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Determinantal Representations for the Crystallographic Point Groups

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Abstract

A table of the values of the determinants of the representation matrices for the crystallographic point groups is given to facilitate the application of some recent theorems concerning determinantal wavefunctions.

A recent paper (Duff 1982) explored the symmetry properties of determinantal wavefunctions constructed from functions selected from the members of bases for representations of a group. Such functions can be important for the description of multi-fermion systems such as, for example, multiple holes bound to a charged impurity in a semiconducting material. Three theorems were presented of which two are relevant to the present considerations. The first theorem ('Filled Shell' Theorem) showed that a determinantal wavefunction, constructed from all of the one-particle functions forming a basis for a representation Γ_u of some group G, is a basis function for a one-dimensional representation Γ_ψ of G, and the characters of Γ_ψ are the values of the determinants of the representation matrices for Γ_u. The second theorem ('Filled Shell Minus n' Theorem) established the connection between the representations generated by determinantal functions constructed from n and from $N-n$ of the N basis functions for Γ_u, and thus this theorem can be useful (provided $n \neq \frac{1}{2}N$) in reducing the size of the group theory problem involved in a multiple fermion system. The equations effecting the connection (equations 19 and 20 of Duff 1982) require for their application the values of the determinants of the representation matrices for Γ_u.

Since both of the aforementioned theorems require the values of the determinants of the relevant representation matrices, and since these theorems may be expected to have utility in diverse areas of solid state physics, it is the purpose of the present work to supply a succinct tabulation of the required determinant values for the crystallographic point groups. So that the table may be as concise as possible without omitting any important detail, we note the following two points: (a) For a one-dimensional representation, the required determinant values are trivially the characters of the representation, and since these are almost universally cited whenever an application is made, it is not necessary to list them here and accordingly results for all one-dimensional representations are omitted from our table. (b) According to the 'Filled

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Shell' theorem described above, the values of the determinants of the representation matrices for a particular representation of a given group themselves form a one-dimensional representation of that group, and so it is not necessary to list the values individually for each group operator; it suffices to simply identify which of the possible one-dimensional representations has characters equal to the required determinant values. Accordingly in Table 1 we list for all of the crystallographic point groups (both single and double groups and excepting those groups that only have one-dimensional representations), the one-dimensional representations whose characters provide the required determinant values.

Table 1. Determinantal representations for crystallographic point groups

To use this table, first identify from the relevant row the group (G) of interest. Under that, select the representation of interest from the relevant row (R). Under that is the one-dimensional representation (DR) whose character for any group operator is the value of the determinant of the representation matrix for that operator

G	D_2, C_{2v}	D_{2h}	D_4, C_{4v}, D_{2d}		D_{4h}		D_3, C_{3v}	
R	Γ_5	Γ_5^+, Γ_5^-	Γ_5	Γ_6, Γ_7	Γ_5^+, Γ_5^-	$\Gamma_6^+, \Gamma_7^+, \Gamma_6^-, \Gamma_7^-$	Γ_3	Γ_4
DR	Γ_1	Γ_1^+	Γ_2	Γ_1	Γ_2^+	Γ_1^+	Γ_2	Γ_1

G	D_{3d}		D_6, C_{6v}, D_{3h}		D_{6h}	
R	Γ_3^+, Γ_3^-	Γ_4^+, Γ_4^-	Γ_5, Γ_6	$\Gamma_7, \Gamma_8, \Gamma_9$	$\Gamma_5^+, \Gamma_6^+, \Gamma_5^-, \Gamma_6^-$	$\Gamma_7^+, \Gamma_8^+, \Gamma_9^+, \Gamma_7^-, \Gamma_8^-, \Gamma_9^-$
DR	Γ_2^+	Γ_1^+	Γ_2	Γ_1	Γ_2^+	Γ_1^+

G	T			T_h			O, T_d	
R	Γ_4, Γ_5	Γ_6	Γ_7	$\Gamma_4^+, \Gamma_4^-, \Gamma_5^+, \Gamma_5^-$	Γ_6^+, Γ_6^-	Γ_7^+, Γ_7^-	Γ_3, Γ_5	$\Gamma_4, \Gamma_6, \Gamma_7, \Gamma_8$
DR	Γ_1	Γ_3	Γ_2	Γ_1^+	Γ_3^+	Γ_2^+	Γ_2	Γ_1

G	O$_h$			
R	Γ_3^+, Γ_5^+	$\Gamma_4^+, \Gamma_6^+, \Gamma_7^+, \Gamma_8^+, \Gamma_6^-, \Gamma_7^-, \Gamma_8^-$	Γ_4^-	Γ_5^-
DR	Γ_2^+	Γ_1^+	Γ_1^-	Γ_2^-

In nearly all cases, the entries in Table 1 may be obtained without explicitly constructing the representation matrices, but rather by use of the multiplication tables of the group representations. Suppose, for example, that for a particular group the multiplication table contains the entry

$$\Gamma_p \times \Gamma_q = \Gamma_r + \Gamma_s + \Gamma_t. \tag{1}$$

Suppose further that the dimensionality of the representation Γ_p and Γ_q is m and n respectively then, as derived in the Appendix, we must have

$$|\Gamma_p|^n \, |\Gamma_q|^m = |\Gamma_r| \, |\Gamma_s| \, |\Gamma_t|, \tag{2}$$

where the notation $|\Gamma_i|$ means the determinant of the representation matrix $a_i(R)$ for representation Γ_i and for group operator R, it being implied in (2) that the same operator R applies to each symbol. As an example, the multiplication table for the group T (Koster *et al.* 1963) contains the entry

$$\Gamma_4 \times \Gamma_4 = \Gamma_1 + \Gamma_2 + \Gamma_3 + 2\Gamma_4.$$

Thus, since Γ_4 is a three-dimensional representation while Γ_1, Γ_2 and Γ_3 are all one dimensional, we have by application of (2)

$$|\Gamma_4|^6 = |\Gamma_1| \, |\Gamma_2| \, |\Gamma_3| \, |\Gamma_4|^2.$$

The character tables for group T show that, for each of the group operators, the product of the characters of the representations Γ_1, Γ_2 and Γ_3 is $+1$, so we immediately deduce that

$$|\Gamma_4|^4 = 1 \quad \text{for each operator of } T.$$

Since unity is the only fourth root of 1 existing as a character of the one-dimensional representations for this group, we deduce immediately that

$$|\Gamma_4| = 1,$$

and thus identify Γ_1 as the one-dimensional representation whose characters are the values of the determinants of the representation matrices for the representation Γ_4 of the group T.

In Table 1 the group and representation designations, and as far as possible the order of appearance of the groups and representations, are those of Koster *et al.* (1963). As an example of the use to which this table can be put, consider the case of two fermions in states belonging to a basis for the representation Γ_5 of group O, a three-dimensional representation of that group. The two-particle state must necessarily be a Γ_4 state, as is easily demonstrated by use of the 'Filled Shell Minus n' theorem (equation 20 of Duff 1982), in the form

$$\chi_n = \chi_d \chi^*_{N-n}, \tag{3}$$

where, for any of the group operators, χ_n and χ_{N-n} are the characters for n particle and $N-n$ particle antisymmetric states respectively and χ_d is the character of the determinantal representation; for the present application $N = 3$ and $n = 2$. From Table 1 we see that the determinantal representation for Γ_5 of group O is Γ_2. In Table 2 we list the characters of the representations Γ_2, Γ_4 and Γ_5, together with the values of χ_2 deduced from equation (3). It is quite clear that the values of χ_2 are identically the characters of the representation Γ_4, and this is all that is required to show that the two-particle antisymmetric states form a basis for a Γ_4 representation.

Table 2. Character table for selected representations of group O, together with the values of χ_2 deduced from equation (3)

Represen-tation	Group operator E	$\bar{E}$	C_3	$\bar{C}_3$	$C_2, \bar{C}_2$	C_4	$\bar{C}_4$	$C_2', \bar{C}_2'$
Γ_2	1	1	1	1	1	-1	-1	-1
Γ_4	3	3	0	0	-1	1	1	-1
Γ_5	3	3	0	0	-1	-1	-1	1
χ_2	3	3	0	0	-1	1	1	-1

References

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Appendix

It is our purpose here to derive equation (2) from equation (1). Let a(R) be an $m \times m$ representation matrix for the operator R for the representation Γ_p, and b(R) the corresponding $n \times n$ matrix for Γ_q. Then the (reducible) representation matrix for the product representation is c(R), the outer product of a(R) and b(R). Explicitly, we write

$$\mathrm{c} = \begin{bmatrix} a_{11}b_{11} & a_{11}b_{12} \cdots a_{11}b_{1n} & a_{12}b_{11} \cdots a_{12}b_{1n} & a_{13}b_{11} & \cdots & a_{1m}b_{1n} \\ a_{11}b_{21} & a_{11}b_{22} \cdots a_{11}b_{2n} & a_{12}b_{21} \cdots a_{12}b_{2n} & a_{13}b_{21} & \cdots & a_{1m}b_{2n} \\ \vdots & \vdots \quad\quad \vdots & \vdots \quad\quad \vdots & \vdots & & \vdots \\ a_{11}b_{n1} & a_{11}b_{n2} \cdots a_{11}b_{nn} & a_{12}b_{n1} \cdots a_{12}b_{nn} & a_{13}b_{n1} & \cdots & a_{1m}b_{nn} \\ a_{21}b_{11} & a_{21}b_{12} \cdots a_{21}b_{1n} & a_{22}b_{11} \cdots a_{22}b_{1n} & a_{23}b_{11} & \cdots & a_{2m}b_{1n} \\ \vdots & \vdots \quad\quad \vdots & \vdots \quad\quad \vdots & \vdots & & \vdots \\ a_{21}b_{n1} & a_{21}b_{n2} \cdots a_{21}b_{nn} & a_{22}b_{n1} \cdots a_{22}b_{nn} & a_{23}b_{n1} & \cdots & a_{2m}b_{nn} \\ a_{31}b_{11} & a_{31}b_{12} \cdots a_{31}b_{1n} & a_{32}b_{11} \cdots a_{32}b_{1n} & a_{33}b_{11} & \cdots & a_{3m}b_{1n} \\ \vdots & \vdots \quad\quad \vdots & \vdots \quad\quad \vdots & \vdots & & \vdots \\ a_{m1}b_{n1} & a_{m1}b_{n2} \cdots a_{m1}b_{nn} & a_{m2}b_{n1} \cdots a_{m2}b_{nn} & a_{m3}b_{n1} & \cdots & a_{mm}b_{nn} \end{bmatrix} \tag{A1}$$

We wish to evaluate the determinant of the matrix c. To do this we first perform a Laplace expansion of c in terms of the first n rows (see Ayres 1962). Every minor formed from these rows contains columns, each element of which has a common factor of one of the elements of the matrix a, and these can then be factored out of the minor. What remain are columns of the matrix b. If any one column is repeated, the value of the minor is zero. Thus the only surviving minors are those with distinct columns, and since the minor is $n \times n$, it must contain all of the columns of b (possibly in a different order) and so its value contains the factor $|\mathrm{b}|$. For each such minor, the complementary minor must be taken which, by an identical process, also consists of a factor of $|\mathrm{b}|$, factors of the elements of a, and a lower level minor. By repeating the process, it is clear that

$$|\mathrm{c}| = |\mathrm{b}|^m f(\{a_{ij}\}), \tag{A2}$$

where f is an as yet undetermined function of the elements of the matrix a.

In like manner $|\mathrm{c}|$ can be expanded by a Laplace expansion in which the m rows all containing b_{11} are chosen. Minors formed from these rows either vanish or contain $|\mathrm{a}|$ along with some factors of the elements of b. Repeating the procedure as before gives

$$|\mathrm{c}| = |\mathrm{a}|^n g(\{b_{ij}\}), \tag{A3}$$

where g is some function of the elements of the matrix b. Comparing equations (A2) and (A3) we must have

$$|\mathrm{c}| = |\mathrm{a}|^n \, |\mathrm{b}|^m \times \text{constant}. \tag{A4}$$

To evaluate the constant in (A4) we calculate from both (A1) and (A4) the coefficient in the expansion of $|\mathrm{c}|$ of the term

$$\prod_{i,j} a_{ii}^n b_{jj}^m .$$

The chosen term is simply the product of the diagonal elements in c, and thus the constant is evaluated to be 1; then

$$|c| = |a|^n \, |b|^m .$$

In the symbolism of equation (2) this is

$$|c| = |\Gamma_p|^n \, |\Gamma_q|^m . \tag{A5}$$

We now derive an alternative expression for $|c|$ by recognizing that the representation $\Gamma_p \times \Gamma_q$ is reducible, and so it is clear that c can be block diagonalized by a suitable similarity transformation. The value of the determinant of c is not affected by the transformation. In the block-diagonalized form the determinant of c can be evaluated by successive Laplace expansions, each of which encompasses only one of the diagonal blocks as one of the minors in the expansion. In this manner the value of the determinant is seen to be simply the product of the determinants of the blocks along the diagonal. With the symbolism of equation (2), this result is

$$|c| = |\Gamma_r| \, |\Gamma_s| \, |\Gamma_t| . \tag{A6}$$

On combining (A5) and (A6) we have directly

$$|\Gamma_p|^n \, |\Gamma_q|^m = |\Gamma_r| \, |\Gamma_s| \, |\Gamma_t| ,$$

and this is equation (2).

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