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A comment on the reality classification of space group representations

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Abstract. A connection between the reality type of a group representation, and the symmetrized and antisymmetrized squares of that representation is noted. The correspondence leads to a simple reality test for space group representations. A detailed analysis reproduces the Herring test.

1. Introduction

It is well known, principally through the work of Wigner (1959), that the recognition of time-reversal symmetry in a quantum-mechanical system may lead to rather more energy degeneracies than can be inferred purely from a consideration of spatial symmetries. In the absence of magnetic effects, the group-theoretical criterion for these extra degeneracies involves knowledge of the reality types, as determined by the Frobenius–Schur test, of the irreducible representations (reps) of the spatial symmetry group of the system. The details of the criterion are given in convenient tabular form on p 146 of Tinkham (1964).

In the application of the above to a crystal, the Frobenius–Schur test becomes unwieldy on account of the infinite summation over the translational subgroup of the relevant space group. However, Herring (1937) was able to simplify the test by explicitly performing this summation. He found that the reality index, with values 1, 0 or -1, corresponding to the property of being (*a*) real, (*b*) complex, or (*c*) pseudo-real, respectively, of the character of the induced rep D of the space group G is given by

$$\frac{1}{|\bar{G}^{k}|}\sum{}' \chi(Q^2), \tag{1}$$

where $\boldsymbol{k}$ is a wavevector of D, $\bar{G}^{k}$ is the little co-group of $\boldsymbol{k}$, χ is the character of an allowable rep of the little group G^{k}, and the prime restricts the summation to those coset representatives of the translation subgroup which send $\boldsymbol{k}$ into $-\boldsymbol{k}$, or an equivalent vector. An empty sum indicates a zero value for the index. Formula (1), usually called the Herring test, makes reality testing a practical proposition for space groups, for it involves only a finite sum over group elements.

The first purpose of the present paper is to draw attention to an alternative expression for the reality indices of the reps of a locally compact group G, which, given tables of symmetrized and antisymmetrized squares of the reps of G, enables the reality testing to be done at a glance. Unfortunately the value of this test is reduced somewhat in the case of space groups, for the realities of the reps of such groups have already been tabulated by Miller and Love (1967) and Bradley and Cracknell (1972). Nevertheless, a detailed analysis of the alternative formulation reproduces the Herring test in a manner which makes transparent the structure of the latter.

2. The reality index

If D is a rep of the finite group G, then Mackey (1953) has shown that

(*a*) D is real $\Leftrightarrow [D\otimes D]$ contains $A(G)$;

(*b*) D is pseudo-real $\Leftrightarrow \{D\otimes D\}$ contains $A(G)$;

(*c*) D is complex $\Leftrightarrow D\otimes D$ does not contain $A(G)$; where the square brackets and braces refer to the symmetrized and antisymmetrized squares of D, respectively, and where $A(G)$ is the totally symmetric (ie trivial) representation of G. Equivalently, since $A(G)$ can be contained at most once in $D\otimes D$, D is real, pseudo-real or complex, according as $A(G)$ has multiplicity 1, -1 or 0, in the generalized representation

$$U = [D\otimes D]-\{D\otimes D\}.$$

Actually the latter characterization follows simply from the Frobenius–Schur test, without reference to Mackey (1953), when it is noted that $\chi(g^2)$ is the value at g of the character of U, where χ is the character of D.

It should be pointed out that although Mackey's result refers to finite groups, its proof is valid more generally. Thus the above characterization certainly applies to space groups, even though such groups are infinite and noncompact.

It follows that should a table of the symmetrized and antisymmetrized squares of a space group G be available, then the reality types of the representations of G can be read off at once. In particular such a table appears in Bradley and Davies (1970) for T_d^2, the group of the zinc-blende structure. For example it is easily seen that $\Delta_1 \uparrow G$ is real, $\Delta_5 \uparrow G$ is pseudo-real, $\Delta_3 \uparrow G$ is complex.

3. The Herring test

A deeper analysis of the above is possible when D is an induced representation, as is the case when G is a space group, for Mackey (1953) showed further how to effect the separation of the square of such a D into its symmetrized and antisymmetrized parts, in such a way that each part can be written as a sum of induced representations. The details of this separation, which require a fairly lengthy statement, have been simplified, made more complete computationally and in particular applied to space groups, by Bradley and Davies (1970). Rather than reproduce that work here, we refer the reader there for the necessary definitions and for the statement of theorem 6 and the equations (4.12) and (4.13).

Now suppose D_p^k is an allowable representation of G^k, the little group of the wave-vector k; then $D_p^k \uparrow G$ is irreducible. By the Frobenius reciprocity theorem, an induced representation contains $A(G)$ if and only if the pre-induced representation contains $A(H)$, where H is the relevant subgroup. Thus the reality type of $D_p^k\uparrow G$ is determined by seeing whether or not any of the pre-induced representations in (4.12) and (4.13) contain a trivial representation. The structure of these equations allows several simplifications in the analysis.

First, noting that $[(D_p^k \uparrow G)\otimes(D_p^k \uparrow G)]$ contains $[D_p^k \otimes D_p^k] \uparrow G$ and that $\{(D_p^k \uparrow G)\otimes(D_p^k \uparrow G)\}$ contains $\{D_p^k \otimes D_p^k\} \uparrow G$, we see that $D_p^k \uparrow G$ is of the same reality type as D_p^k if the latter is real or pseudo-real. By restriction of $D_p^k \otimes D_p^k$ to the translation group it is evident that D_p^k is complex if $2\boldsymbol{k} \not\equiv \boldsymbol{0}$. We shall see presently that if $2\boldsymbol{k} \equiv \boldsymbol{0}$ (ie $2\boldsymbol{k} = \boldsymbol{0}$ or a reciprocal lattice vector), then $A(G)$ cannot be contained in the second or third terms of (4.12) and (4.13). Then follows, if $2\boldsymbol{k} = \boldsymbol{0}$, the stronger result that $D_p^k \uparrow G$ has the same reality type as D_p^k, which, again because $2\boldsymbol{k} \equiv \boldsymbol{0}$, has the reality type of the associated projective representation of the little co-group $\bar{G}^k$. Of course if G is symmorphic, or $\boldsymbol{k}$ is interior to the Brillouin zone (which cannot be the case if $2\boldsymbol{k} \equiv \boldsymbol{0}$) then the latter representation is a vector representation and hence may be tested for reality by the usual Frobenius–Schur test. Otherwise, the projective generalization of this test, noted by Backhouse (1970) and Brown (1970), may be employed. In either case the Frobenius–Schur test reduces at once to the special case of the Herring test (1) in which $2\boldsymbol{k} \equiv \boldsymbol{0}$, for then the summation can only be taken over the coset representatives of the translation subgroup in the little group.

We are left to consider the cases when D_p^k is complex and $2\boldsymbol{k} \not\equiv \boldsymbol{0}$, where it is necessary to look at the second and third terms of (4.12) and (4.13). Actually the third term in each equation is not relevant here, because we have already remarked that the square of an irreducible representation can contain $A(G)$ no more than once. Thus it is sufficient to check whether or not, for each self-inverse double coset α, the characters $\chi_{\alpha p}^{k\pm}$, given by (4.15) and (4.16), contain $A(M_\alpha^k)$. Recalling that the allowable representations of the little groups act like scalars for the translations, it is a prerequisite for one or other of these characters to contain $A(M_\alpha^k)$ that $R_\alpha \boldsymbol{k}+\boldsymbol{k} \equiv \boldsymbol{0}$. We can now see the reason for the separation of the cases $2\boldsymbol{k} \not\equiv \boldsymbol{0}$ and $2\boldsymbol{k} \equiv \boldsymbol{0}$, for the latter denies the existence of R_α, never an element of $\bar{G}^k$. Now, from § 2, the reality index is the frequency of $A(M_\alpha^k)$ in $\chi_{\alpha p}^{k+} - \chi_{\alpha p}^{k-}$, which takes zero value on L_α^k, but $2\chi_p^k[(\{A|\boldsymbol{a}\}\{S|\boldsymbol{w}\})^2]$ on the other coset of L_α^k in M_α^k. The condition $R_\alpha \boldsymbol{k}+\boldsymbol{k} \equiv \boldsymbol{0}$ implies that this character is independent of the translation $\boldsymbol{w}$, and hence that the index is the frequency of $A(\bar{M}_\alpha^k)$ in the representation of $\bar{M}_\alpha^k = M_\alpha^k/T$ whose character vanishes on $\bar{L}_\alpha^k = L_\alpha^k/T$, but which has value $2\chi_p^k[(\{A|\boldsymbol{a}\}\{S|\boldsymbol{0}\})^2]$ on the other coset of $\bar{L}_\alpha^k$ in $\bar{M}_\alpha^k$. Thus the index is

$$\frac{1}{|\bar{L}_\alpha^k|}\sum \chi_p^k[(\{A|\boldsymbol{a}\}\{S|\boldsymbol{0}\})^2], \tag{2}$$

since $|\bar{M}_\alpha^k| = 2|\bar{L}_\alpha^k|$, where the summation is over $S \in \bar{L}_\alpha^k$. Now, bearing in mind $R_\alpha \boldsymbol{k} \equiv -\boldsymbol{k}$, which implies $\bar{L}_\alpha^k = \bar{G}^k$ and $A\boldsymbol{k} \equiv R_\alpha \boldsymbol{k} \equiv -\boldsymbol{k}$, we see that this summation is identical to that given by the Herring test for $2\boldsymbol{k} \not\equiv \boldsymbol{0}$.

4. Conclusion

We have pointed out an alternative to the Frobenius–Schur and Herring methods for the reality testing of group representations, which becomes particularly useful if tables of symmetrized and antisymmetrized squares are available. We have also shown that an analysis of the alternative method leads to the Herring test in the case of space groups. One novel feature of this analysis is that the infinite translation subgroup is accounted for without the need for the mathematically unrigorous infinite summation in the reduction of the Frobenius–Schur test to the Herring test.

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