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Some Theorems Concerning Group Representations Generated by Determinantal Wavefunctions

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Abstract

Theorems are developed which extend to representations more general than those of the rotation group the usefulness of the concept of filled fermion shells, and the relationships between shells containing and shells lacking n fermions.

1. Introduction

Spectroscopy in widely diverse systems of fermions has profited greatly from the interpretive analytic techniques of group theory and from the use of determinantal wavefunctions. In the case of isolated atoms, the spherical symmetry of the Hamiltonian reduces the group theory problem to that of the familiar task of the addition of the angular momenta of the individual fermions to form eigenfunctions of the usual total angular momentum operators. For impurities in solids, spherical symmetry does not apply, so angular momentum addition procedures are not relevant. One nevertheless must determine a total wavefunction satisfying the appropriate symmetry requirements, by combining the symmetries of the one-particle states. For example, a Group I impurity such as copper in a Group IV semiconductor will behave as a triple acceptor and the wavefunction of the resulting entity will describe three holes bound to the impurity site. For Cu in Ge, the orbital for each hole will be a member of a $\Gamma_8(\overline{T}_d)$ manifold (Jones and Fisher 1970) (where Γ_8 is a four-dimensional representation of $\overline{T}_d$, Koster *et al.* 1963). For the construction of the ground state wavefunctions, four possible choices can be made of three one-particle functions drawn from a single Γ_8 manifold and the four choices lead to four distinct antisymmetric system wavefunctions. The representation(s) thus generated by the three holes must be one of the following alternatives: $2\times\Gamma_6$, $2\times\Gamma_7$, $\Gamma_6+\Gamma_7$ or Γ_8 (where Γ_6 and Γ_7 are two-dimensional representations of $\overline{T}_d$, Koster *et al.* 1963). Which of those alternatives describes the three-hole ground state? Answers to such questions can be resolved, while recognizing the requirements of the Pauli principle, by examining the symmetry properties of determinantal wavefunctions formed from states participating in the basis (or bases) for the representation(s) of the appropriate symmetry group. The theorems presented below are directed at simplifying such tasks.

2. Definitions and Mathematical Preliminaries

Assume that $u_1(\boldsymbol{r}), u_2(\boldsymbol{r}), \ldots, u_M(\boldsymbol{r})$ constitute a basis for some representation Γ_u of group G. We wish to explore representations of G generated by determinantal functions constructed from these functions. We define

$$\psi = \begin{vmatrix} u_1(\boldsymbol{r}_1) & u_2(\boldsymbol{r}_1) & \ldots & u_M(\boldsymbol{r}_1) \\ u_1(\boldsymbol{r}_2) & u_2(\boldsymbol{r}_2) & \ldots & u_M(\boldsymbol{r}_2) \\ \vdots & \vdots & & \vdots \\ u_1(\boldsymbol{r}_M) & u_2(\boldsymbol{r}_M) & \ldots & u_M(\boldsymbol{r}_M) \end{vmatrix}. \tag{1}$$

Complementary minors of this determinant can be defined by selecting rows numbered $i_1, i_2, \ldots, i_m$ $(i_1 < i_2 < \ldots < i_m, m < M)$ and columns $j_1, j_2, \ldots, j_m$ $(j_1 < j_2 < \ldots < j_m)$. Designate by p and q respectively the ordered sets $i_1, \ldots, i_m$ and $j_1, \ldots, j_m$, and by p' and q' respectively the complements of p and q. The minor ψ_p^q is the determinant of the $m \times m$ matrix whose (α, β) element is the (i_α, j_β) element (where $i_\alpha \in p, j_\beta \in q$) of the array on the RHS of equation (1). The minor complementary to ψ_p^q is $\psi_{p'}^{q'}$ defined in a similar way with respect to the sets p', q'. We also designate the sum of the subscripts in a set such as p or q as

$$S(p) = i_1 + i_2 + \ldots + i_m, \qquad S(q) = j_1 + j_2 + \ldots + j_m, \qquad \text{etc.} \tag{2a, b}$$

The transformation properties of ψ and ψ_p^q under the operations of the group are determined by the transformation properties of $\{u_i\}$, which may be defined by

$$R u_i = \sum_{j=1}^{M} \mathrm{a}_{ji}(R) u_j, \tag{3}$$

where R is any of the operators of G, and the matrices $\mathrm{a}(R)$ can in general be taken to be unitary. The determinant of the matrix $\mathrm{a}(R)$ will be designated $|\mathrm{a}(R)|$. Again it is convenient to specify a notation for the minors of $\mathrm{a}(R)$, which, for the sets p and q as above, will be designated $\mathrm{a}_p^q(R)$, and the complementary minor is $\mathrm{a}_{p'}^{q'}(R)$. Since $\mathrm{a}(R)$ is a matrix with definite values for each of its elements, $\mathrm{a}_p^q(R)$ is a determinant with a definite value once the sets p and q have been designated. The values of these determinants can be arranged into a matrix $\mathrm{A}(R)$ with elements $\mathrm{A}_{p,q}(R)$, in which the rows and columns of $\mathrm{A}(R)$ are labelled unambiguously by the set labels p and q. In like manner we can arrange the values of $\mathrm{a}_{p'}^{q'}(R)$ into a matrix $\mathrm{A}'(R)$ with elements $\mathrm{A}'_{p',q'}(R)$. The matrices $\mathrm{A}(R)$ and $\mathrm{A}'(R)$ are of dimensionality $M!/(M-m)!m!$ corresponding to the number of ways the sets p and q can be chosen.

It will be shown below that for fixed m, $\{\mathrm{A}(R) : R \in G\}$ forms a representation of G. Anticipating this result, and using the unitarity of $\{\mathrm{a}(R)\}$, we can show that each $\mathrm{A}(R)$ is unitary. The group property requires

$$\mathrm{A}(R^{-1}) = \mathrm{A}^{-1}(R) \qquad \text{and} \qquad \mathrm{a}(R^{-1}) = \mathrm{a}^{-1}(R), \tag{4a, b}$$

and the unitarity of the members of $\{\mathrm{a}(R)\}$ requires

$$\mathrm{a}_{ij}(R) = \mathrm{a}_{ji}^*(R^{-1}). \tag{5}$$

Now $a_p^q(R)$ is the determinant of a matrix of selected elements of $a(R)$. By virtue of the selection procedure and the above property, $a_p^q(R^{-1})$ is the determinant of the Hermitian conjugate of the matrix of which $a_p^q(R)$ is the determinant. The value of $a_q^p(R^{-1})$ is unaltered by transposing the matrix, in which case the elements are then simply the complex conjugates of the elements making up the determinant $a_p^q(R)$. That is, we have

$$a_q^p(R^{-1}) = (a_p^q(R))^*, \qquad A_{qp}(R^{-1}) = A_{pq}^*(R), \qquad A_{qp}^{-1}(R) = A_{pq}^*(R). \tag{6a, b, c}$$

In like manner the members of $\{A'(R)\}$ are unitary matrices.

In addition to the above functions, matrices and determinants we will have need of another set of functions $v_1(\boldsymbol{r}), v_2(\boldsymbol{r}), \ldots, v_N(\boldsymbol{r})$ which form a basis for the representation Γ_v of G. A determinantal function ϕ can be constructed from these in the manner in which ψ is formed from $\{u_i(\boldsymbol{r})\}$. Minors $\phi_f^g, \phi_{f'}^{g'}$ are constructed by following identical procedures to those above; f, g are two ordered sets of n subscripts chosen from N in the same way that p, q are sets of m subscripts selected from M, and f' and g' are the ordered complements of f and g respectively. The transformation properties under G of $\{v_i(\boldsymbol{r})\}$ are taken to be

$$Rv_i = \sum_{j=1}^{N} b_{ji}(R)\, v_j, \tag{7}$$

where $b(R)$ are unitary matrices. Minors of $b(R)$ are designated $b_f^g(R)$ and $b_{f'}^{g'}(R)$, and their values arranged into matrices $B_{fg}(R)$ and $B'_{f'g'}(R)$, where the dimensionality of $B(R)$ and $B'(R)$ is $N!/(N-n)!n!$ As above, $B(R)$ and $B'(R)$ are unitary.

3. Theorems

Theorem 1 ('Filled Shell' Theorem): ψ is a basis function for a one-dimensional representation of G, and the characters of this representation are $\{|a(R)|\}$.

Proof: Operate with any R on ψ:

$$R\psi = \det\left[\begin{bmatrix} u_1(\boldsymbol{r}_1) & u_2(\boldsymbol{r}_1) & \ldots & u_m(\boldsymbol{r}_1) \\ u_1(\boldsymbol{r}_2) & u_2(\boldsymbol{r}_2) & \ldots & u_m(\boldsymbol{r}_2) \\ \vdots & \vdots & & \vdots \\ u_1(\boldsymbol{r}_m) & u_2(\boldsymbol{r}_m) & \ldots & u_m(\boldsymbol{r}_m) \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & \ldots & a_{1m} \\ a_{21} & a_{22} & \ldots & a_{2m} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \ldots & a_{mm} \end{bmatrix}\right]. \tag{8}$$

Since the determinant of a product is the product of the determinants, we have

$$R\psi = \psi\,|a(R)|. \tag{9}$$

To demonstrate the group properties, we note that if I is the identity operator, $|a(I)|$ is the determinant of a unit matrix and is trivally unity, and if T is an operator of G, not necessarily distinct from R, then

$$\begin{aligned} T(R\psi) &= |a(R)|\, T\psi = |a(T)|\,|a(R)|\,\psi \\ &= |a(T)\, a(R)|\,\psi \\ &= |a(TR)|\,\psi = (TR)\psi. \end{aligned}$$

It should be noted that, although the unitarity of the members of $\{a(R)\}$ requires each determinant to have a magnitude of unity, for some representations of some groups, for example those containing both proper and improper rotations, there may be more than one value in the character set $\{|a(R)|\}$, so that ψ does not necessarily generate the totally symmetric representation. Designate the representation generated as Γ_{ψ}.

Theorem 2 ('Filled Shell Minus n' Theorem): For fixed p, $\{\psi_p^q\}$ constitutes a basis for the representation of G, and so does $\{\psi_{p'}^{q'}\}$; the representations generated by $\{\psi_p^q\}$ and $\{\psi_{p'}^{q'}\}$ are simply related.

Proof: Operate with R on any ψ_p^q. The result is similar to equation (8) except that in the present case the first matrix would consist solely of the rows of ψ specified by p, and the second matrix would consist solely of the columns of $a(R)$ specified by q. Thus the first matrix is $m \times M$ and the second is $M \times m$. By a theorem on determinants (Muir 1960), the determinant of such a product is the sum of the determinants of all products of pairs of $m \times m$ matrices in which the first matrix of the pair is formed by choosing m columns from the $m \times M$ matrix (retaining their sequence of appearance), and the second matrix of the pair is formed by taking the *corresponding* m rows from the $M \times m$ matrix (again preserving the sequence of appearance). Thus, for fixed p, we have

$$R\psi_p^q = \sum_k \psi_p^k a_k^q(R) = \sum_k A_{kq}(R)\,\psi_p^k. \tag{10}$$

In equation (10), k is a set of m ordered subscripts, there being ${}^M C_m$ such sets possible. Since each $R\psi_p^q$ is a linear combination of the members of $\{\psi_p^k\}$, it follows that $\{\psi_p^k\}$ is a candidate for a basis of a representation of G, with the representation matrices being $\{A(R)\}$. We now verify that the group properties are satisfied.

(1) Consider first $R = I$, the identity operation. If the sets k and q are identical, then $a_k^q(I)$ is the determinant of a unit matrix and has the value 1. If k and q are not identical, then $a_k^q(I)$ is a determinant with at least one row and one column of zeros, and its value is necessarily zero. Thus $A(I)$ is the unit matrix.

(2) We demonstrate the group multiplication property by considering the operators T and TR, both of which are operators of G, not necessarily distinct or different from R:

$$\begin{aligned} T(R\psi_p^q) &= \sum_k A_{kq}(R)\,T\psi_p^k = \sum_k A_{kq}(R)\sum_l A_{lk}(T)\,\psi_p^l \\ &= \sum_l (A(T)\,A(R))_{lq}\,\psi_p^l, \end{aligned} \tag{11}$$

while

$$(TR)\psi_p^q = \sum_l A_{lq}(TR)\,\psi_p^l. \tag{12}$$

We must show $A(T)A(R) = A(TR)$. Since $\{a(R)\}$ form a representation of G, we have

$$a_{ij}(TR) = \sum_t a_{it}(T)\,a_{tj}(R). \tag{13}$$

In order to evaluate the determinant $a_l^q(TR)$ we construct the matrix of its elements by selecting from $a(TR)$ all elements indicated by the set of row subscripts l and column subscripts q. It is clear from (13) that this matrix can be expressed as the product of an $m \times M$ matrix consisting of all the elements of the rows l of $\mathrm{a}(T)$, and an $M \times m$ matrix consisting of all the elements of columns q of $\mathrm{a}(R)$. Thus $\mathrm{A}_{lq}(TR)$ is the determinant of this product. Using the determinant theorem cited above for such products, we have immediately

$$\mathrm{A}_{lq}(TR) = \sum_k \mathrm{A}_{lk}(T)\,\mathrm{A}_{kq}(R), \tag{14}$$

which is the desired result.

(3) It follows from the results in (1) and (2) that

$$\mathrm{A}(R^{-1}) = \mathrm{A}^{-1}(R). \tag{15}$$

In like manner $\{\mathrm{A}'(R)\}$ forms a representation of G. To establish the relationship between the representations $\{\mathrm{A}(R)\}$ and $\{\mathrm{A}'(R)\}$, we construct another set of determinants $\{\mathrm{C}_\alpha^\beta(R)\}$ as follows. Let α and β be two ordered sets of m subscripts, and let α' and β' be the ordered complements of these sets respectively. Then $\mathrm{C}_\alpha^\beta(R)$ is the determinant of the $M \times M$ array whose columns are specified by the following recipe: if $i \in \alpha'$, then column i of $\mathrm{C}_\alpha^\beta(R)$ is taken to be column i of $\mathrm{a}(R)$; if $i \in \alpha$, suppose it to be the tth member of the ordered set α, choose the tth member of the ordered set β, suppose it to be j, then column i of $\mathrm{C}_\alpha^\beta(R)$ is column j of $\mathrm{a}(R)$. If $\alpha \neq \beta$ then $\mathrm{C}_\alpha^\beta(R)$ must necessarily have two identical columns, and such a determinant has a value of zero. That is, we get

$$\mathrm{C}_\alpha^\beta(R) = \delta_{\alpha\beta}\,|\,\mathrm{a}(R)\,|\,. \tag{16}$$

Using the Laplace expansion of the determinant (Ayres 1962), and utilizing the definition of the sum function given in equations (2), gives

$$\begin{aligned}\delta_{\alpha\beta}\,|\,\mathrm{a}(R)\,| = \mathrm{C}_\alpha^\beta(R) &= \sum_k (-1)^{S(\beta)+S(k)}\mathrm{a}_k^\beta(R)\,\mathrm{a}_{k'}^{\alpha'}(R)\\ &= \sum_k (-1)^{S(\beta)+S(k)}\mathrm{A}_{k\beta}(R)\,\mathrm{A}'_{k'\alpha'}(R).\end{aligned} \tag{17}$$

Defining the matrices E and F by the relations

$$\mathrm{E}_{\beta k} = (-1)^{S(\beta)+S(k)}\mathrm{A}_{k\beta}(R)/|\,\mathrm{a}(R)\,|, \qquad \mathrm{F}_{k\alpha} = \mathrm{A}'_{k'\alpha'}(R), \tag{18a, b}$$

equation (17) becomes

$$\delta_{\alpha\beta} = \sum_k \mathrm{E}_{\beta k}\,\mathrm{F}_{k\alpha} \qquad \text{or} \qquad 1 = \mathrm{EF},$$

so that $\mathrm{E} = \mathrm{F}^{-1}$. That is, from (18) we write

$$\begin{aligned}\mathrm{A}_{k\beta}(R) &= (-1)^{S(\beta)+S(k)}|\,\mathrm{a}(R)\,|\,(\mathrm{A}'(R))^{-1}_{\beta k}\\ &= (-1)^{S(\beta)+S(k)}|\,\mathrm{a}(R)\,|\,\mathrm{A}'_{\beta'k'}(R^{-1}).\end{aligned} \tag{19}$$

The characters of the representations are found by taking the traces of the representation matrices, and therefore

$$\begin{aligned}\mathrm{Tr}(\mathrm{A}(R)) &= |\,\mathrm{a}(R)\,|\,\mathrm{Tr}(\mathrm{A}'(R^{-1}))\\ &= |\,\mathrm{a}(R)\,|\,\mathrm{Tr}(\mathrm{A}'(R))^*.\end{aligned} \tag{20}$$

Equations (19) and (20) are the connections between the representation generated by the determinantal functions formed by selecting m functions at a time from the M functions in $\{u_i(r)\}$, and the representation generated by the determinantal functions formed by selecting $M-m$ functions from the $\{u_i(r)\}$. These relations will be especially useful in the special case $m = M-1$, in which the determinantal wavefunctions will have symmetry properties closely similar to those of the single particle states. In some cases equation (20) will reveal the two character sets to be identical, which is all that is required to prove the representations to be equivalent. Thus, equation (20) can be used to answer the question raised in the Introduction concerning the three-hole ground state of Cu in Ge: the ground state must necessarily be a Γ_8 state, just as the single particle states are, and not any of the other alternatives listed.

Theorem 3 ('Two Shell' Theorem): For fixed m and n, the set of all determinantal functions of the type

$$\theta^{qg} = \begin{vmatrix} u_{i_1}(r_1) & u_{i_2}(r_1) & \dots & u_{i_m}(r_1) & v_{j_1}(r_1) & \dots & v_{j_n}(r_1) \\ \vdots & \vdots & & \vdots & \vdots & & \vdots \\ u_{i_1}(r_{m+n}) & u_{i_2}(r_{m+n}) & \dots & u_{i_m}(r_{m+n}) & v_{j_1}(r_{m+n}) & \dots & v_{j_n}(r_{m+n}) \end{vmatrix}$$

forms a basis for the representation of G, and this representation is simply the product of the representations generated by $\{\psi_p^q\}$ and $\{\phi_f^g\}$.

Proof: θ^{qg} can be represented symbolically as

$$\theta^{qg} = |\psi_{m+n}^q \phi_{m+n}^g|. \tag{21}$$

Operate with R on θ^{qg}, so that using the same symbolism,

$$R\theta^{qg} = \left| (\psi_{m+n}\, \phi_{m+n}) \begin{pmatrix} \mathrm{a}^q & 0 \\ 0 & \mathrm{b}^g \end{pmatrix} \right| \tag{22}$$

$$= \sum_{k,h} |\psi_{m+n}^k \phi_{m+n}^h| \begin{vmatrix} \mathrm{a}_k^q & 0 \\ 0 & \mathrm{b}_h^g \end{vmatrix}. \tag{23}$$

Here k is an ordered set of m subscripts and h is an ordered set of n subscripts. In proceeding from equation (22) to (23), the theorem cited above concerning the determinant of products of non-square matrices has been used, and in doing so certain terms have been omitted from the expansion because they are recognized to be zero. These terms are the ones in which the number of columns containing u functions in the first matrix of the products in (23) differs from m (with the consequence that the number of columns containing v functions differs from n). It is recognized that the operation of the symmetry operator R cannot replace a u with a v (or *vice versa*); in terms of the mathematical properties such terms are eliminated by the vanishing of the determinant of the coefficients as is easily seen by consideration of an appropriate Laplace expansion (Ayres 1962), in which a row or column of zeros in one of the minors of each product in the expansion guarantees that the determinant vanishes. Thus, we get

$$R\theta^{qg} = \sum_{k,h} \theta^{kh} \, |\mathrm{a}_k^q| \, |\mathrm{b}_h^g|$$
$$= \sum_{k,h} \mathrm{A}_{kq} \mathrm{B}_{hg} \theta^{kh}. \tag{24}$$

It is therefore seen that the transformation properties of $\{\theta^{qg}\}$ are those of the products of members of $\{\psi_p^q\}$ with members of $\{\phi_f^g\}$, and thus the product representation is generated. This result can obviously be extended to any number of sets of functions.

Corollary ('Filled Shell Plus n' Theorem): If $m = M$, the representation generated is $\Gamma_\psi \times \Gamma_n$, where Γ_n is the representation generated by $\{\phi_f^g\}$. It will frequently occur that Γ_ψ is the totally symmetric representation, in which case the product representation is Γ_n, but this is not a general result.

4. Conclusions

Techniques for the generation of properly antisymmetrized functions from a set of products of one-particle orbitals are well known and widely used. Most expositions of this topic concentrate on the development of spin orbitals with emphasis on angular momentum properties. Considerable understanding has flowed from the concept of filled shells, and the relationships between shells containing and shells lacking n particles. The present work is intended to underscore, as far as possible, the extension of such concepts to representations of a more general nature. In this respect equations (19) and (20) are the central results, providing as they do a way to replace a problem involving many ('filled shell minus n') particles with one involving fewer ('n') particles, a considerable advantage. The other results have been included for completeness, and their exposition implies a useful caution: that in determining the symmetry properties of a multiparticle system, filled shells cannot be neglected unless it can be shown that Γ_ψ is the totally symmetric representation, a requirement which is not met in all cases.

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