integral is $+1$ and for j half an odd integer its value is -1. When j is an integer (single-valued representations) there are an even number of fermions and $\omega=+1$; when j is half an odd integer (double-valued representations) there are an odd number of fermions and $\omega=-1$. Hence for every representation Δ^j we are in case (a). Thus when the Hamiltonian has the full symmetry of the rotation group the addition of time-reversal symmetry causes no further degeneracy.

As a third example we take one for which the time-reversal operator Θ is not itself a member of the magnetic group. It is an example already introduced as an illustration in Sec. 2.1, namely the magnetic group $\mathbf{C}_{4v}(\mathbf{C}_{2v})$. We study the relationship between its irreducible corepresentations and the irreducible representations of the unitary subgroup $\mathbf{C}_{2v}$. We only consider the single-valued representations of these groups. In order to prevent us having to introduce definitions of the operators we use for them exactly the same notation as Altmann and Cracknell.[31] Thus the 8 operations of $\mathbf{M}$ are E, C_{2z}, σ_x, σ_y, ΘC_{4z}^+, ΘC_{4z}^-, $\Theta\sigma_{da}$, $\Theta\sigma_{db}$, the first four of these forming the unitary subgroup $\mathbf{G}$. In Table II we list the characters of $\mathbf{G}(\mathbf{C}_{2v})$. In accordance with Eq. (2.1) we fix $A=\Theta C_{4z}^+$. Since $(\Theta C_{4z}^{\pm})^2=C_{2z}$ and $(\Theta\sigma_{da})^2=(\Theta\sigma_{db})^2=E$ the sum involved in Eq. (2.40) is equal to 4 for A_1 and A_2 and is equal to 0 for B_1 and B_2. Thus the corepresentations $D(A_1)$ and $D(A_2)$ belong to case (a) and since in these cases $\bar{\Delta}(R)=\Delta(R)$ we can choose $P=1$. The actual forms of $D(A_1)$ and $D(A_2)$ then follow from Eq. (2.34) and are given in Table III (in which the plus sign is chosen for the representative of ΘC_{4z}^+). For $D(B)$ we choose $\Delta=B_1$ and then, since $A^{-1}EA=E$, $A^{-1}C_{2z}A=C_{2z}$, $A^{-1}\sigma_yA=\sigma_x$, and $A^{-1}\sigma_xA=\sigma_y$, it follows that $\bar{\Delta}=B_2$. We are in case (c), the irreducible corepresentation $D(B)$ is of dimension 2 and contains both B_1 and B_2. Its actual form follows at once from Eq. (2.36) and is also given in Table III.

A compatibility table between the representations and corepresentations of the groups $(\mathbf{C}_{4v}+\Theta\mathbf{C}_{4v})$, $\mathbf{C}_{4v}$, $\mathbf{C}_{2v}$, and $\mathbf{C}_{4v}(\mathbf{C}_{2v})$ is given in Table IV. From the first and fourth lines of this table we can see that if there was a direct transition from a system with symmetry group $(\mathbf{C}_{4v}+\Theta\mathbf{C}_{4v})$ to one with a magnetic sublattice involving the symmetry group $\mathbf{C}_{4v}(\mathbf{C}_{2v})$ there would be no alteration in the degeneracies of the energy levels of the systems. Such a transition might occur at the Néel point of an antiferromagnetic crystal. However if in either case the symmetry was reduced to that of the group $\mathbf{C}_{2v}$ the degenerate levels E or $D(B)$ would split into the two non-degenerate levels B_1 and B_2.

A compatibility analysis similar to the above has been carried out for all the magnetic point groups by Dimmock and Wheeler[12] and their corepresentations are given in full by Cracknell.[32]

2.6. The Symmetry of Tensors in Magnetic Crystals

Not all the physical problems connected with magnetic crystals that can be simplified or solved by group theory depend on corepresentation theory. This is because corepresentation theory arises out of the antiunitary nature of time reversal in quantum mechanics. In problems of classical physics associated with macroscopic bodies time reversal is to be regarded simply as the operator which transforms t into $-t$ and has the property therefore of changing the sign of certain physical quantities which depend on the time, simple examples being velocity, current density, and magnetic field. For problems such as these it is often appropriate to use the representations of the unitary group $\mathbf{M}'$ isomorphic with $\mathbf{M}$. To illustrate this we consider the problem of determining the simplest possible form of tensors describing static properties of magnetic crystals. Piezomagnetism, pyromagnetism, and magnetoelectricity are a few examples of static phenomena of crystals that can be described by means of tensors. The problem has been solved, the most comprehensive accounts being given by Birss[8] and Bhagavantam.[9] The first of these authors gives in his book a good bibliography complete up to 1964. Work since then, for example by Kleiner,[33] has been devoted to tensors describing transport phenomena. We would emphasize that we deal here only with those cases which are described by tensors invariant under the magnetic point groups such as the static phenomena mentioned above.

It is worthwhile summarizing the methods used by previous authors for solving this problem. Birss[8] demonstrates how to simplify a given tensor in a magnetic point group, by showing that its form is the same as that of some other tensor of the same rank in one of the classical point groups. For tensors of both even and odd rank for all magnetic groups a prescription is given for identifying requisite tensors and the corre-

[31] S. L. Altmann and A. P. Cracknell, Rev. Mod. Phys. **37**, 19 (1965).

[32] A. P. Cracknell, Progr. Theoret. Phys. **35**, 196 (1966).
[33] W. H. Kleiner, Phys. Rev. **142**, 318 (1966).

TABLE III. The corepresentations of $C_{4v}(C_{2v})-4\underline{mm}$.

$C_{4v}(C_{2v})$	E	C_{2z}	σ_x	σ_y	ΘC_{4z}^+	ΘC_{4z}^-	$\Theta\sigma_{da}$	$\Theta\sigma_{db}$
$D(A_1)$	1	1	1	1	1	1	1	1
$D(A_2)$	1	1	-1	-1	1	1	-1	-1
$D(B)$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&1\\-1&0\end{pmatrix}$	$\begin{pmatrix}0&1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\-1&0\end{pmatrix}$

sponding classical groups. The problem then devolves on to the same problem for the classical point groups, and, for this, one is able to invoke the magnificent sets of tables of Fumi,[34] Fieschi and Fumi,[35] and Fieschi,[36] which are complete for all tensors up to and including rank 6. Bhagavantam[9] shows how to use group theory to calculate the number of independent components that tensors can display in a magnetic environment but he uses a descriptive and rather lengthy *ad hoc* analysis to obtain their precise form. Many authors have investigated particular cases. One who has influenced our approach is Indenbom,[37] who examined the magnetoelectric case and showed how to obtain the form of the corresponding tensor in any magnetic point group by finding invariants of $\mathbf{E}\cdot\mathbf{H}$, where $\mathbf{E}$ and $\mathbf{H}$ are respectively the electric and magnetic field vectors. However he also used a method of inspection, when a group theoretical method would have been more powerful. We have made a slight generalization of the work of Indenbom[37] and Bhagavantam[9] using the full power of group theory. The method may be used for any tensor in any magnetic point group; it is simple to use even for tensors of high rank.

For magnetic point groups which are a direct product of a classical point group and time-reversal there is no problem at all, the results for i tensors are the same as for such tensors in the classical point groups and clearly all c tensors invariant under such groups vanish

TABLE IV. Compatibility between the groups $(C_{4v}+\Theta C_{4v})$, C_{4v}, C_{2v}, and $C_{4v}(C_{2v})$. [*Notes*: (i) The notation in the last three rows of the table corresponds to that used in Tables I, II, and III. (ii) The first row of the table lists the corepresentations of the magnetic group $(C_{4v}+\Theta C_{4v})$. Since the representations of C_{4v} are of type (a) with respect to this magnetic group, the corepresentation $D(A_1)$ of $(C_{4v}+\Theta C_{4v})$ has the same dimension as the representation A_1 of C_{4v} and so on.]

$(C_{4v}+\Theta C_{4v})$	$D(A_1), D(B_1)$	$D(A_2), D(B_2)$	$D(E)$	$D(E)$
C_{4v}	A_1, B_1	A_2, B_2	E	E
C_{2v}	A_1	A_2	B_1	B_2
$C_{4v}(C_{2v})$	$D(A_1)$	$D(A_2)$	$D(B)$	$D(B)$

[34] F. G. Fumi, Phys. Rev. **83**, 1274 (1951); **86**, 561 (1952); Acta Cryst. **5**, 44 (1952); Nuovo Cimento **9**, 739 (1952).
[35] R. Fieschi and F. G. Fumi, Nuovo Cimento, **10**, 865 (1953).
[36] R. Fieschi, Physica **24**, 972 (1957).
[37] V. L. Indenbom, Soviet Phys.—Cryst. **5**, 493 (1960)..

identically. (We follow Birss[8] and call tensors which transform symmetrically and antisymmetrically under Θ i tensors and c tensors, respectively.) This leaves us to discuss the 58 magnetic groups $\mathbf{M}$ whose structures are of the second type, as introduced in Sec. 2.1. Using the same notation, let $\mathbf{M}'$ be the unitary group isomorphic with $\mathbf{M}$ and let $\mathbf{G}$ be the unitary subgroup of index 2 common to both $\mathbf{M}$ and $\mathbf{M}'$. When considering $\mathbf{M}$ we use the following labels for the representations of $\mathbf{M}'$: Γ_s, the totally symmetric representation; Γ_m, the representation that corresponds to $\mathbf{M}$—as explained in Sec. 2.1 this is the one-dimensional representation in which all elements of $\mathbf{G}$ are represented by $+1$; Γ_p, the pseudoscalar representation—it has all proper rotations represented by $+1$ and all improper rotations represented by -1. In certain cases Γ_p may coincide with Γ_m or Γ_s, but this does not matter. We shall write $\Gamma_{m\times p}$ for the direct product representation $\Gamma_m\otimes\Gamma_p$. For example, for the magnetic group $C_{4v}(C_{2v})$, we see from Tables I and II that the representations of C_{4v} given in Table I are to be relabelled for the present purpose $A_1=\Gamma_s$, $A_2=\Gamma_p$, $B_1=\Gamma_m$, and $B_2=\Gamma_{m\times p}$. The setting of the group C_{2v} with respect to fixed axes is critical. If the alternative setting of $C_{4v}(C_{2v})$ is used then the labels of B_1 and B_2 get reversed, and the detailed form of the results are changed. The form of the results often depends on the orientation of the axes chosen. We use the same right-handed orthogonal axes in our examples as Altmann and Cracknell.[31] Similarly for the magnetic group $C_{4v}(C_4)$ the labels of the representations of C_{4v} would be $A_1=\Gamma_s=\Gamma_{m\times p}$ and $A_2=\Gamma_m=\Gamma_p$.

Tensors of a given rank fall into four categories: (i) polar i tensors, (ii) polar c tensors, (iii) axial i tensors, and (iv) axial c tensors. These correspond in a simple way that we shall now describe to the four representations Γ_s, Γ_m, Γ_p, and $\Gamma_{m\times p}$, respectively.

Let $\mathcal{R}$ be an element of $\mathbf{M}$ and R the element in $\mathbf{M}'$ that corresponds to $\mathcal{R}$ in the isomorphism between $\mathbf{M}$ and $\mathbf{M}'$. The coordinates (x_1, x_2, x_3) of a point in the frame of the chosen right-handed orthogonal system will transform under R according to the vector representation V of $\mathbf{M}'$:

$$x_i'=\sum_{j=1}^{3} R_{ij}x_j, \tag{2.44}$$

where (R_{ij}) is the orthogonal matrix representing R

in V. Let $\chi_\alpha(R)$ be the character of R in the representation $\Gamma_\alpha[\alpha=s,\ m,\ p,$ or $(m\times p)]$. Then we define an α tensor of rank k in $\mathbf{M}$ to be one that transforms like the direct product V^k of k vector representations V multiplied by the phase factor χ_α; thus, d is an α tensor of rank k if it is transformed by $\mathfrak{R}$ into d' where

$$d_{ab\cdots k}'=\chi_\alpha(R)\sum_{pq\cdots z}R_{ap}R_{bq}\ldots R_{kz}d_{pq\cdots z}. \quad (2.45)$$

From definition and from Eq. (2.45) it is clear that an s tensor is a polar i tensor, an m tensor is a polar c tensor, a p tensor is an axial i tensor, and an $(m\times p)$-tensor is an axial c tensor. It is also clear from Eq. (2.45) that if there were not further restrictions on d its components would form a basis for the direct product representation $\Gamma_\alpha\otimes V^k$. However we also require the tensor to be invariant under all the operations of $\mathbf{M}$. This forces various relationships to hold between the components of the tensor. When these relations have been satisfied we have the tensor in its simplest form. If the relations cannot be satisfied nontrivially then the physical effect described by the tensor is forbidden in crystals invariant under the given magnetic group.

Standard group theoretical arguments provide us not only with the number of independent components of the tensor but also with its precise form. The number of independent components τ is equal to the dimension of the space spanned by components of d that are left invariant by all the operations of $\mathbf{M}$ and which therefore transform as basis functions for the representation Γ_s. This is equal to the number of times Γ_s appears in the reduction of $\Gamma_\alpha\otimes V^k$. Writing χ for the character of V and $|\mathbf{M}|$ for the order of $\mathbf{M}$ this means that

$$\tau=|\mathbf{M}|^{-1}\sum_{R\in\mathbf{M}'}\chi_\alpha(R)\{\chi(R)\}^k. \quad (2.46)$$

Since χ_α is real, this is also the number of times Γ_α appears in the reduction of V^k.

In order to find the precise form of an α tensor of rank k that is invariant under $\mathbf{M}$ we have to find functions from the space spanned by $\Gamma_\alpha\otimes V^k$ that transform as basis functions for the representation Γ_s. To do this we must use the projection operator

$$P_s=|\mathbf{M}|^{-1}\sum_{\mathfrak{R}\in\mathbf{M}}\chi_s(R)\mathfrak{R} \quad (2.47)$$

and apply it to functions $d_{ab\cdots k}$ that transform under $\mathfrak{R}$ as given by Eq. (2.45). From this equation we see that this imposes on the coefficients of $d_{ab\cdots k}$ exactly the same relationships as are imposed by applying the projection operator

$$P_\alpha=|\mathbf{M}|^{-1}\sum_{\mathfrak{R}\in\mathbf{M}}\chi_\alpha(R)\mathfrak{R} \quad (2.48)$$

on a polar i tensor of rank k. All that happens is that the factor $\chi_\alpha(R)$ gets transferred from Eq. (2.45) to Eq. (2.48). Hence an α tensor which is invariant under $\mathbf{M}$ suffers exactly the same restrictions and therefore has the same simple form as a polar i tensor which transforms not under Γ_s but under Γ_α. This is not surprising in view of the remark following Eq. (2.46). A typical polar i tensor of rank k is given by the direct product of k coordinates $x_ax_b\cdots x_k$, where with all such products the order of the factors must be preserved. If we apply P_α to such a product we obtain from Eqs. (2.44) and (2.48) the following α-scalars (α tensors of zero rank)

$$|\mathbf{M}|^{-1}\sum_R\chi_\alpha(R)R_{ap}R_{bq}\cdots R_{kz}x_px_q\cdots x_z. \quad (2.49)$$

By varying $a, b, \cdots, k$ we eventually obtain τ linearly independent α scalars of this form, say

$$\sum_{pq\cdots z}C_{pq\cdots z}{}^\sigma x_px_q\cdots x_z,\qquad \sigma=1,2,\cdots,\tau. \quad (2.50)$$

The most general α scalar that can be constructed is therefore

$$\sum_{\sigma=1}^{\tau}\lambda^\sigma c_{pq\cdots z}{}^\sigma x_px_q\cdots x_z, \quad (2.51)$$

in which the λ^σ are real arbitrary constants. But $x_px_q\cdots x_z$ is a typical polar i tensor of rank k and since we are dealing with Cartesian tensors it follows by the principle of contraction that the coefficients of $x_px_q\cdots x_z$ in the expression (2.51) form the most general α tensor of rank k that is invariant under $\mathbf{M}$.

Hence the components of $d_{ab\cdots k}$ are related by the 3^k equations

$$d_{ab\cdots k}=\sum_{\sigma=1}^{\tau}\lambda^\sigma c_{ab\cdots k}{}^\sigma, \quad (2.52)$$

where the coefficients $C_{ab\cdots k}{}^\sigma$ are to be obtained from Eq. (2.51) and the λ^σ are τ real arbitrary constants. The validity of this method of obtaining the form of the tensor required rests on the simple fact that if $d_{ab\cdots k}$ is the most general α tensor of rank k invariant under $\mathbf{M}$ then

$$\sum_{ab\cdots k}d_{ab\cdots k}x_ax_b\cdots x_k$$

is the most general α scalar which includes $x_ax_b\cdots x_k$.

We illustrate the theory with an example using once again the magnetic point group $\mathbf{C}_{4v}(\mathbf{C}_{2v})$ and we determine the form of the magnetoelectric tensor. Since $\mathbf{E}$ is a polar i tensor of rank 1 and $\mathbf{H}$ is an axial c tensor of rank 1 the magnetoelectric tensor is an axial c tensor of rank 2. The appropriate representation of $\mathbf{C}_{4v}$ is therefore $\Gamma_{m\times p}=B_2$ its characters being given in Table I. The projection operator corresponding to Eq. (2.48) is therefore

$$P_{m\times p}=\tfrac{1}{8}(E+C_{2z}-C_{4z}^+-C_{4z}^--\sigma_x-\sigma_y+\sigma_{da}+\sigma_{db}). \quad (2.53)$$

The vector representation V [the set of matrices R_{ij} appearing in Eq. (2.44)] is determined by the following set of equations

$$\begin{aligned}
E(x_1,x_2,x_3)&=(x_1,x_2,x_3),\\
C_{2z}(x_1,x_2,x_3)&=(-x_1,-x_2,x_3),\\
C_{4z}^{+}(x_1,x_2,x_3)&=(-x_2,x_1,x_3),\\
C_{4z}^{-}(x_1,x_2,x_3)&=(x_2,-x_1,x_3),\\
\sigma_x(x_1,x_2,x_3)&=(-x_1,x_2,x_3),\\
\sigma_y(x_1,x_2,x_3)&=(x_1,-x_2,x_3),\\
\sigma_{da}(x_1,x_2,x_3)&=(-x_2,-x_1,x_3),\\
\sigma_{db}(x_1,x_2,x_3)&=(x_2,x_1,x_3).
\end{aligned} \tag{2.54}$$

Using formula (2.46) and the characters as obtained from Table I and Eqs. (2.54) we find the number of independent components to be

$$\tau=\tfrac{1}{8}(3^2+1^2-1^2-1^2-1^2-1^2+1^2+1^2)=1. \tag{2.54}$$

And applying the operator (2.53) to products $x_ax_b(a, b=1, 2, 3)$ we find the only nonvanishing axial c scalar to be of the form $\frac{1}{2}(x_1x_2+x_2x_1)$. From Eq. (2.52) we deduce that all d_{ab} vanish except $d_{12}=d_{21}=\lambda$. The magnetoelectric tensor therefore has the form

$$\begin{pmatrix} 0 & \lambda & 0\\ \lambda & 0 & 0\\ 0 & 0 & 0\end{pmatrix}.$$

As an example the reader may like to check that for the alternative setting of the magnetic group $\mathbf{C}_{4v}(\mathbf{C}_{2v})$ the magnetoelectric tensor has the form

$$\begin{pmatrix} \mu & 0 & 0\\ 0 & -\mu & 0\\ 0 & 0 & 0\end{pmatrix}.$$

Certain property tensors in addition to their invariance under operations of the magnetic group $\mathbf{M}$ must be symmetric or antisymmetric (for physical reasons) under the interchange of pairs of indices. These extra conditions can be imposed *either* by operating with P_α only on products which already have the appropriate symmetry or antisymmetry taken into account *or* by imposing the appropriate conditions on the final form of the tensor. For example, if one is looking for an antisymmetric axial c tensor of rank 2 one is only allowed to operate on antisymmetric products of the form $(x_ax_b-x_bx_a)$. Alternatively one can note simply that all axial c tensors of rank 2 (see the form of the magneto electric tensor above) are necessarily symmetric. Either approach leads quickly to the conclusion that there is no nonnull antisymmetric axial c tensor of rank 2 invariant under this group.

3. MAGNETIC LITTLE GROUPS

3.1. Groups with an Invariant Abelian Subgroup

We return now to the development of corepresentation theory for the case when $\mathbf{G}$ has an invariant Abelian subgroup $\mathbf{T}$. For example, $\mathbf{G}$ might be a space group and $\mathbf{T}$ the subgroup of lattice translations: then $\mathbf{M}$ would be a magnetic space group. Indeed we shall apply the general theory of this section to the case of magnetic space groups in Sec. 4. However we keep the theory at present perfectly general so that it can be applied to a wider class of groups. The spin-space groups of Brinkman and Elliott[20] already provide such an example of magnetic groups of this category whose corepresentations are needed. Since the number of groups of interest in physics is for ever increasing it seems likely that there will be plenty of other examples. The motive behind the analysis of this section is to define what is meant by a magnetic little group and to describe its significance.

Given $\mathbf{G}$ and $\mathbf{T}$ (an invariant Abelian subgroup of $\mathbf{G}$) we may write

$$\mathbf{G}=\sum_\alpha r_\alpha\mathbf{T}, \tag{3.1}$$

where, as in all such decompositions, the coset representatives r_α, once chosen, remain fixed. The coset $r_\alpha\mathbf{T}$ in the quotient group $\mathbf{G}/\mathbf{T}$ is denoted for convenience by α. An element $R\in\mathbf{G}$ has, according to Eq. (3.1), a unique decomposition of the form $(r_\alpha t_a)$, where $t_a\in\mathbf{T}$ and $\alpha\in\mathbf{G}/\mathbf{T}$.

Write

$$r_\alpha r_\beta=r_{\alpha\beta}t_{\alpha\beta}\in r_{\alpha\beta}\mathbf{T}, \tag{3.2}$$

and define

$$[t_a]_\beta=r_\beta^{-1}t_ar_\beta\in\mathbf{T}. \tag{3.3}$$

Also we denote the coset representative corresponding to the inverse of α in $\mathbf{G}/\mathbf{T}$ by $r_{\bar\alpha}$. With this notation the reader may verify that the following relations hold: The law of multiplication is

$$(r_\alpha t_a)(r_\beta t_b)=(r_{\alpha\beta}t_{\alpha\beta}[t_a]_\beta t_b). \tag{3.4}$$

The inverse of $(r_\alpha t_a)$ is

$$(r_\alpha t_a)^{-1}=(r_{\bar\alpha}[t_a^{-1}]_{\bar\alpha}t_{\alpha\bar\alpha}^{-1}). \tag{3.5}$$

And associativity implies (amongst other things) that

$$r_{\alpha,\beta\gamma}=r_{\alpha\beta,\gamma} \tag{3.6}$$

and

$$t_{\alpha\beta,\gamma}[t_{\alpha\beta}]_\gamma=t_{\alpha,\beta\gamma}t_{\beta\gamma}. \tag{3.7}$$

3.2. Little Groups and Irreducible Representations

Before proceeding to describe how the irreducible representations of $\mathbf{G}$ are classified it is appropriate to define what is meant by *subduced* and *induced* representations.

Let $\mathbf{L}$ be a group and $\mathbf{H}$ a subgroup of $\mathbf{L}$. If P is a representation of **L** then the set of matrices $\{P(h):h\in\mathbf{H}\}$ is called the representation of **H** *subduced* by P. We shall denote this representation by $P\downarrow\mathbf{H}$.

Suppose further that C is a representation of **H** with basis $\langle\phi_1, \phi_2, \cdots, \phi_d|$ so that, for all $h\in\mathbf{H}$, we have equations of the form

$$h\phi_i=\sum_{j=1}^{d}\phi_jC(h)_{ji} \tag{3.8}$$

then, writing

$$\mathbf{L}=\sum_\sigma p_\sigma\mathbf{H} \tag{3.9}$$

the $d|\mathbf{L}|/|\mathbf{H}|$ functions $p_\sigma\phi_i$, $i=1$ to d, $\sigma=1$ to $|\mathbf{L}|/|\mathbf{H}|$, forms a basis for a representation of **L** which is called the *induced* representation of C in **L**. We denote this representation by $C\uparrow\mathbf{L}$. This representation is unique in the sense that a representation induced from C using a different choice of coset representatives in the decomposition (3.9) turns out to be equivalent to the one already defined; and so the notation is unambiguous.

The upward and downward arrow notation is convenient and is becoming fairly standard. It was first used to a large extent by Coleman,[38] who was impressed by its use in the lectures of G. de B. Robinson. For further information about subduced and induced representations the reader is referred to Bradley[21] or to Chap. V of the book by Lomont.[30] Both these references give amplifications or proofs of the results we now survey.

Since **G** has an invariant Abelian subgroup its irreducible representations are most appropriately classified within the framework of little-group theory. To define the little group proceed as follows:

Select an irreducible representation F of **T** (which is, of course, 1-dimensional, since **T** is Abelian). Select the irreducible representations F_α of **T** defined by the equations

$$F_\alpha(t_a)=F([t_a]_\alpha). \tag{3.10}$$

The set of all those γ for which $F_\gamma(t_a)=F(t_a)$, for all $t_a\in\mathbf{T}$, forms a subgroup of $\mathbf{G}/\mathbf{T}$ called the *little co-group* of F in **G** and which we denote by $\bar{\mathbf{K}}_F$. The subgroup $\mathbf{K}_F$ of **G** defined by

$$\mathbf{K}_F=\sum_{\gamma\in\bar{\mathbf{K}}_F}r_\gamma\mathbf{T} \tag{3.11}$$

is called the *little group* of F in **G**.

If we decompose **G** in terms of its left cosets with respect to $\mathbf{K}_F$:

$$\mathbf{G}=\sum_\sigma r_\sigma\mathbf{K}_F \tag{3.12}$$

then the set of representations F_σ, as σ runs over the terms in the sum (3.12), forms what is called the *star* (or *orbit*) of F. It is easily shown that the stars so defined are the classes of an equivalence relation on the irreducible representations of **T**. In this way every irreducible representation of **T** is assigned to one and only one star. Any unitary irreducible representation $\Gamma_F{}^j$ of $\mathbf{K}_F$ for which

$$\Gamma_F{}^j\downarrow\mathbf{T}=\lambda_F{}^jF \tag{3.13}$$

(i.e., whose subduction to **T** yields an integral multiple $\lambda_F{}^j$ of the representation F) is called a *small* (or *allowed*) representation of $\mathbf{K}_F$. Then follows the *key little group theorem*: The representations induced from $\mathbf{K}_F$ into **G**:

$$\Delta_F{}^j=\Gamma_F{}^j\uparrow\mathbf{G} \tag{3.14}$$

(all allowed j for each star, and running through all possible stars) are all of them irreducible, and furthermore all unitary irreducible representations of **G** are obtained in this way once and once only. It is only because the key little group theorem holds and that it produces for us a completely unambiguous classification of all the unitary irreducible representations of **G** that the little group is defined as it is. In the same way later on the magnetic little group must produce for us a similar classification of the unitary irreducible corepresentations of **M**.

3.3. Character of Representations Induced from Little Groups

We now enumerate some of the properties of $\Delta_F{}^j$ (see Sec. 2 of Bradley[21]). Let $\psi_F{}^j$ be the character of $\Gamma_F{}^j$. Then the character $\chi_F{}^j$ of $\Delta_F{}^j$ is, for all $R\in\mathbf{G}$,

$$\chi_F{}^j(R)=\sum_\sigma{}'\psi_F{}^j(r_\sigma^{-1}Rr_\sigma), \tag{3.15}$$

where the prime means that the sum over σ is restricted to those σ in the sum (3.12) for which $Rr_\sigma\in r_\sigma\mathbf{K}_F$, that is those σ for which $\mathbf{K}_F{}^\sigma\equiv r_\sigma\mathbf{K}_Fr_\sigma^{-1}$ contains R. In particular if $R=t_a\in\mathbf{T}$ there is no restriction on σ, the sum is over all σ appropriate to the star of F and

$$\chi_F{}^j(t_a)=\sum_\sigma\psi_F{}^j([t_a]_\sigma)=\sum_\sigma\lambda_F{}^jF_\sigma(t_a). \tag{3.16}$$

This is a famous result: an irreducible representation of **G** contains one complete star an integral number of times.

3.4. The Relationship between Small Representations and Projective Representations of the Little Co-group

Finally we look for a moment at the form of the small representations $\Gamma_F{}^j$. From Eq. (3.13) we know that

$$\Gamma_F{}^j(t_a)=F(t_a)1_F{}^j, \tag{3.17}$$

where $1_F{}^j$ is the unit matrix of dimension $\lambda_F{}^j$. This means that we know $\Gamma_F{}^j$ for all elements of $\mathbf{K}_F$ once $\Gamma_F{}^j(r_\gamma)$ is known for all $\gamma\in\bar{\mathbf{K}}_F$. Also since the matrices (3.17) are diagonal it follows that the set of matrices

[38] A. J. Coleman, Report No. 102, Quantum Chemistry Group, Uppsala University, Uppsala, Sweden.

$\Gamma_F{}^j(r_\gamma)$, $\gamma\in\mathbf{K}_F$, must be irreducible. Also from Eqs. (3.2) and (3.17) they must satisfy the relations

$$\Gamma_F{}^j(r_\gamma)\Gamma_F{}^j(r_\delta)=F(t_{\gamma\delta})\Gamma_F{}^j(r_{\gamma\delta}). \qquad (3.18)$$

Furthermore, by virtue of Eq. (3.7) the complex numbers $F(t_{\gamma\delta})$ satisfy the equations

$$F(t_{\beta\gamma,\delta})F([t_{\beta\gamma}]_\delta)=F(t_{\beta,\gamma\delta})F(t_{\gamma\delta}). \qquad (3.19)$$

But $\delta\in\bar{\mathbf{K}}_F$ so $F([t_{\beta\gamma}]_\delta)=F_\delta(t_{\beta\gamma})=F(t_{\beta\gamma})$ and Eq. (3.19) becomes

$$F(t_{\beta\gamma,\delta})F(t_{\beta\gamma})=F(t_{\beta,\gamma\delta})F(t_{\gamma\delta}). \qquad (3.20)$$

From Eqs. (3.18) and (3.20) it follows that the matrices $\Gamma_F{}^j(r_\gamma)$, considered as functions of γ, form an irreducible projective representation of $\bar{\mathbf{K}}_F$ with factor system F, and conversely any such irreducible projective representation can be taken over to yield a small representation of the little group $\mathbf{K}_F$. The dimensions of these projective representations j are $\lambda_F{}^j$ and as Rudra[39] has shown, they satisfy

$$\sum_j(\lambda_F{}^j)^2=|\bar{\mathbf{K}}_F|, \qquad (3.21)$$

the order of the little co-group of F. The problem of finding all the irreducible representations of $\mathbf{G}$ is thus simplified to that of finding all the irreducible projective representations j of the little co-groups $\bar{\mathbf{K}}_F$ of all the stars. Since $\mathbf{G}$ is usually a group of large order and the $\bar{\mathbf{K}}_F$ are groups of much smaller order this is indeed a great simplification.

3.5. The Three Types of Corepresentation Classified According to the Characters of the Small Representation

We now consider the group $\mathbf{M}$, as defined by Eq. (2.1), for the case when $\mathbf{M}$ has a unitary invariant Abelian subgroup $\mathbf{T}$. If we were to follow the procedure of Sec. 2 to determine the corepresentations of $\mathbf{M}$ the first step would be to obtain the irreducible representations Δ of $\mathbf{G}$. This would be done as indicated in the previous parts of this section. (For greater clarity we now drop the indices j and F, writing Δ instead of $\Delta_F{}^j$, and so on.) The next step would be to take χ, the character of Δ, and to evaluate

$$\sum_{B\in A\mathbf{G}}\chi(B^2):$$

the result would determine, according to Eq. (2.40), the type of corepresentation. In principle given Δ this sum could be calculated, but it turns out that this would be a matter of doing more than is necessary. Indeed we have seen how Δ is determined by the small representation Γ of the little group $\mathbf{K}$. It would obviously be better to simplify, if possible, the criterion (2.40) so that it involves only the character ψ of Γ and fewer of the elements of $\mathbf{M}$: in other words to determine the type of corepresentation from Γ rather from Δ. To this end we write

$$J=|\mathbf{G}|^{-1}\sum_{B\in A\mathbf{G}}\chi(B^2)$$
$$=|\mathbf{G}|^{-1}\sum_{R\in\mathbf{G}}\chi(ARAR). \qquad (3.22)$$

Using Eq. (3.15) we obtain

$$J=|\mathbf{G}|^{-1}\sum_{R\in\mathbf{G}}\sum_\sigma{}'\psi(r_\sigma{}^{-1}ARARr_\sigma), \qquad (3.23)$$

where the prime means that for fixed R the sum over σ is restricted to those σ for which $\mathbf{K}^\sigma\equiv r_\sigma\mathbf{K}r_\sigma{}^{-1}$ contains $ARAR$.

Reversing the order of summation Eq. (3.23) becomes

$$J=|\mathbf{G}|^{-1}\sum_\sigma\sum_{R\in\mathbf{G}}{}'\psi(r_\sigma{}^{-1}ARARr_\sigma), \qquad (3.24)$$

in which the prime now means that for fixed σ the sum over R is restricted for those R for which $ARAR\in\mathbf{K}^\sigma$. Now if AS is such that $ASAS\in\mathbf{K}$ then $r_\sigma ASr_\sigma{}^{-1}=AR$ (for some $R\in\mathbf{G}$) is such that $ARAR=r_\sigma ASASr_\sigma{}^{-1}\in\mathbf{K}^\sigma$. Furthermore, for this σ, $\psi(r_\sigma{}^{-1}ARARr_\sigma)=\psi(ASAS)$. This means that J splits up into $|\mathbf{G}|/|\mathbf{K}|$ equal parts, one part for each σ; that is, one part for each member of the star. Thus

$$J=|\mathbf{K}|^{-1}\sum_{S\in\mathbf{G}}{}'\psi(ASAS), \qquad (3.25)$$

in which the prime now means that the sum over S is restricted to those S for which $ASAS\in\mathbf{K}$.

Now, if we write

$$Ar_\alpha=r_{\alpha'} \qquad (3.26)$$

for all α, it follows from Eq. (2.1) that

$$\mathbf{M}=\sum_\alpha r_\alpha\mathbf{T}+\sum_{\alpha'}r_{\alpha'}\mathbf{T} \qquad (3.27)$$

and further the suffices $\alpha,\beta\cdots,\alpha',\beta'\cdots$ form a group isomorphic with $\mathbf{M}/\mathbf{T}$. With this provision we can extend the notation of Eqs. (3.1) to (3.7) to include the primed suffices. Now if $AS=r_{\alpha'}t_a$ then $ASAS=r_{\alpha'\alpha'}t_{\alpha'\alpha'}[t_a]_{\alpha'}t_a$, so that $ASAS\in\mathbf{K}$ if $\alpha'^2\in\bar{\mathbf{K}}$. Equation (3.25) now becomes

$$J=|\mathbf{K}|^{-1}\sum_{\alpha'^2\in\mathbf{K}}\sum_{t_a\in\mathbf{T}}\psi(r_{\alpha'\alpha'}t_{\alpha'\alpha'}[t_a]_{\alpha'}t_a), \qquad (3.28)$$

which, using Eq. (3.17), yields

$$J=|\mathbf{K}|^{-1}\sum_{\alpha'^2\in\mathbf{K}}\sum_{t_a\in\mathbf{T}}F(t_{\alpha'\alpha'})F([t_a]_{\alpha'})F(t_a)\psi(r_{\alpha'\alpha'}). \qquad (3.29)$$

Now $F([t_a]_{\alpha'})=F_{\alpha'}(t_a)$ and the sum over t_a in Eq. (3.29) will vanish by virtue of orthogonality relations over $\mathbf{T}$ unless α' is such that $F_{\alpha'}(t_a)=[F(t_a)]^{-1}$. Note that all such α' satisfy $\alpha'^2\in\bar{\mathbf{K}}$: so the sum over $\bar{\mathbf{K}}$ in (3.29) contains no further restriction. When the sum

[39] P. Rudra, J. Math. Phys. 6, 1273 (1965).

over t_a does not vanish its value is $|\mathbf{T}|$, the order of $\mathbf{T}$. Hence

$$J=|\mathbf{K}|^{-1}\sum_{\alpha'}\psi(r_{\alpha'}^2), \qquad (3.30)$$

in which the sum over α' is restricted to those α' such that $F_{\alpha'}=F^{-1}$, and $|\bar{\mathbf{K}}|$ is the order of the little co-group. Of course it can be that no such α' exist in which case $J=0$ immediately from Eq. (3.29).

To summarize: in order to determine which of the three cases the irreducible corepresentation of $\mathbf{M}$ derived from Δ belongs to, determine those coset representatives $r_{K'}$ in Eq. (3.27) which satisfy $F_{K'}=F^{-1}$ and evaluate the sum

$$\sum_{K'}\psi(r_{K'}^2),$$

where ψ is the character of Γ in $\mathbf{K}$. Then restricting the sum to those K' the criterion for the type of corepresentation is

$$\begin{aligned}\sum_{K'}\psi(r_{K'}^2)&=\ \ |\bar{\mathbf{K}}| &&\text{in case (a)}\\ &=-|\bar{\mathbf{K}}| &&\text{in case (b)}\\ &=\ \ 0 &&\text{in case (c)},\end{aligned} \qquad (3.31)$$

where we include the special case that if no such K' exist then the sum is zero.

3.6. Magnetic Little Groups and Irreducible Co-representations

The similarity between the criteria (3.31) and (2.40) gives us the clue to the definition of the magnetic little group.

We define the *magnetic little co-group* $\bar{\mathbf{Q}}$ to be the group of all suffices γ for which $F_\gamma=F$ together with all suffices K' for which $F_{K'}=F^{-1}$. Two cases occur: either no such K' exist at all and then $\bar{\mathbf{Q}}=\bar{\mathbf{K}}$; or there exist an equal number of primed and unprimed suffices so that $\bar{\mathbf{K}}$ is a subgroup of $\bar{\mathbf{Q}}$ of index 2. The *magnetic little group* $\mathbf{Q}$ is then defined to have the same relation to $\bar{\mathbf{Q}}$ as $\mathbf{K}$ has to $\bar{\mathbf{K}}$: thus, if no K' exist $\mathbf{Q}=\mathbf{K}$; but, in the alternative case when both sets of suffices appear in equal numbers

$$\mathbf{Q}=\sum_{\gamma\in\mathbf{K}}r_\gamma\mathbf{T}+\sum_{K'\in\mathbf{Q}-\mathbf{K}}r_{K'}\mathbf{T}. \qquad (3.32)$$

In the case in which the magnetic little group coincides with the little group it has the following significance. We are bound to be in case (c). The appropriate corepresentation D is derived from the small representation Γ by first using Eq. (3.14) to find Δ, and then Eq. (2.36) to find D. In this case there is always a doubling of degeneracy due to the presence of antiunitary operators. Of course this method is open to us in the alternative case also, where we use Eq. (2.34) to Eq. (2.36) in the second step as appropriate. What is interesting and important is that in this case another method of obtaining the irreducible corepresentation of $\mathbf{M}$ containing Δ presents itself. In order to see why note first that $\mathbf{Q}$ is a magnetic group and that $\mathbf{K}$ is its unitary subgroup. Γ is an irreducible representation of $\mathbf{K}$. So it is possible to form an irreducible corepresentation Λ of $\mathbf{Q}$ containing Γ. According to Eq. (2.40) the type of Λ depends on the sum

$$\sum_{B\in\mathbf{Q}-\mathbf{K}}\psi(B^2).$$

Indeed the criterion is

$$\begin{aligned}\sum_{B\in\mathbf{Q}-\mathbf{K}}\psi(B^2)&=\ \ |\mathbf{K}| &&\text{in case (a)}\\ &=-|\mathbf{K}| &&\text{in case (b)}\\ &=\ \ 0 &&\text{in case (c)},\end{aligned} \qquad (3.33)$$

which on performing the sum over the elements of $\mathbf{T}$ reduces to

$$\begin{aligned}\sum_{K'\in\bar{\mathbf{Q}}-\bar{\mathbf{K}}}\psi(r_{K'}^2)&=\ \ |\bar{\mathbf{K}}| &&\text{in case (a)}\\ &=-|\bar{\mathbf{K}}| &&\text{in case (b)}\\ &=\ \ 0 &&\text{in case (c)}.\end{aligned} \qquad (3.34)$$

And this is exactly the same criterion (3.31) that governs the type of irreducible corepresentation of $\mathbf{M}$ that contains Δ.

It seems appropriate to call Λ a *small corepresentation* of the magnetic little group $\mathbf{Q}$. The alternative method for determining the irreducible corepresentation of $\mathbf{M}$ that contains Δ should now be clear: *it can also be derived by inducing the small corepresentation Λ into* $\mathbf{M}$. It may not be entirely clear what is meant by an induced corepresentation since this is a new concept. What it means here is as follows: we are given a corepresentation Λ of $\mathbf{Q}$. Since $\mathbf{M}$ is to $\mathbf{Q}$ as $\mathbf{G}$ is to $\mathbf{K}$ we can write

$$\mathbf{M}=\sum_\sigma r_\sigma\mathbf{Q}, \qquad (3.35)$$

where the r_σ that appear in Eq. (3.35) are the same as the r_σ in Eq. (3.12), and are therefore unitary. Let the basis of Λ be $\langle\alpha|$; then, for all $q\in\mathbf{Q}$,

$$q\langle\alpha|=\langle\alpha|\Lambda(q). \qquad (3.36)$$

Furthermore, since Λ is a corepresentation, we have from Eqs. (2.14), for $k_1, k_2\in\mathbf{K}$ and $a_1, a_2\in\mathbf{Q}-\mathbf{K}$,

$$\Lambda(k_1)\Lambda(k_2)=\Lambda(k_1k_2), \qquad (3.37a)$$

$$\Lambda(k_1)\Lambda(a_1)=\Lambda(k_1a_1), \qquad (3.37b)$$

$$\Lambda(a_1)\Lambda^*(k_1)=\Lambda(a_1k_1), \qquad (3.37c)$$

$$\Lambda(a_1)\Lambda^*(a_2)=\Lambda(a_1a_2). \qquad (3.37d)$$

Define for each σ in (3.35) the set of functions

$$\langle\alpha_\sigma|=r_\sigma\langle\alpha|. \qquad (3.38)$$

Then the totality of all functions that appear in these sets as σ varies over the star of F forms the basis of a vector space which is invariant under $\mathbf{M}$. To see this let $m\in\mathbf{M}$ and suppose

$$mr_\tau = r_\gamma q, \tag{3.39}$$

where $q\in\mathbf{Q}$; then

$$\begin{aligned} m\langle\alpha_\tau| &= mr_\tau\langle\alpha|,\\ &= r_\gamma q\langle\alpha|,\\ &= r_\gamma\langle\alpha|\Lambda(q),\\ &= \langle\alpha_\gamma|\Lambda(q),\\ &= \langle\alpha_\gamma|\Lambda(r_\gamma^{-1}mr_\tau), \end{aligned} \tag{3.40}$$

in which we have used Eqs. (3.36), (3.38), and (3.39). In keeping with Eq. (3.40) we define, for all $m\in\mathbf{M}$, the block matrices

$$(\Lambda\uparrow\mathbf{M})_{\gamma\tau}(m) = \Lambda(r_\gamma^{-1}mr_\tau)\delta_{\gamma,m\tau}, \tag{3.41}$$

where $\delta_{\gamma,m\tau}$ is the unit matrix if $mr_\tau\in r_\gamma\mathbf{Q}$ and is the zero matrix otherwise. (Notice the exact parallel between these equations and ideas and induced representations as defined in Sec. 2 of Bradley.[21]) Note that m and $r_\gamma^{-1}mr_\tau$ are both of them unitary or both of them antiunitary. Using this fact and writing $H=(\Lambda\uparrow\mathbf{M})$ it soon follows from Eqs. (3.37) and (3.41) that Eqs. (2.14) holds for H for all R, $S\in\mathbf{G}$ and for all B, $C\in\mathbf{M}-\mathbf{G}$. This means that $(\Lambda\uparrow\mathbf{M})$ is a corepresentation of $\mathbf{M}$ and is said to be *induced* from Λ.

We now have to establish our assertion that $(\Lambda\uparrow\mathbf{M})$ is equivalent to the corepresentation D of $\mathbf{M}$ derived from Δ. First we remember that Δ and Γ are of the same type, that is, they lead to corepresentations of the same type. Since $\Delta=(\Gamma\uparrow\mathbf{G})$ it follows at once that D and H are of the same dimension. Secondly the induction $(\Lambda\uparrow\mathbf{M})$ is performed using exactly the same r_σ as the induction $(\Gamma\uparrow\mathbf{G})$: see Eqs. (3.12) and (3.35). And since Λ contains Γ it follows immediately that H contains Δ. But we have proved H is a corepresentation of $\mathbf{M}$. Furthermore it contains Δ and is of the same dimension as D, which is irreducible and which also contains Δ. Since (up to equivalence) there is only one corepresentation of $\mathbf{M}$ containing Δ of the same dimension as D it follows that $H=(\Lambda\uparrow\mathbf{M})$ is equivalent to D.

Not until this point in the analysis is the definition of the magnetic little group $\mathbf{Q}$ really justified. But now it is seen to be of as fundamental significance for magnetic groups, which have an invariant Abelian subgroup of unitary elements, as is the little group for unitary groups with the same property. *Indeed we have proved that the irreducible corepresentations of such magnetic groups are induced from the small corepresentations of the magnetic little groups*; and this can be made to include the special case in which the magnetic little group $\mathbf{Q}$ is nothing more than the little group $\mathbf{K}$, for then $\mathbf{Q}$ contains no antiunitary elements, the small corepresentations become small representations, and *since we are in case (c)*, the required results are obtained by inducing them straight into $\mathbf{M}$, the intermediate step to $\mathbf{G}$ being unnecessary.

3.7. The Relationship between Small Corepresentations and Projective Corepresentations of the Magnetic Little Co-group

Finally we look at the form of the small corepresentations of $\mathbf{Q}$ and prove a result analogous to the fact that the small representations of $\mathbf{K}$ are the irreducible projective representations of the little co-group $\bar{\mathbf{K}}$.

In case (a), from Eqs. (2.34) and (3.17),

$$\Lambda(t_a) = \Gamma(t_a) = F(t_a)1. \tag{3.42}$$

In case (b), from Eqs. (2.35) and (3.17),

$$\Lambda(t_a) = \begin{pmatrix} \Gamma(t_a) & 0 \\ 0 & \Gamma(t_a) \end{pmatrix} = F(t_a)1. \tag{3.43}$$

And in case (c), from Eq. (2.34), for some fixed K',

$$\Lambda(t_a) = \begin{pmatrix} \Gamma(t_a) & 0 \\ 0 & \Gamma^*(r_{K'}^{-1}t_ar_{K'}) \end{pmatrix}. \tag{3.44}$$

Now

$$\begin{aligned} \Gamma^*(r_{K'}^{-1}t_ar_{K'}) &= F^*([t_a]_{K'})\\ &= F_{K'}^*(t_a)1\\ &= (F^{-1})^*(t_a)1 = F(t_a)1, \end{aligned}$$

where we have used the fact that, since $K'\in\bar{\mathbf{Q}}-\mathbf{K}$, $F_{K'}=F^{-1}$. Hence in case (c) also

$$\Lambda(t_a) = F(t_a)1. \tag{3.45}$$

Thus in all cases $(\Lambda\downarrow\mathbf{T})$ is a scalar matrix. This means that we know Λ for all elements of $\mathbf{Q}$ once $\Lambda(r_\gamma)$ is known for all $\gamma\in\bar{\mathbf{K}}$ and $\Lambda(r_{K'})$ for all $K'\in\mathbf{Q}-\bar{\mathbf{K}}$. Also from Eq. (3.2) and the fact that Λ is a corepresentation it follows that, for γ, $\delta\in\bar{\mathbf{K}}$ and K', $L'\in\mathbf{Q}-\bar{\mathbf{K}}$,

$$\Lambda(r_\gamma)\Lambda(r_\delta) = F(t_{\gamma\delta})\Lambda(r_{\gamma\delta}), \tag{3.46a}$$

$$\Lambda(r_\gamma)\Lambda(r_{K'}) = F^*(t_{\gamma K'})\Lambda(r_{\gamma K'}), \tag{3.46b}$$

$$\Lambda(r_{K'})\Lambda^*(r_\gamma) = F^*(t_{K'\gamma})\Lambda(r_{K'\gamma}), \tag{3.46c}$$

$$\Lambda(r_{K'})\Lambda^*(r_{L'}) = F(t_{K'L'})\Lambda(r_{K'L'}). \tag{3.46d}$$

Furthermore, by virtue of Eq. (3.7), the complex numbers F satisfy

$$F(t_{\mu\nu,\gamma})F(t_{\mu\nu}) = F(t_{\mu,\nu\gamma})F(t_{\nu\gamma}), \tag{3.47a}$$

for all μ, $\nu\in\bar{\mathbf{Q}}$ and $\gamma\in\bar{\mathbf{K}}$, and

$$F(t_{\mu\nu,K'})F^*(t_{\mu\nu}) = F(t_{\mu,\nu K'})F(t_{\nu K'}), \tag{3.47b}$$

for all μ, $\nu\in\bar{\mathbf{Q}}$ and $K'\in\bar{\mathbf{Q}}-\bar{\mathbf{K}}$.

Equations (3.46) and (3.47) imply that Λ considered as a function on the elements of $\bar{\mathbf{Q}}$ forms an irreducible projective corepresentation of $\mathbf{Q}$ with factor system F. Irreducible projective corepresentations have recently been studied by Karavaev *et al.*,[16] Kudryavtseva,[40] and Murthy,[41] who have obtained them for certain of the magnetic crystallographic point groups, and have outlined their general theory. Each such irreducible projective corepresentation of $\bar{\mathbf{Q}}$ can be derived from an irreducible projective representation of the unitary subgroup $\mathbf{K}$, of character, say, ψ and once more there are three cases according to the criterion (3.31). In the present context these facts follow immediately from the preceding theory so there is no need to pursue the general theory here.

4. MAGNETIC SPACE GROUPS

4.1. The General Form of Magnetic Space Groups

A good description of the general form of magnetic space groups (or Shubnikov groups) appears in the book by Shubnikov and Belov.[4] As mentioned in Sec. 1 these groups were derived first by Zamorzaev,[2] but the independent derivation by Belov, Neronova and Smirnova[3] is the one most authors usually lean upon for their material.

Of the 1651 magnetic space groups, 230 correspond to the classical space groups, 230 to these groups together with time reversal and the remaining 1191 to groups in which time reversal occurs only in combination with other operations and not by itself. This classification into different types of magnetic groups is explained in general terms at the beginning of Sec. 2. However in order to understand the general form of magnetic space groups it is necessary to consider the classification in rather more detail.

Type I

These are the crystallographic space groups $\mathbf{G}$ of which there are 230. They have an invariant Abelian subgroup $\mathbf{T}$ of pure translations which characterizes the *Bravais lattice* of the crystal. There are 14 possible distinct Bravais lattices. Different space groups on the same Bravais lattice are further characterized by having different sets of rotations, reflections, screw axes, or glide planes which leave the given Bravais lattice invariant. A good account of these groups and tabulation of their elements appears in Lyubarskii.[18]

Type II

These are of the form [see Eq. (2.2)]

$$\mathbf{M}=\mathbf{G}+\Theta\mathbf{G}, \tag{4.1}$$

where $\mathbf{G}$ is of Type I. There are clearly 230 of these groups and they too are based on one or other of 14 Bravais lattices.

Type III

These are of the form

$$\mathbf{M}=\mathbf{G}+\Theta R\mathbf{G}, \tag{4.2}$$

where $\mathbf{G}$ is of Type I and R cannot be chosen to be the identity. In this case the group [see Eq. (2.3)]

$$\mathbf{M}'=\mathbf{G}+R\mathbf{G} \tag{4.3}$$

must also be a group of Type I. Groups of this type can be found by running through the classical space groups $\mathbf{M}'$ and locating subgroups $\mathbf{G}$ of index 2. There turn out to be 1191 which are crystallographically distinguishable. However there is a convenient subdivision of groups of Type III.

Type IIIa

This is when the element R in Eq. (4.3) cannot be chosen to be a pure translation of the Bravais lattice of $\mathbf{M}'$. From Eq. (4.2) it can be seen that in this case the Bravais lattice of $\mathbf{M}$ coincides with the Bravais lattice of $\mathbf{G}$ and is therefore one of the 14 Bravais lattices previously mentioned. Altogether there are 674 distinguishable groups of Type IIIa. They are tabulated by Shubnikov and Belov.[4]

Type IIIb

This is when the element R in Eq. (4.3) can be chosen to be a pure translation (but cannot be chosen equal to the identity). In this case R^2 must be a translation of $\mathbf{T}$: so what happens in this case is that only half the translations of $\mathbf{M}'$ belong to $\mathbf{G}$. $\mathbf{T}$, the unitary invariant Abelian subgroup of pure translations of $\mathbf{G}$, still characterizes one of the 14 Bravais lattices above. But the magnetic group $\mathbf{M}$ includes an equal number of translations which are antiunitary. The group $\mathbf{S}$ of all the translations, given by

$$\mathbf{S}=\mathbf{T}+\Theta R\mathbf{T}, \tag{4.4}$$

characterizes what is called the magnetic Bravais lattice. There are 22 distinct magnetic Bravais lattices of this kind; their classification and diagrams illustrating their form are given by Shuvnikov and Belov.[4] These authors also tabulate the 517 groups of Type IIIb.

A very thorough account of the classification of magnetic groups is given by Opechowski and Guccione.[7] They also tabulate the magnetic space groups of Type III. Our Type IIIa groups correspond to groups they designate by the symbol $\mathbf{M}_{\mathbf{T}}$. Our Type IIIb groups they subdivide further into groups for which the antiunitary primitive translations never appear as nonprimitive translations associated with screw axis rotations or glide plane reflections of $\mathbf{G}$: these they designate by $\mathbf{M}_{\mathbf{R}0}$. The remainder they label with the

[40] N. V. Kudryavtseva, Soviet Phys.—Solid State **7**, 803 (1965).
[41] M. V. Murthy, J. Math. Phys. **7**, 853 (1966).

symbol $\mathbf{M}_{R\alpha}$. This further subdivision is useful if one embarks upon performing a complete tabulation but is not of primary significance as far as this article is concerned.

4.2. Magnetic Crystals

In this paragraph we give a brief description of the types of structure whose symmetry groups are the magnetic space groups of the various types described above.

Consider first groups of Type II. In all such groups Θ itself is a symmetry operation. Since no axial c vector can be left invariant by Θ it follows that no structure with a symmetry group of Type II can have atoms with localized magnetic moments. Hence groups of Type II describe paramagnetic crystals, that is to say, crystals without any long-range magnetic order.

As the temperature of a paramagnetic crystal is lowered it is possible that the condition of minimum free energy will impose some long range magnetic order. The atoms of the crystal lock together through some exchange effect with their intrinsic magnetic moments arranged in some symmetrical way. If this magnetic ordering persists throughout the whole crystal the symmetry group of the structure will be a magnetic space group of Types I or III. Since Θ is no longer an element of the symmetry group the total symmetry of the magnetically ordered structure is lower than before. The transition temperature is called the Néel temperature T_N. The transitions are second order and this means that the state of the system must change continuously through T_N even though the symmetry is altered discontinuously. This fact can be used to draw some conclusions about the compatibility of symmetries in the magnetic and nonmagnetic states of a given crystal; we shall return to this point again in Sec. 5.

When the magnetic order has set in there may be a net average magnetic moment for the whole crystal. The crystal is then ferromagnetic or ferrimagnetic. On the other hand if there is no net average magnetic moment the crystal is antiferromagnetic.

It turns out that antiferromagnetic spin arrangements can persist (in theory, at any rate) in all groups of Types I or III, but that only a limited number (275, to be precise) can entertain ferromagnetic or ferrimagnetic spin arrangements. In fact groups of Type IIIb must necessarily be antiferromagnetic. In order to see this one must remember that groups of Type IIIb have equal numbers of unitary and antiunitary pure translations: this means that whatever net average magnetic moment there may be in one chemical unit cell of the crystal is necessarily cancelled out exactly by an equal and opposite net average magnetic moment in a chemical unit cell separated from the first by an antiunitary pure translation. Thus each magnetic unit cell (consisting of two chemical unit cells) has zero net average magnetic moment and the whole structure is therefore antiferromagnetic.

The excellent account by Opechowski and Guccione[7] in Chap. IV of their article describes how to build invariant spin arrangements for the various magnetic space groups. In order to understand the limitation on the groups of Types I and IIIa that is imposed in order that a ferromagnetic spin arrangement can exist it is not necessary however to use the full power of their analysis.

Groups of Types I and IIIa have only unitary pure translations. This means that any net average magnetic moment that exists in one chemical unit cell of the magnetic crystal will appear in the next cell and so on throughout the whole crystal. It is sufficient therefore to concentrate on obtaining a ferromagnetic arrangement in one unit cell. Now the total magnetic moment within a unit cell depends only on the magnitudes and directions of the various component magnetic moments that combine together to form the total magnetic moment and not on the precise spatial positions of the atoms carrying the magnetic moments. What this means is that the total magnetic moment within a unit cell transforms under a magnetic space group operation only under the magnetic point group part of the operation: for the question at hand all translational parts of the operations (both primitive and nonprimitive) can be suppressed. Hence the question of whether a ferromagnetic spin arrangement exists reduces to the question of whether an axial c vector can be left invariant under all the operations of a given magnetic point group. For groups of Type I the relevant point groups are the 32 crystallographic point groups, and for groups of Type IIIa they are the 58 magnetic crystallographic point groups. The question of whether such an axial c vector can exist in these point groups can be answered by employing the analysis in the last paragraph of Sec. 2. The answer is that 31 of the 90 groups can exhibit a nonvanishing axial c vector. They are listed, for example, by Tavger and Zaitzev.[5] Also the 275 magnetic space groups based on these point groups are listed by Opechowski and Guccione.[7]

Certain further points of physical significance ought to be noted. First of all these 275 magnetic space groups are not necessarily ferromagnetic. They can, for example, carry two or more interlocking ferromagnetic spin arrangements in different directions. If their separate moments cancel out the resulting structure is antiferromagnetic. If their separate moments only partially cancel the resulting structure is ferrimagnetic. Secondly it is notable that no cubic point group can be ferromagnetic. This means that if a cubic paramagnetic crystal becomes ferromagnetic at low temperatures it must get slightly distorted and lose its cubic structure at the transition point.

Finally we mentioned some of the experimental work that has gone into determining magnetic structures. This work was initiated by Donnay *et al.*[6] who used magnetic space groups to characterize invariant spin arrangements as obtained from neutron diffraction experiments. Corliss and Hastings[42] list all the available data up to 1963 that has been obtained from such neutron diffraction experiments. Other methods can also be used to study invariant spin arrangements, for example, Rudel and Spence,[43] who obtain data from the orientation dependence of nuclear magnetic resonance spectra.

4.3. The Corepresentations of Magnetic Space Groups

We now interpret the theory given in Sec. 3 for the case in which **M** is a magnetic space group. **G** is then one of the 230 crystallographic space groups of Type I and **T** is the subgroup of lattice translations of **G**. The theory in Sec. 3 is appropriate because **T** is a unitary Abelian invariant subgroup of **M**. To save trouble with notation we use the same conventions as Bradley,[21] which in turn are in keeping with those first introduced by Seitz.[44] Elements of **T** are written in the form $\{E \mid \mathbf{t}\}$, where $\mathbf{t}$ is a lattice translation. An element $r_\alpha \in \mathbf{G}$ is of the form $\{R_\alpha \mid \mathbf{v}_\alpha\}$, where R_α is a point group operation. An element $r_{\alpha'} \in \mathbf{M}-\mathbf{G}$ is of the form $\Theta\{\mathbf{S}_{\alpha'} \mid \mathbf{w}_{\alpha'}\}$, where Θ is the time-reversal operator and $\mathbf{S}_{\alpha'}$ is a point group operation; $\mathbf{v}_\alpha$ and $\mathbf{w}_{\alpha'}$ are either zero or nonprimitive translations. From Eq. (3.26) it will be seen that we are writing

$$A\{R_\alpha \mid \mathbf{v}_\alpha\} = \Theta\{S_{\alpha'} \mid \mathbf{w}_{\alpha'}\}, \qquad (4.5)$$

where A is defined by Eq. (2.1). This very general nomenclature permits us to deal simultaneously with all types of magnetic space groups; that is, no distinctions need to be drawn between Types II, IIIa, and IIIb groups.

Each irreducible representation $F^{\mathbf{k}}$ of **T** is labeled with a vector **k** from the first Brillouin zone and is such that

$$F^{\mathbf{k}}(\{E \mid \mathbf{t}\}) = \exp(-i\mathbf{k}\cdot\mathbf{t}). \qquad (4.6)$$

Now the conjugate of $\{E \mid \mathbf{t}\}$ by $\{R_\alpha \mid \mathbf{v}_\alpha\}$ is

$$\{R_\alpha \mid \mathbf{v}_\alpha\}^{-1}\{E \mid \mathbf{t}\}\{R_\alpha \mid \mathbf{v}_\alpha\} = \{E \mid R_\alpha^{-1}\mathbf{t}\}, \qquad (4.7)$$

so from Eq. (3.10)

$$\begin{aligned} F_\alpha{}^{\mathbf{k}}(\{E \mid \mathbf{t}\}) &= F^{\mathbf{k}}(\{E \mid R_\alpha^{-1}\mathbf{t}\}) \\ &= \exp(-i\mathbf{k}\cdot R_\alpha^{-1}\mathbf{t}) \\ &= \exp(-iR_\alpha\mathbf{k}\cdot\mathbf{t}) \\ &= F^{R_\alpha\mathbf{k}}(\{E \mid \mathbf{t}\}). \end{aligned} \qquad (4.8)$$

The little cogroup of $F^{\mathbf{k}}$ now denoted by $\bar{\mathbf{G}}^{\mathbf{k}}$ is therefore to be thought of as consisting of all those point group operations R_γ such that $F^{R_\gamma\mathbf{k}} = F^{\mathbf{k}}$, that is, which satisfy

$$R_\gamma\mathbf{k} = \mathbf{k}+\mathbf{g}, \qquad (4.9)$$

where $\exp(-i\mathbf{g}\cdot\mathbf{t}) = 1$ for all **t**. Such vectors **g** are called *reciprocal lattice vectors* and vectors of the form $(\mathbf{k}+\mathbf{g})$ are said to be *equivalent* to **k**. The condition (4.9) is therefore that $R_\gamma\mathbf{k}$ should be equivalent to **k**. The little group of $F^{\mathbf{k}}$ in **G**, often called the group of **k** and now denoted by $\mathbf{G}^{\mathbf{k}}$ can then be written as

$$\mathbf{G}^{\mathbf{k}} = \sum_{R_\gamma \in \bar{\mathbf{G}}^{\mathbf{k}}} \{R_\gamma \mid \mathbf{v}_\gamma\}\mathbf{T}. \qquad (4.10)$$

If we decompose **G** with respect to $\mathbf{G}^{\mathbf{k}}$:

$$\mathbf{G} = \sum_\sigma \{R_\sigma \mid \mathbf{v}_\sigma\}\mathbf{G}^{\mathbf{k}} \qquad (4.11)$$

then it follows immediately that the set of representations $F^{R_\sigma\mathbf{k}}$ forms the star of $F^{\mathbf{k}}$. Geometrically one may interpret the star as consisting of all vectors $R_\sigma\mathbf{k}$ appropriate to this decomposition. The irreducible representations of **G** now follow immediately from the theory in paragraphs 2, 3, and 4 of Sec. 3. These representations are given for all the 230 space groups by Kovalyev.[45] The more familiar structures are analysed in the classic papers by Bouckaert, Smoluchowski and Wigner,[46] and Herring.[47] More recently very comprehensive accounts have been given by Koster[22] and Slater.[48]

We proceed now to the definition of the magnetic little group. Since Θ commutes with all space group operations the conjugate of $\{E \mid \mathbf{t}\}$ by $\Theta\{S_{\alpha'} \mid \mathbf{w}_{\alpha'}\}$ is $\{E \mid S_{\alpha'}^{-1}\mathbf{t}\}$. Hence it follows, exactly as with Eq. (4.8), that

$$F_{\alpha'}{}^{\mathbf{k}}(\{E \mid \mathbf{t}\}) = F^{S_{\alpha'}\mathbf{k}}(\{E \mid \mathbf{t}\}). \qquad (4.12)$$

In order that $S_{\alpha'}$ should belong to the magnetic little co-group $\mathbf{M}^{\mathbf{k}}$ it is necessary for this to be equal to $(F^{\mathbf{k}})^{-1} = F^{-\mathbf{k}}$. Hence in addition to the $R_\gamma \in \mathbf{G}^{\mathbf{k}}$ the magnetic little co-group consists of all $S_{K'}$ such that $S_{K'}\mathbf{k}$ is equivalent to $-\mathbf{k}$. If no such $S_{K'}$ exist then $\mathbf{M}^{\mathbf{k}} = \mathbf{G}^{\mathbf{k}}$. Finally the magnetic little group $\mathbf{M}^{\mathbf{k}}$ can be written as

$$\mathbf{M}^{\mathbf{k}} = \sum_{R_\gamma \in \bar{\mathbf{G}}^{\mathbf{k}}} \{R_\gamma \mid \mathbf{v}_\gamma\}\mathbf{T} + \sum_{S_{K'} \in \bar{\mathbf{M}}^{\mathbf{k}}-\mathbf{G}^{\mathbf{k}}} \Theta\{S_{K'} \mid \mathbf{w}_{K'}\}\mathbf{T}. \qquad (4.13)$$

The irreducible corepresentations of **M** now follow immediately from the theory in paragraphs 5, 6, and 7 of Sec. 3. No systematic tabulation of all the various types of irreducible corepresentations has yet been made for all the magnetic space groups. This task rests entirely on the relatively easy classification into type of the irreducible projective corepresentations of the magnetic point groups.

In connection with the magnetic little group we make some comments about an equation which is often

[42] L. M. Corliss and J. M. Hastings, *American Institute of Physics Handbook*, D. E. Gray, Ed. (McGraw-Hill Book Co., New York, 1963), Table 5g-22.

[43] E. P. Rudel and R. D. Spence, Physica **26**, 1174 (1960).

[44] F. Seitz, Ann. Math. **37**, 17 (1936).

[45] O. V. Kovalyev, *Irreducible Representations of the Space Groups* (University of Kiev, 1961, and Gordon and Breach Science Publishers, Inc., New York, 1965).

[46] L. P. Bouckaert, R. Smoluchowski, and E. Wigner, Phys. Rev. **50**, 58, (1936).

[47] C. Herring, J. Franklin Inst. **233**, 525 (1942).

[48] J. C. Slater, *Quantum Theory of Molecules and Solids*, (McGraw-Hill Book Co., New York, 1965), Vol. 2.

written down in the literature without explanation. This is the equation

$$\Theta\mathbf{k} = -\mathbf{k}. \tag{4.14}$$

This equation is *not* an analog of Eq. (4.9) because $\Theta^{-1}\{E\mid\mathbf{t}\}\Theta = \{E\mid\mathbf{t}\}$ and hence $F_{\Theta}{}^{\mathbf{k}}(\{E\mid\mathbf{t}\}) = F^{\mathbf{k}}(\Theta^{-1}\{E\mid\mathbf{t}\}\Theta) = F^{\mathbf{k}}(\{E\mid\mathbf{t}\})$ and not $F^{-\mathbf{k}}(\{E\mid\mathbf{t}\})$ as Eq. (4.14) might lead us to suppose if it was an analogue of Eq. (4.9). This does not imply that Eq. (4.14) has no meaning: what it does mean is that, for example,

$$\Theta^{-1}\exp(i\mathbf{k}\cdot\mathbf{r})\Theta = \exp(-i\mathbf{k}\cdot\mathbf{r}), \tag{4.15}$$

that is, Θ transforms a wave function of quasi-momentum $\hbar\mathbf{k}$ into a wave function of quasi-momentum $-\hbar\mathbf{k}$. The meaning is connected with the physical interpretation of $\hbar\mathbf{k}$ as a quasi-momentum rather than the geometrical interpretation of $\mathbf{k}$ as a reciprocal length. Any argument about corepresentation theory which used Eq. (4.14) as a basic postulate and which went on to use it geometrically would be at best a plausibility argument and could conceivably be wrong altogether. (As mentioned in the Introduction this did happen in one case.)

Finally, if $\Gamma_p{}^{\mathbf{k}}$ is a small representation of $\mathbf{G}^{\mathbf{k}}$ with character $\psi_p{}^{\mathbf{k}}$ and $\Delta_p{}^{\mathbf{k}}$ is the irreducible representation of $\mathbf{G}$ induced from $\Gamma_p{}^{\mathbf{k}}$ then the corepresentation of $\mathbf{M}$ derived from $\Delta_p{}^{\mathbf{k}}$ has a type which depends on the following criterion:

$$\begin{aligned}\sum_{S_{K'}}\psi_p{}^{\mathbf{k}}(\{S_{K'}\mid\mathbf{w}_{K'}\}^2) &= \omega\mid\bar{\mathbf{K}}\mid && \text{in case (a)}\\ &= -\omega\mid\bar{\mathbf{K}}\mid && \text{in case (b)}\\ &= 0 && \text{in case (c),}\end{aligned} \tag{4.16}$$

where ω is defined by Eq. (2.42), and $\mid\bar{\mathbf{K}}\mid$ is the order of $\bar{\mathbf{G}}^{\mathbf{k}}$, and in which the sum over $S_{K'}$ is restricted to those point group operations $S_{K'}$ in the set $(\mathbf{M}^{\mathbf{k}}-\mathbf{G}^{\mathbf{k}})$ for which $S_{K'}$ is restricted to those point group operations $S_{K'}$ in the set $(\bar{\mathbf{M}}^{\mathbf{k}}-\mathbf{G}^{\mathbf{k}})$ for which $S_{K'}\,\mathbf{k}$ is equivalent to $-\mathbf{k}$, and where for purposes of evaluation one chooses for each $S_{K'}$ *any one* element $\{S_{K'}\mid\mathbf{w}_{K'}\}$ such that $\Theta\{S_{K'}\mid\mathbf{w}_{K'}\}\in\mathbf{M}$. This agrees, of course, with the formulas of Dimmock and Wheeler.[12–15] And for the case of Type II groups it reduces to the criterion given by Herring[49] for time-reversal degeneracies in paramagnetic space-group structures. To conclude it should perhaps be remarked as a warning that if one works with the magnetic little co-group $\mathbf{M}^{\mathbf{k}}$ the operators $R_\gamma\in\mathbf{G}^{\mathbf{k}}$ must be taken as unitary and the operators $S_{K'}\in(\mathbf{M}^{\mathbf{k}}-\mathbf{G}^{\mathbf{k}})$ must be taken as antiunitary. (Alternatively one could maintain the unitarity of $S_{K'}$ and write $\Theta S_{K'}$ for $S_{K'}$ in the magnetic little co-group.)

[49] C. Herring, Phys. Rev. **52**, 361 (1937).

4.4. Physical Applications

The fundamental ideas which relate the theory of energy spectra with corepresentations have already been dealt with at some length in paragraph 5 of Sec. 2, and need not be repeated here. The theory in the last paragraph extends those ideas to cover quantum systems involving magnetic space groups, in particular the classification of electron states in magnetic crystals.

The prime example is the sticking together of electron energy bands in paramagnetic crystals due to time-reversal being an allowed symmetry operation for Type II groups. This work due to Herring[49] is generalized to cover degeneracies induced by antiunitary operators in Type III groups and appears in some length in the papers of Kudryartseva and his co-authors.[11,16] An instructive artificial example is given by Dimmock and Wheeler[12] who consider the transition between a paramagnetic and an antiferromagnetic (or ferromagnetic) Kronig–Penney model. In this case the translational symmetry is reduced at the transition and this has the effect of producing discontinuities in the magnetic bands which do not appear in the paramagnetic bands.

Other types of quantum spectra are also influenced by magnetic symmetry. A case which has received attention lately is the spin-wave spectrum. For this subject the reader is referred to the interesting papers by Brinkman and Elliott.[20]

5. KRONECKER PRODUCTS OF COREPRESENTATIONS

The next problem is the definition and reduction of the inner Kronecker product of any two irreducible corepresentations of $\mathbf{M}$. In keeping with the notation of Sec. 2 we shall write Δ^i for an irreducible representation of the unitary subgroup $\mathbf{G}$ and for notational convenience later we define

$$\Delta^{i\prime}(R) = \bar{\Delta}^i(R) = \Delta^{i*}(A^{-1}RA). \tag{5.1}$$

We denote by D^i the irreducible corepresentation of $\mathbf{M}$ derived from Δ^i.

We assume the decomposition of Inner Kronecker products within the unitary subgroup are known. That is to say, the Clebsch–Gordan coefficients $C_{ij,k}$ in the reduction

$$\Delta^i\otimes\Delta^j = \sum_k C_{ij,k}\Delta^k \tag{5.2}$$

are supposed known. Writing ψ^i for the character of Δ^i the well-known formula for $C_{ij,k}$ is

$$C_{ij,k} = \mid\mathbf{G}\mid^{-1}\sum_{R\in\mathbf{G}}\psi^i(R)\psi^j(R)\psi^{k*}(R). \tag{5.3}$$

A detailed analysis of how to obtain $C_{ij,k}$ from this formula in the case in which $\mathbf{G}$ is a crystallographic space group is given by Bradley.[21] Other treatments are given by Elliott and Loudon,[50] Lax and Hopfield,[51]

[50] R. J. Elliott and R. Loudon, J. Phys. Chem. Solids **15**, 146 (1960).
[51] M. Lax and J. Hopfield, Phys. Rev. **124**, 115 (1961).

Lax,[52] and Birman.[53] Tables of the reduction coefficients $C_{ij,k}$ appear so far for very few space groups because of the tediousness of their calculation. Birman[53] does however include tables for the Diamond and Zinc-Blende structures. The lack of such tables severely limits the practical application that can at present be made of the work in this Section.

Define now, for all $m\in\mathbf{M}$, and for any two irreducible corepresentations D^i and D^j the matrix D^{ij} whose elements are

$$D^{ij}(m)_{pq,rs}=D^i(m)_{pr}D^j(m)_{qs} \tag{5.4}$$

so that D^{ij} is the Kronecker product of the matrices D^i and D^j:

$$D^{ij}(m)=D^i(m)\otimes D^j(m). \tag{5.5}$$

Then it is soon verified that D^{ij} is a corepresentation of $\mathbf{M}$. That is to say, D^{ij} satisfied equations of the form (2.14).

We know from Sec. 2 that a corepresentation is uniquely determined (up to equivalence) by the characters of the elements of the unitary subgroup. Writing χ^i for the character of D^i (when restricted to $\mathbf{G}$), then from Eq. (5.4) we obtain, for all $R\in\mathbf{G}$,

$$\chi^{ij}(R)=\chi^i(R)\chi^j(R), \tag{5.6}$$

and these values characterize completely the corepresentation D^{ij}. In general the corepresentative D^{ij} will be reducible under $\mathbf{M}$. Suppose therefore

$$D^{ij}=D^i\otimes D^j=\sum_k d_{ij,k}D^k. \tag{5.7}$$

The sum over k in Eq. (5.2) will be over all superfixes both primed and unprimed, whereas the sum over k in Eq. (5.7) is restricted to unprimed superfixes. Our problem is to determine the coefficients $d_{ij,k}$. The first step is to relate $d_{ij,k}$ to the characters χ^i, χ^j and χ^k of the unitary subgroup. This comes as a very simple generalization of Eq. (5.3) (bearing in mind that D^k is possibly reducible under $\mathbf{G}$), and the formula (see also Karavaev[25]) is

$$d_{ij,k}=|\mathbf{G}|^{-1}\sum_{R\in G}\chi^i(R)\chi^j(R)\chi^{k*}(R)/|\mathbf{G}|^{-1}\sum_{R\in G}\chi^k(R)\chi^{k*}(R). \tag{5.8}$$

Next we assert that if D^k is of type (a), (b), or (c) then the denominator of Eq. (5.8) is 1, 4, or 2, respectively. This follows from Eqs. (2.34) to (2.36), and is a consequence of the fact that D^k contains in case (a) just one irreducible representation of $\mathbf{G}$, in case (b) one irreducible representation twice, and in case (c) two inequivalent irreducible representations once. Indeed

$$\begin{aligned}\chi^k(R)&=\psi^k(R) &&\text{in case (a)}\\ &=2\psi^k(R) &&\text{in case (b)}\\ &=\psi^k(R)+\psi^{k'}(R) &&\text{in case (c).}\end{aligned} \tag{5.9}$$

Thus using the orthogonality relations for characters,

$$\begin{aligned}|\mathbf{G}|^{-1}\sum_{R\in G}\chi^k(R)\chi^{k*}(R)&=1 &&\text{in case (a)}\\ &=4 &&\text{in case (b)}\\ &=2 &&\text{in case (c).}\end{aligned} \tag{5.10}$$

The second step is to convert formula (5.8) into a relationship between $d_{ij,k}$ and the $C_{ij,k}$ of Eq. (5.2). Since the $C_{ij,k}$ are known (at any rate in principle) the problem is then solved for all magnetic groups. A laborious evaluation of the numerator of Eq. (5.8) for each particular case is then unnecessary. In particular, for magnetic space groups, the rather involved method of Karavaev[25] is unnecessary provided the values for $C_{ij,k}$ are first derived using the formulas of Bradley.[21]

There are, taking account of the relation

$$d_{ij,k}=d_{ji,k} \tag{5.11}$$

eighteen different cases to consider according to whether D^i, D^j, D^k are of types (a), (b), (c). The formulas are quite straightforward to establish: one has to substitute Eqs. (5.9) and (5.10) into (5.8) and to simplify the result using Eq. (5.3). It is also necessary to use the fact that if D^k is of type (c) then a corepresentation D^{ij} containing Δ^k contains $\Delta^{k'}$ an equal number of times. The values of the $d_{ij,k}$ are given in Table V.

As an example of the use of Table V let us consider the group $\mathbf{C}_{4v}(\mathbf{C}_{2v})$ in terms of its unitary subgroup $\mathbf{C}_{2v}$. To make the notation coincide with that of this Section denote the representations A_1, A_2, B_1, and B_2 of $\mathbf{C}_{2v}$ (see Table II) by Δ_1, Δ_2, Δ_3, and $\Delta_{3'}$, respectively, and the corepresentations $D(A_1)$, $D(A_2)$, and $D(B)$ of $\mathbf{C}_{4v}(\mathbf{C}_{2v})$ (see Table III) by D_1, D_2, and D_3, respectively.

We assume the Clebsch–Gordan coefficients for the Kronecker products of $\mathbf{C}_{2v}$ are known. These are

$$\begin{aligned}C_{11,1}&=C_{12,2}=C_{13,3}=C_{13',3'}=C_{22,1}=C_{23,3'}\\ &=C_{23',3}=C_{33,1}=C_{33',2}=C_{3'3',1}=1,\end{aligned} \tag{5.12}$$

and all other $C_{ij,k}$ not derived from these by the relation

$$C_{ij,k}=C_{ji,k} \tag{5.13}$$

are zero.

Remembering Δ_1 and Δ_2 are of type (a) and Δ_3 is of type (c) (see paragraph 5 of Sec. 2) we use appropriate

[52] M. Lax, Phys. Rev. **138**, A793 (1965).
[53] J. L. Birman, Phys. Rev. **127**, 1093 (1962).

lines of Table V to obtain

$$d_{11,1}=C_{11,1}=1,$$

$$d_{12,2}=C_{12,2}=1,$$

$$d_{13,3}=C_{13,3}+C_{13',3}=1,$$

$$d_{22,1}=C_{22,1}=1,$$

$$d_{23,3}=C_{23,3}+C_{23',3}=1,$$

$$d_{33,1}=C_{33,1}+C_{33',1}+C_{3'3,1}+C_{3'3',1}=2,$$

$$d_{33,2}=C_{33,2}+C_{33',2}+C_{3'3,2}+C_{3'3',2}=2, \quad (5.14)$$

and all other $d_{ij,k}$ not derived from these by Eq. (5.11) vanish. Thus the Clebsch–Gordan decomposition for $\mathbf{C}_{4v}(\mathbf{C}_{2v})$ is

$$D_1\otimes D_1=D_1,$$

$$D_1\otimes D_2=D_2,$$

$$D_1\otimes D_3=D_3,$$

$$D_2\otimes D_2=D_1,$$

$$D_2\otimes D_3=D_3,$$

$$D_3\otimes D_3=2D_1+2D_2. \quad (5.15)$$

TABLE V. Clebsch–Gordan coefficients for Kronecker products of irreducible corepresentations. *Notes*: (i) The formulas are for *irreducible* corepresentations only. (ii) Each row of the table supplies a formula for $d_{ij,k}$, as defined by Eq. (5.7). (iii) The appropriate row of the table to use depends on the types of the corepresentations involved. The first three entries in each row are, respectively, the types of D^i, D^j, and D^k [as defined by Eqs. (2.34) to (2.36)]. (iv) The fourth entry in each row is the value of $d_{ij,k}$ in terms of the $C_{ij,k}$ as defined by Eq. (5.2). (v) Primed suffices refer to primed representations: see Eq. (5.1). Thus $C_{ij',k}$ is the number of times Δ^k appears in the decomposition of $\Delta^i \otimes \Delta^{j'}$.

D^i	D^j	D^k	$d_{ij,k}$
(a)	(a)	(a)	$C_{ij,k}$
(a)	(a)	(b)	$\frac{1}{2}C_{ij,k}$
(a)	(a)	(c)	$C_{ij,k}$
(a)	(b)	(a)	$2C_{ij,k}$
(a)	(b)	(b)	$C_{ij,k}$
(a)	(b)	(c)	$2C_{ij,k}$
(a)	(c)	(a)	$C_{ij,k}+C_{ij',k}$
(a)	(c)	(b)	$\frac{1}{2}C_{ij,k}+\frac{1}{2}C_{ij',k}$
(a)	(c)	(c)	$C_{ij,k}+C_{ij',k}$
(b)	(b)	(a)	$4C_{ij,k}$
(b)	(b)	(b)	$2C_{ji,k}$
(b)	(b)	(c)	$4C_{ji,k}$
(b)	(c)	(a)	$2C_{ij,k}+2C_{ij',k}$
(b)	(c)	(b)	$C_{ij,k}+C_{ij',k}$
(b)	(c)	(c)	$2C_{ij,k}+2C_{ij',k}$
(c)	(c)	(a)	$C_{ij,k}+C_{ij',k}+C_{i'j,k}+C_{i'j',k}$
(c)	(c)	(b)	$\frac{1}{2}C_{ij,k}+\frac{1}{2}C_{ij',k}+\frac{1}{2}C_{i'j,k}+\frac{1}{2}C_{i'j',k}$
(c)	(c)	(c)	$C_{ij,k}+C_{ij',k}+C_{i'j,k}+C_{i'j',k}$

One possible physical application of the Kronecker products of corepresentations lies in the study of the restrictions that apply to magnetic structures which can arise when a crystal undergoes a single second-order phase transition from the paramagnetic state to the magnetic state in question. An extensive treatment of the thermodynamic properties of second-order phase transitions in magnetic crystals has been given by Belov.[54]

More recently Dimmock[19] has written an instructive article on this subject. These references taken together with the fundamental work of Landau and Lifschitz[17] explain how it is that the product representations arise. We do not wish to pursue this topic further for as we have pointed out earlier in this section detailed practical analysis is at present out of the question. We are indebted to Cracknell (private correspondence) for pointing out a second possible physical application, namely the development of crystal field theory to situations involving a magnetic environment. Whatever applications do emerge from time to time one thing however seems abundantly clear and forms a common feature which threads its way throughout the whole analysis: whatever the application, if it depends for its analysis in the first place on the corepresentation theory of a magnetic group, the analysis can be so organized that it can be made to depend on the ordinary representations of the unitary subgroup of index 2 and a knowledge of their classification into types with respect to the magnetic group as a whole. Table V is a clear example of a case in point.

ACKNOWLEDGMENTS

The authors wish to express thanks to Dr. S. L. Altmann for his encouragement with this work, to Dr. R. J. Elliott for discussion, and to Dr. A. P. Cracknell for correspondence. One of us (B.L.D.) wishes to express his gratitude to the British Science Research Council for a grant during the tenure of which this article was prepared.

[54] K. P. Belov, *Magnetic Transitions* (Consultants Bureau Enterprises Inc., New York, 1961).