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REDUCED MATRIX ELEMENTS
AND REPRESENTATION OF WAVE FUNCTIONS

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Résumé. — On suggère d'étendre les représentations de fonctions d'onde qui ont un ensemble minimal de termes intermédiaires de structure arborescente ou dendritique, à des structures polygonales simples, ou même plus élaborées, avec un grand nombre de termes intermédiaires. Ces représentations se conservent sans référence explicite à axe privilégié dans les espaces de quasispin, de spin et angulaires. Dans le traitement d'une couche seule, un opérateur à symétrie de fermion, en général multilinéaire, doit se trouver à chaque sommet de la représentation. Les coefficients des sommets sont alors des éléments de sous-matrices de ces opérateurs, c'est-à-dire des coefficients de parenté fractionnelle pour des structures appropriées. Il est alors utile d'introduire un petit élément de sous-matrice pour étudier ces coefficients. Il est également pratique d'adopter un ordre des termes selon le poids des quasispins et des spins, en particulier pour la détermination des phases. Pour la couche p on trouve quelques cas de coefficients de parenté fractionnelle indépendants de nombres avec des propriétés reliées aux adjoints et aux compléments.

Abstract. — An extension is suggested from wave function representations with a minimal set of intermediate terms, treeform or dendritic in structure, to simply polygonal or more elaborate structures, with a larger number of intermediates. These representations are maintained without explicit reference to axis orientation, in quasispin, spin, and angular spaces. In treatment of a single shell, a fermion operator, multilinear in general, must occur at each vertex of the representation. The vertex coefficients are then submatrix elements of these operators, or coefficients of fractional parentage for appropriate structures. Here it is useful to introduce a small submatrix element for the study of the coefficients. It is also convenient to adopt an ordering of terms with use of quasispin and spin weights particularly for assignment of phases. The p-shell provides a few instances of number-free parentage coefficients with properties relating to adjoint and complement.

1. Introduction. — The study of principal-parent wave functions and their generalizations leads immediately to more elaborate structures, characterized by several internal terms. In one of the simplest of these, the tetragon wave function, which may occur if there are just two outer momenta in addition to the initial and the final, there are evidently four inner momenta; while in the dendrite there is but one, the principal parent in that case. However an extended discussion is needed. For if there are five outer momenta, one may revert to branched structures, which, again minimal, here contain only two inner momenta. In any such study, one recalls that as the number of outer momenta becomes larger, the number of accessible structures increases very rapidly indeed.

The need and search for clarity in treatment early indicated that representations of wave functions should be cleared of dependence of \( N \), the number of orbitals, and clear also of other component quantum numbers. The use of quasispin then requires construction operators in the representations for terms within a shell. Coefficients of fractional parentage (cfp) appear as matrix elements, fundamentally, and as vertex coefficients. The whole study, as it now stands, should be considered exploratory. The use of \( N \)-independent cfp (number free, in the sense of quasispin) and the rationalization of various sorts of submatrix elements may finally prove of most interest. Separation of matrix elements into quasispin-spin (QSS) and angular (W, WU) factors should be thoroughly studied.

Discussion is confined to a single shell in the \( \Gamma = QSL \) coupling scheme. Also the arrangement is homogenous, i.e., the same format serves for each of the three spaces. In addition these spaces are treated as distinct. It will be finally necessary to proceed with the view that the angular structure must differ from the quasispin-spin structure, but such a development is not attempted at present. There is quite enough new material in the number-free coefficients that are needed, and in some tentative phasing procedures, to inhibit more distant exploration at this moment.
2. Submatrix Elements in Several Weights. — Coefficients of fractional parentage are most conveniently studied by sum-rule methods. The intermediate state expansion is usually given in terms of coupled submatrix elements. Now some utility resides in the use of several kinds of these submatrix elements which may differ in weighting factors and in phases. For there are already a number of conventions in the literature and they can be classified as to weight with but little expense and some advantage. Racah’s double-barred element is the largest. If one takes out the roots of the weights there appears the small submatrix element \((r : T; r')\).\(^2\) \(\langle r' | \langle T | r \rangle \rangle \equiv (r' \parallel T \parallel r)^2\). Quite a number of familiar forms, cf. for example, lie between these cases, weighted on one side or the other. Here an exceptional submatrix element is that of TAS \([1]\). It bears relation to a few others, to the unit operator of Racah \([2]\) (or the similar operators used by Judd \([3]\)), for example. But these set to one side, the various submatrix elements can be described as small, medium, or large.

The sum rules and orthogonality relations in \(jm\)-coefficients (or of Wigner) and \(j\)-coefficients \([4]\) involve the weight of the summed parameter just as do similar sorts of relations in the small submatrix elements now introduced. The statement of the Wigner-Eckart theorem involves a large and a small submatrix elements. The integral \(C_{\alpha \nu \nu}^\alpha\) (TAS \(9^6S\)) is a small coefficient squared. In general the symmetric forms, small or large, are best suited for graphical treatment; while medium forms find a place as vertex coefficients in treeform graphs. Finally, the symmetric forms are convenient in questions of phase, particle-hole conjugation, reciprocity, and complementarity.

The assimilation of cfp to submatrix elements raises a problem so soon as the elements are factored. Reciprocity and the adjoint relation are identified now. In the usual factoring as in R IV, the nature of the related QSS- and W-operators requires further study. One may ask again concerning separation of quasispin and spin, but it is another and different problem.

3. Submatrix Elements and CFP without Particle Counting. — The sum-rule expansion is, \([5]\),

\[
(F : X^{(3)} : T) = (-)^T \langle T | F^{(3)} \rangle \sum (F^{(3)} | F^{(2)} \gamma' : F^{(2)} \gamma : T) \times \langle F^{(2)} : a^{(2)} : F^{(2)} \rangle (F^{(3)} : a^{(2)} : T).
\]

If \(T\) equal zero, and with \(a^{(3)}\) antithermitean

\[
\sum (F^{(3)} | F^{(2)} : a^{(2)} : F) = \{F\}.
\]

Number-free cfp are found upon normalizing and taking medium forms. There are two connections of particular interest, that with the adjoint and with the complement \([6]\). Since submatrix elements of \(a^{(3)}\) are sometimes such that the adjoint and complement are the same (\(F\) and \(F'\) are complements), a condition exists on the phases. These elements may be written \((QSL : \langle \gamma | : SQL\rangle\). The simplest plausible phase exponent is \(\gamma + 1\), recalling the study of particle-hole conjugation in R II. This formula can lead to a curious result in the \(p\)-shell as noted in Section 5. Indeed it may well prove too simple in other cases.

Complementarity can be studied by finding a universal QSS cfp from results given in R IV. This remark serves but to point out that certain submatrix elements can be factored in two or more parts. There is no quasispin cfp or spin cfp in this analysis, simply a QSS submatrix element which will exhibit the evident symmetry to its adjoint or complement.

It is helpful to have a standard ordering of terms. To that end, Hund’s rules can be extended to quasispin. With the expression \(\langle Q \rangle - \langle S \rangle\) as guide, the highest term in a shell, the \(1^2S\) or \(1^4I+1^2S\), is least negative and the deepest is its complement, \(1^6I+1^2S\), clearly. For assignment of free phases, one proceeds from the top, setting out a tree to encompass the terms of positive weights, \(Q > S\). For the \(p\)-shell this merely proceeds from \(4^3S\) to \(3^5P\) to \(2^3D\), for there is no complication in \(L\)-values in this simple instance. The matrix elements of \(a^{(3)}\) are sufficient for the terms of a halfshell, but other operators, compounded from a number of \(a^{(2)}\), are useful. The extreme and thus very simple one couples the highest and the deepest term. Indeed it should couple any term with (maximum)

\[
Q + S = l + \frac{1}{2}
\]

to its complement. The \(2^1S\) occurs for \(l \neq 1\) and will not be coupled to its complement by \(a^{(2)}\), except \(l = 0\). Evidently three such operations are required to proceed from \(2^3S\) to \(2^1S\) if \(l = 2\). Further elaboration evidently occurs for \(l = 3\).

After having sketched out a set of operators for wave functions within a halfshell, to be limited to products of not more than \(l\) quasispin operators, it may finally be noted that there must exist connections between the matrix elements of the nature of Redmond’s formula \([5, 6]\) for each subset of these operators designated by a rank in each of the three spaces.

4. Representations of Wave Functions. — The vertex coefficients which comprise \(jm\)-coefficients \([4]\) and submatrix elements as noted above, and the \(j\)-coefficients which are integrals and sums over these, and must appear upon expansion of any wave function so represented, are not all generally available at this writing. They are known for expansions in dendrites of the simplest sort, which are analogous to customary parentage expansions.

The occurrence of quasispin operators within the representation of a wave function is a facet of the quasispin formalism, which essentially deals with matrix elements of such operators. The existence of a number-free representation is limited, with allowance for complementarity, by the seniority numbers which can be extracted at any stage. There is no other comparable number-free method for orbitals within equivalence sets.
It is evident that seniority and quasispin are the same, for a single shell. Clearly operators must appear in analysis of wave functions or the structure be artificial, if the seniority scheme is retained. The other possibilities are to be content with a treatment of \( S, L \), or \( J \) alone, or go on to quasiparticles. In any case there is no number free treatment in the present sense. The advantage of such a treatment is in its unity and simplicity, for the number of independent elements in a shell is rather few. Of course these submatrix elements should be factored, though first the properties of the separate operators must be reconsidered.

In the previous section and in the one to follow, there is discussion of submatrix elements and their phases. It is possible to take a different line into these structures and ask about phases in the representations of the wave functions themselves. The present position is that a representation is essentially a graph, descriptive of a coupling situation, and here these are taken as the cubic graphs of \( SU_2 \). The process of attachment, or of operating upon one representation to yield another, is essentially cubic (or trivalent) and the simplest of formats are lineal trees, in which a number of operations are taken in order upon an initial, \( i \), with a resultant final, \( f \), and a number of intermediates, \( m \), conformable to the number of these operations. It is these treeform structures which can be formalized to provide phases for individual wave functions within a shell, without reference to particular \( z \)-components in the spaces involved.

In all these operational graphs, in which the operators are compounds of the quasispin operators, \( a_{ij} \) antisymmetrization is imposed. The vertex coefficients take care of the coupling, of course, and also renormalize as required within the given shell. It is in this way that the occurrence of parentage coefficients as vertex coefficients is first seen.

The expansion techniques of Jucys et al. [4] are essential to these methods. Upon expanding a more complicated representation, possibly polygonal in format, into treeform graphs or dendrites, it is quickly noted that several modes are possible, in general. The mode of expansion must be indicated. The complete representation thus provides the format, the assigned quantum numbers for the various momenta and operators, and the mode of expansion. Questions remain on normalization. In every case a construction-operator graph may be replaced by a number of unsymmetrized graphs.

The limitations of principal-parent wave functions have been discussed, as in [3]. These must in some degree characterize all graphical methods, as here considered. Interesting results can be obtained, however. The use of construction operators was forced by adoption of the QSL scheme. But these operators have advantages in the general case, in the properties of their submatrix elements.

5. Submatrix Elements in the \( p \)-Shell. — Since \( Q \) and \( S \) here suffice for the elements in \( a_{ij} \), except for a phase, the study of the \( p \)-shell is largely of phases. The magnitudes in Table I are according to the writer [5]; the phases have been built up with a view to the work of Racah, particularly in R IV, where there is a prescription for \( l = 3 \) that can be applied to \( l = 1 \) directly.

Now this application can lead to a phase change in terms with \( r = 3 \), the \( ^{14}S \) and \( ^{12}D \). The phases of their complements, \( ^{41}S \) and \( ^{21}D \), might have been changed instead, but one would avoid such a change in the \(^{1}S\), perhaps as a matter of taste. When this version of the CFP phases is combined with the phases given in [5], the results must follow the rules for taking the adjoint and the complement in the submatrix elements. There are also a few phases, three of them in the \( p \)-shell, which are chosen to conform to those found in R III. That is the program in outline. But there is little to be found on the complementarity phase. In any event it does not involve \( L, L' \) [6]. There are certain matrix elements, however, which have the same adjoint as complement. For the present, take the phase exponent \( \gamma + 1 + \Gamma - \Gamma' \) for the adjoint and delete \( \Gamma \) and \( \Gamma' \) for the complement. This goes.

| \( \Gamma \) | \( \Gamma' \) | \( (\Gamma | \gamma | \Gamma') \) |
|---|---|---|
| 1. \( ^{32}p \) | \( ^{41}S \) | \(-1/\sqrt{3}\) |
| 2. \( ^{41}S \) | \( ^{32}p \) | \(-1/\sqrt{5}\) |
| 3. \( ^{21}D \) | \( ^{32}p \) | \(+1/\sqrt{6}\) |
| 4. \( ^{23}p \) | \( ^{32}p \) | \(+1/\sqrt{3}\) |
| 5. \( ^{32}p \) | \( ^{21}D \) | \(-1/\sqrt{6}\) |
| 6. \( ^{12}D \) | \( ^{21}D \) | \(+\sqrt{3}/\sqrt{10}\) |
| 7. \( ^{21}D \) | \( ^{12}D \) | \(-\sqrt{3}/\sqrt{10}\) |

Table I

p-Shell Submatrix Elements
well in the p-shell, for the simplest of operators, \( a^\dagger \). It may not survive severer tests. A phase exponent \( \gamma + 1 \) is indeed familiar, in particle-hole conjugation.

It was already noted that three phases would be assigned in the p-shell. These are that of

\[ (12^p : 41^S) (-) \]

the \( (21^D : 32^P) (+) \), and the \( (23^P : 32^P) (+) \). There is another, indeed two more, which come under question. They are of the \( (14^S : 41^S) \), which is not coupled by \( \gamma \) and so falls outside the present view, and

\[ (12^D : \gamma : 21^D) \].

These phases appear dependent upon those already set. It is plausible to make the second of them \( (+) \). A close accord so is found with those of R III.

The consequence of these tentative is that only one phase from the p-shell as given in R III, that of the \( 14^S \), need be changed to attain conformity. Adoption of a complementarity phase in Q and S, to resemble that of R IV(53), for example, seems not to lead to any closer or better result.

The emergence of complementarity, already noted in R IV, has cut in half the number of "new" terms in a shell, as can be seen in Table I, in which the last six elements are entered only for emphasis. Note that the entries have been folded back to show complements side by side. There are here three new terms: \( 41^S, 33^P, \) and \( 21^D \). According to the definition no new term is found in any half-filled shell, \( N = \lfloor \rfloor \), though there are some in each of the other sets of a halfshell.

6. Conclusions. — It is hoped these innovations will assist in the formalities of shell structure. Graph theory seems so to lie near the origins of the model that the most flexible development of vertex coefficients must be needed. It seems just possible that a construction-operator method can serve to analyze purely orbital (angular) wave functions in any \( l \)-shell. For the impression persists that restriction to homogeneity over spin and orbital spaces too severely confines these applications.

References


