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Reduction of angular momentum expressions by matrix arithmetic

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Abstract. In perturbation calculations using basis states defined in terms of spherically symmetric potentials it is often necessary to simplify complicated expressions involving n - j symbols. A well known graphical technique can be used to aid in this process. We represent the graphs by their incidence matrices, so that the algebraic manipulations can be carried out by matrix arithmetic. It is shown that the sequence of operations required to simplify a given graph can be determined from structural considerations based on the properties of certain polynomials in the adjacency matrix. This provides a method of performing complete perturbation calculations of this type on a computer.

1. Introduction

The work of Yutsis[§] *et al* (1962) put graphical methods for carrying out angular momentum calculations on a rigorous basis. Their techniques have an advantage over the algebraic manipulations they represent in that they give a visual impression of the moves necessary to simplify a complicated expression. There is also a simple expression of the relationship between angular momentum expressions and the corresponding Feynman diagram forms of terms in the perturbation series (Judd 1967).

Recent expositions of this theory (notably those of Brink and Satchler 1968, and Sandars 1969) have established some generalizations as well as defining a fairly standard notation for angular momentum diagrams and making the theory more easily understood. We shall assume the reader to be familiar with this work.

One disadvantage of graphical manipulations is that they can become confusing in cases when the graphs are large, as in the case of higher order perturbation contributions. The purpose of this article is to show that in situations of this kind some standard techniques of mathematical graph theory can be used to reduce graphical manipulations to arithmetical manipulations of matrices.

In § 1 we describe the representation of angular momentum graphs by their incidence matrices. The rules for manipulating incidence matrices are given in § 2 and § 3. We then present in § 4 an algorithm for computer control of the process of reducing a complicated angular momentum expression to a sum of products of 6 - j symbols. An example is given in § 5.

[§] Although this name is more properly spelt 'Jucys', we shall adhere to the spelling used in our reference.

2. Representation of angular momentum graphs by incidence matrices

The main difference between angular momentum graphs and the graphs studied by mathematicians is that the latter are always *closed*, in the sense that every edge joins two vertices, while the former may be *open*, so that the ends of some edges do not end at vertices. Nevertheless, the incidence matrix, which merely tabulates the edges incident at each vertex, allows us to represent edges which are incident at a single vertex. For example, figure 1(a) is represented by the incidence matrix:

<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>	<i>e</i>	<i>f</i>
1	.	.	1	1	.
.	.	1	.	1	1
.	1	.	1	.	1

(2.1)

We have not labelled the vertices (corresponding to the rows of the matrix) because they are not distinguished in angular momentum diagrams, although the edges correspond to specific angular momentum values.

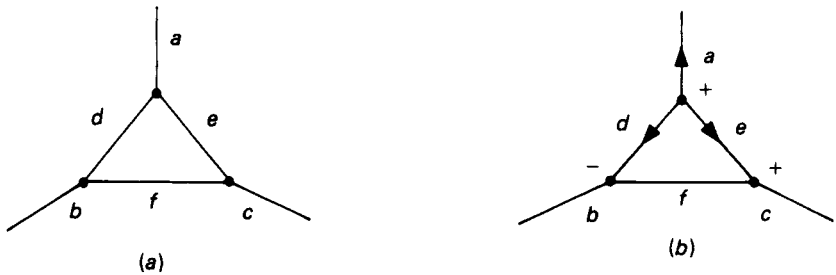


Figure 1.

One consequence of representing open edges in incidence matrices is that directed edges (arcs) can no longer be indicated in the usual way by writing -1 for one end and 1 for the other. Figure 1(b), containing some directed edges, will be represented (for example) by

α	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>	<i>e</i>	<i>f</i>
+	$-i$.	.	$-i$	1	.
+	.	.	1	.	i	1
+	.	1	.	1	.	1

(2.2)

where $\pm i$ is used to denote the insertion of arrows, $-i$ for arrows pointing out and $+i$ for arrows pointing in. In this matrix we have also indicated the 'parity' of the nodes in the left-hand column of the matrix. This symbol is used in the diagrams to distinguish between an anticlockwise (+) and clockwise ($-$) ordering of the 3 edges incident at a vertex. This ordering of edges is specified by a linear ordering in the matrix and (for convenience) has been changed relative to figure 1(b) at one vertex.

The position occupied by α in (2.2) can be used for overall multiplying factors, which are a problem in graphical notation. No method of treating these factors has been standardized. Brink and Satchler (1968) include them explicitly, while Sandars (1969) indicates such factors by carets, so that \hat{j} is used to show that a factor $\sqrt{2j+1}$ is implied. When the angular momentum values a, b, c , etc are known numerically such factors can be included in α .

It is also possible to include numerical factors in α when a, b, c etc are not known numerically. In this case each distinct angular momentum value (j) can be represented by a prime number (p_j). The inclusion of a factor p_j in α can then be used to represent the overall factor $\sqrt{2j+1}$. Negative primes can be used to indicate summation over all angular momenta obeying the triangle rules. Phases can be accommodated by suitable insertion of directed edges, the rearrangement of columns and the use of parity signs in the left-hand column.

3. Rules of manipulation expressed in terms of incidence matrices

Angular momentum diagrams may be modified by a series of rules which leave their value unchanged, but allow them to be simplified or be expressed in terms of tabulated functions enabling their evaluation. These rules form the core of the work of Yutsis *et al* (1962), and we now seek to re-express them in terms of incidence matrices.

We first consider the rules for *phase manipulations*, which do not alter the form of a graph, but which may introduce or remove arrows, change their direction or change vertex phases. As mentioned previously, a change of vertex phase, associated with a factor $(-1)^{j_1+j_2+j_3}$, where j_1, j_2 and j_3 correspond to edges incident at the vertex, is equivalent to a change in the cyclic order of the labels j_1, j_2, j_3 in the matrix. The introduction of an arrow into a graph, pointing out from a vertex, changes the sign of the m value associated with the line and introduces a phase factor $(-1)^{j+m}$ (see Sandars 1969 for examples of these manipulations). Arrows may be introduced into all lines pointing into, or pointing out of, a given vertex without changing the value of a graph. The corresponding equalities for a 3- j symbol† are given below:

$$\begin{array}{l}
 \boxed{\begin{array}{ccc} & j_1 & j_2 & j_3 \\ + & 1 & 1 & 1 \end{array}} = \boxed{\begin{array}{ccc} & j_1 & j_3 & j_2 \\ - & 1 & 1 & 1 \end{array}} \quad \text{(change in order of } j\text{'s)} \\
 \\
 = \boxed{\begin{array}{ccc} & j_1 & j_2 & j_3 \\ + & i & i & i \end{array}} \quad \text{(arrows inserted pointing in)} \\
 \\
 = \boxed{\begin{array}{ccc} & j_1 & j_2 & j_3 \\ + & -i & -i & -i \end{array}} \quad \text{(arrows inserted pointing out).}
 \end{array}$$

† This symbol is also sometimes referred to as the 3- jm symbol in order to establish a general nomenclature (Yutsis *et al* 1962).

Arrows pointing in opposite directions on an edge (j) cancel out, and two pointing in the same direction reduce to a factor $(-1)^{2j}$, so that the following single edge subgraphs are equivalent:

$$\begin{array}{|c|c|} \hline 1 & j_n \\ \hline + & i \\ \hline + & -i \\ \hline \end{array} = \begin{array}{|c|c|} \hline 1 & j_n \\ \hline + & 1 \\ \hline + & 1 \\ \hline \end{array} = \begin{array}{|c|c|} \hline (-1)^{2j_n} & j_n \\ \hline + & i \\ \hline + & i \\ \hline \end{array} .$$

The orthogonality theorems for the 3- j symbols allow us to modify graphs in two ways as indicated by the equalities below (which correspond to figures 2(a) and (b)):

$$\begin{array}{|c|c|c|} \hline 1 & a & b \\ \hline \mu & 1 & \\ \hline \nu & & 1 \\ \hline \kappa & & 1 \\ \hline \tau & 1 & \\ \hline \end{array} = \begin{array}{|c|c|c|c|c|c|} \hline [c] & a & b & (-c) & b & a \\ \hline \mu & 1 & & & & \\ \hline \nu & & 1 & & & \\ \hline \kappa & & & & 1 & \\ \hline \tau & & & & & 1 \\ \hline + & 1 & 1 & 1 & & \\ \hline + & & & 1 & 1 & 1 \\ \hline \end{array} \quad \text{ORTH 1}$$

The minus sign in the top row indicates that the angular momentum c is summed over all possible values. The factor $[c] = 2c + 1$, in the conventional notation. Following the *prime number convention* previously described, $[c]$ would be replaced by the square of the prime representing c :

$$\begin{array}{|c|c|c|c|c|} \hline 1 & a & b & c & c \\ \hline \mu & & & 1 & \\ \hline \nu & & & & 1 \\ \hline + & 1 & 1 & 1 & \\ \hline + & 1 & 1 & & 1 \\ \hline \end{array} = \begin{array}{|c|c|} \hline [c]^{-1} & c \\ \hline \mu & 1 \\ \hline \nu & 1 \\ \hline \end{array} . \quad \text{ORTH 2}$$

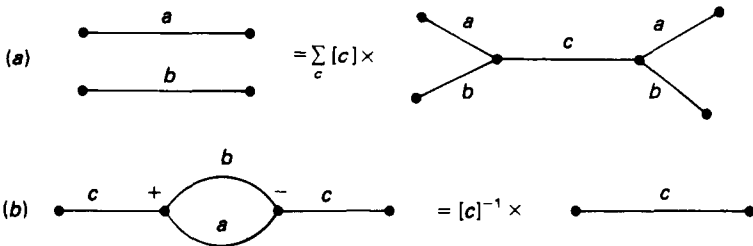


Figure 2.

The following rules have been denoted YLV1, YLV2 and YLV3 by Sandars (1969) (see figures 3(a, b and c) respectively). They are the basic rules necessary for separating graphs which are connected only on one, two or three edges. Graphs with higher connectivity may need to be treated using ORTH 1 to reduce connectivity to three. It

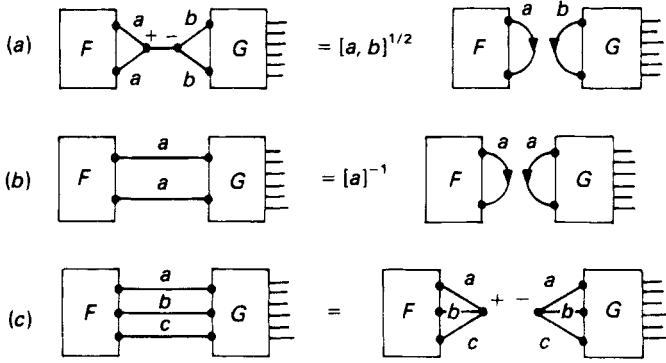


Figure 3.

should be remembered that these rules are only appropriate for separating off closed graphs; they cannot be used to divide open graphs into two open parts. In each case we include a minimal number of extra vertices to make the rule clear. By convention the section of the graph labelled *G* contains all the open edges.

$ \begin{array}{c} \begin{array}{cccccc} & 1 & a & a & j & b & b \\ F & \left[\begin{array}{cc} \mu & 1 \\ \nu & 1 \end{array} \right. \\ & + & 1 & 1 & 1 & & \\ & + & & & 1 & 1 & 1 \\ G & \left[\begin{array}{cc} \kappa & 1 \\ \tau & 1 \end{array} \right. \end{array} \end{array} $	=	$ \begin{array}{c} \begin{array}{ccc} & [a, b]^{-1/2} & a & b \\ F & \left[\begin{array}{cc} \mu & 1 \\ \nu & i \end{array} \right. \\ G & \left[\begin{array}{cc} \kappa & 1 \\ \tau & i \end{array} \right. \end{array} \end{array} $	YLV1
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$ \begin{array}{c} \begin{array}{ccc} & 1 & a & a \\ F & \left[\begin{array}{cc} \mu & 1 \\ \nu & 1 \end{array} \right. \\ G & \left[\begin{array}{cc} \kappa & 1 \\ \tau & 1 \end{array} \right. \end{array} \end{array} $	=	$ \begin{array}{c} \begin{array}{ccc} & [a]^{-1} & a & a \\ F & \left[\begin{array}{cc} \mu & 1 \\ \nu & i \end{array} \right. \\ G & \left[\begin{array}{cc} \kappa & 1 \\ \tau & i \end{array} \right. \end{array} \end{array} $	YLV2
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Similar matrices to those on the left-hand side, where the equalities in angular momentum values implied by the repetition of *a* and *b* are not satisfied, are identically zero.

themselves. Fold backs provide the only possibility of repeating given edges, for we do not investigate the n -edge paths until all cycles of n -edges and less have been eliminated.

The path structure of a graph can be visualized most easily by constructing a truncated 'path tree'. This is determined by choosing an arbitrary origin vertex and then letting each possible fold-free path (up to a predetermined number of edges) end at a distinct vertex in the tree. The path tree for a given graph is unique (but infinite), even though the finite subgraphs produced by truncation are labelled in different ways. An example of such a tree (truncated after 3 edges) is shown in figure 4 for the graph in figure 5. Note that the path tree will reproduce some vertices and edges of the original graph many times. Nevertheless, a fold-free path on the tree always corresponds to a fold-free path on the original tree, so long as the path-graph is truncated at $(n - 1)$ for a graph with n -edge cycles.

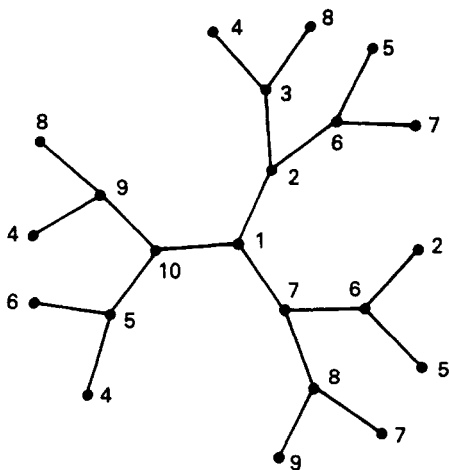


Figure 4.

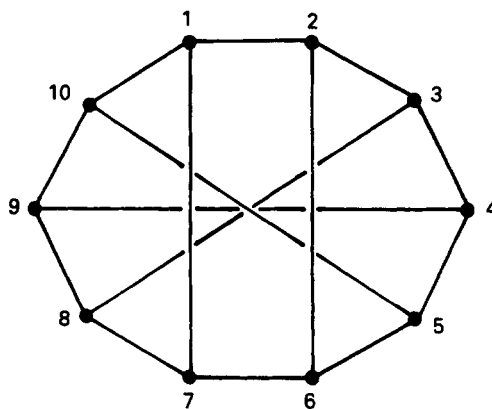


Figure 5.

The polynomials P_n for small values of n are easily determined by inspection of the path tree:

$$P_1 = A$$

$$P_2 = A^2 - 3I,$$

where $3I$ corresponds to the paths of A^2 where a single edge is repeated.

$$P_3 = A^3 - 5A$$

as there are just 5 ways of moving one step in a path containing 3 edges.

Higher degree polynomials are difficult to derive in this way, but may be obtained from the following recurrence relation†:

$$P_{n+1} = AP_n - 2P_{n-1}. \tag{4.1}$$

† See Biggs (1971, p 79), where the corresponding relation for a general k -valent graph is given. Biggs refers to fold-free paths as *proper* paths.

Proof. Consider a typical vertex n edges away from the origin vertex (see figures 4 and 6). The n -edge fold-free path from the origin vertex to this vertex is represented by an

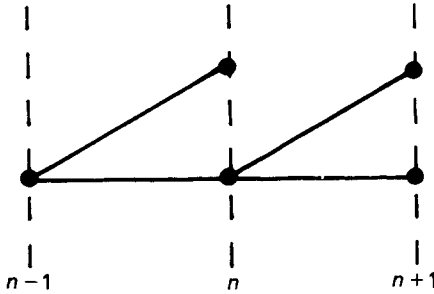


Figure 6.

entry in \mathbf{P}_n . The expression $\mathbf{A}\mathbf{P}_n = \mathbf{P}_n\mathbf{A}$ has entries for all the paths obtained by adding one more edge to those in \mathbf{P}_n . Hence it contains all the paths in \mathbf{P}_{n+1} as well as paths in \mathbf{P}_{n-1} due to folded back $(n + 1)$ -edge paths. Each $(n - 1)$ -edge fold-free path can be obtained from just two initial n th vertices by folding back a single edge. Hence

$$\mathbf{A}\mathbf{P}_n = \mathbf{P}_{n+1} + 2\mathbf{P}_{n-1},$$

which is a rearrangement of the formula given above.

Successive application of this formula gives

$$\mathbf{P}_4 = \mathbf{A}^4 - 7\mathbf{A}^2 + 6\mathbf{I}$$

$$\mathbf{P}_5 = \mathbf{A}^5 - 9\mathbf{A}^3 + 16\mathbf{A}$$

$$\mathbf{P}_6 = \mathbf{A}^6 - 11\mathbf{A}^4 + 30\mathbf{A}^2 - 12\mathbf{I}$$

and higher degree expressions which can readily be generated from equation (4.1) as required by the computer.

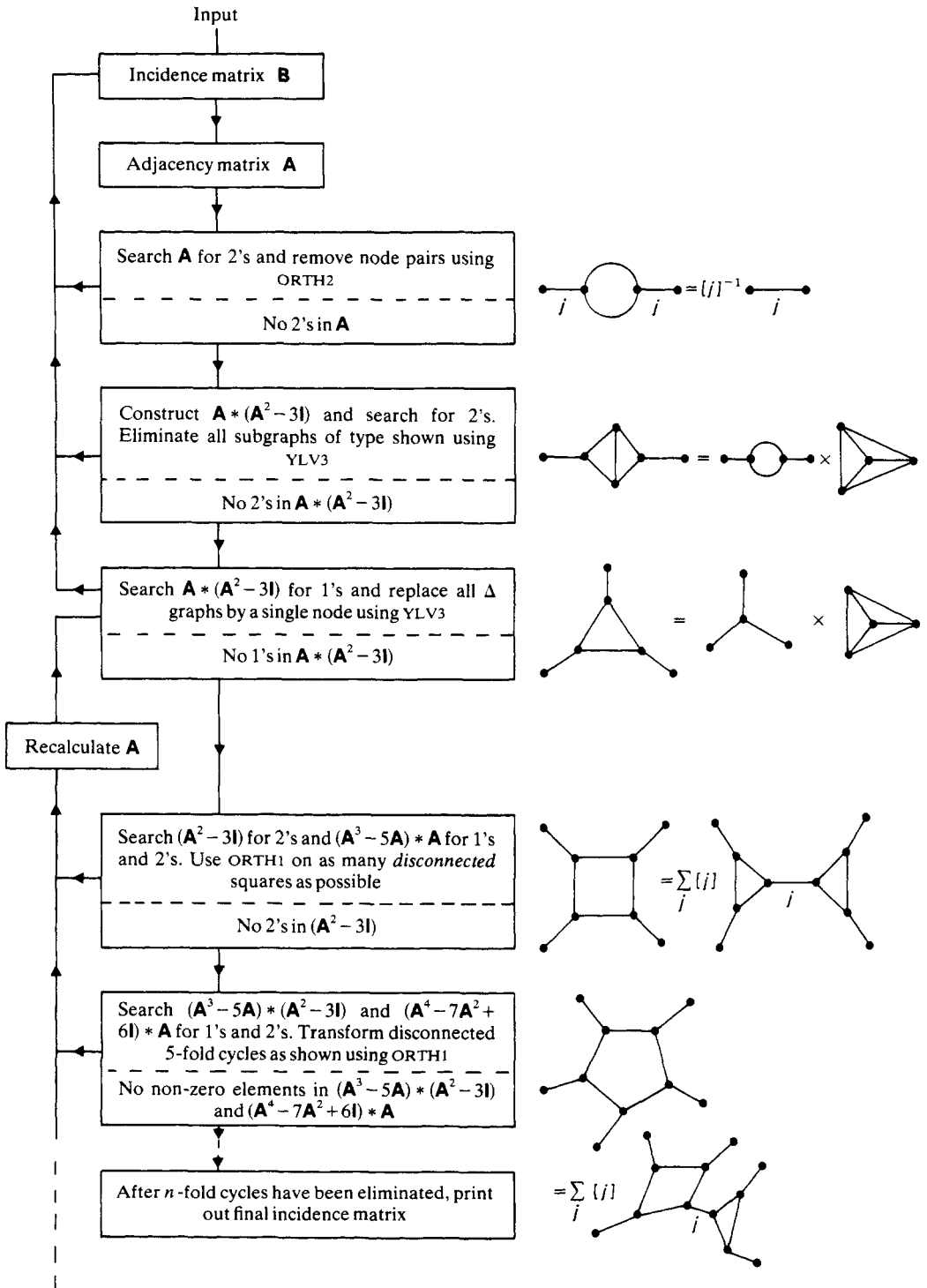
In many evaluations, we begin with an open graph, so that the reduction may be separated into two parts:

(a) All open edges are removed to form the simplest possible open graph which corresponds to the effective operator for the process being calculated.

(b) The remaining complex closed graph is then systematically reduced to sums of products of $6-j$ symbols (corresponding to K_4 graphs) for evaluation using either tabulated values or a subroutine.

For the first step it is only necessary to identify the open edges of the graph using the incidence matrix, and then to use ORTH 1 and YLV3 repeatedly until complete separation occurs. There may be some preference for a given form for the final open graph, so that it corresponds to a standard form of the effective operator.

Reduction (b) requires a systematic method of separating off $6-j$ symbols, without the introduction of more summations than necessary. An algorithm for this process is outlined below. Its main characteristic is the use of the polynomials \mathbf{P}_n in the adjacency matrix to recognize features of the graph, allowing the appropriate arithmetical operations to be carried out on the incidence matrix.



$$\mathbf{P}_2 = \begin{array}{cccccccc|c}
 . & . & 1 & . & 1 & 2 & . & 1 & 1 & . & 1 \\
 . & . & . & 1 & 1 & . & 2 & 1 & . & 1 & 2 \\
 1 & . & . & . & 1 & 1 & 1 & . & 2 & . & 3 \\
 . & 1 & . & . & . & 1 & . & 2 & . & 2 & 4 \\
 1 & 1 & 1 & . & . & . & 1 & . & 2 & . & 5 \\
 2 & . & 1 & 1 & . & . & . & 1 & . & 1 & 6 \\
 . & 2 & 1 & . & 1 & . & . & . & 1 & 1 & 7 \\
 1 & 1 & . & 2 & . & 1 & . & . & . & 1 & 8 \\
 1 & . & 2 & . & 2 & . & 1 & . & . & . & 9 \\
 . & 1 & . & 2 & . & 1 & 1 & 1 & . & . & 10
 \end{array}$$

and

$$\mathbf{P}_3 * \mathbf{A} = \begin{array}{cccccccc|c}
 . & 1 & . & . & . & . & 1 & . & . & . & 1 \\
 1 & . & . & . & . & . & 1 & . & . & . & 2 \\
 . & . & . & 1 & . & . & . & 1 & . & . & 3 \\
 . & . & 1 & . & 1 & . & . & . & 2 & . & 4 \\
 . & . & . & 1 & . & . & . & . & . & 1 & 5 \\
 . & 1 & . & . & . & . & 1 & . & . & . & 6 \\
 1 & . & . & . & . & . & 1 & . & . & . & 7 \\
 . & . & 1 & . & . & . & . & . & 1 & . & 8 \\
 . & . & . & 2 & . & . & . & 1 & . & 1 & 9 \\
 . & . & . & . & 1 & . & . & . & 1 & . & 10
 \end{array}$$

The absence of 3-edge cycles is shown by the fact that $\mathbf{A} * \mathbf{P}_2 = 0$. \mathbf{P}_2 identifies opposite corners in 4-edge cycles by its '2' entries. In cases where there are two '2' entries in a row, the vertex corresponding to that row must lie at the junction of two 4-edge cycles. Nevertheless, it is not straightforward to identify the sets of vertices in each cycle from a consideration of \mathbf{P}_2 . This information is given directly by the expression $\mathbf{P}_3 * \mathbf{A}$, which tells us which pairs of vertices are joined by both a 3-edge path and a 1-edge path. The '2' entries in $\mathbf{P}_3 * \mathbf{A}$ identify pairs of vertices which are linked by two alternative 3-edge paths and a single 1-edge path. It is thus straightforward to identify the subgraphs shown in figure 7.

By applying ORTH 1 and YLV3 to these diagrams it is possible to get several expressions for the 15- j symbol in terms of n - j symbols with $n \leq 12$. For example, the process shown in figure 8 gives the result quoted by Yutsis *et al* (1962, equation (20.6)), where the open subgraph in the final expression is part of a 9- j symbol (with 6 vertices). The computational technique described in the previous section could easily be adapted to search automatically for algebraic relations of this type.

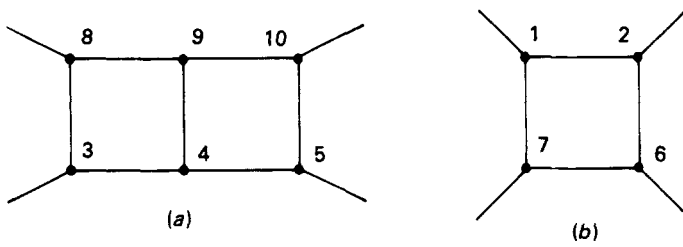


Figure 7.

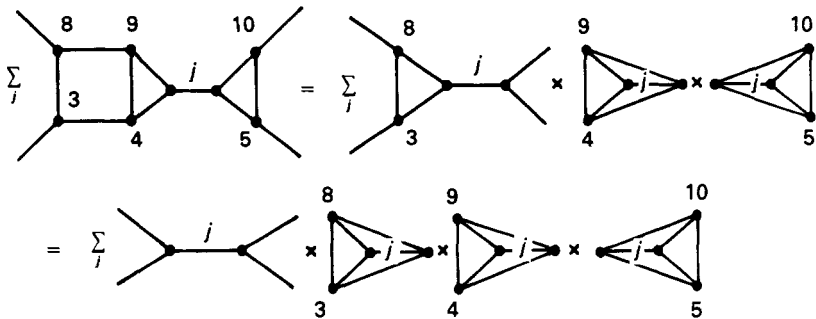


Figure 8.

6. Conclusion

We have demonstrated the existence of a simple one-to-one correspondence between the manipulations of angular momentum graphs and manipulations with their incidence matrices. In addition, polynomials of the adjacency matrix have been defined which provide a technique for controlling a computer program aimed at carrying out specific processes, such as the evaluation of complex expressions.

Rosensteel *et al* (1975) have discussed the characterization, generation and counting of *n*th single-particle Green function graphs using the properties of permutation groups. We shall demonstrate, in a later publication, that their procedures can be generalized to graphs representing *n*-particle operators. If we then make use of the fact that the angular momentum graphs are isomorphic to the corresponding Feynman diagrams (Judd 1967), the methods outlined in this paper provide a means of calculating perturbation contributions on a computer, without the need to perform a separate algebraic analysis of angle-dependent factors.

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