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1976 J. Phys. A: Math. Gen. 9 1999

(http://iopscience.iop.org/0305-4470/9/12/007)

J. Phys. A: Math. Gen., Vol. 9, No. 12, 1976. Printed in Great Britain. © 1976

A diagram technique for basis functions and their transformation, with application to group–subgroup bases and crystal tensors

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Received 2 June 1976, in final form 4 August 1976

Abstract. We develop graphical techniques in the case that the labels on legs (or edges) span a representation of a compact group. This generalizes previous work, in which the labels had to be irreducible representation labels, to cover many matrices or reducible tensors arising in theoretical physics. Diagrams corresponding to tensors are defined so that basis transformations, such as group operations or parity interchange, may be performed by standard graphical operations. Bipartite diagrams play a central role in the theory. The Jucys diagrammatic reduction theorems may be generalized so as to cover reducible tensors. As one example, we discuss group–subgroup bases, developing graphical representations for the Racah factorization lemma and isoscalar factors. As another example, we give a graphical approach to group-theoretic restrictions on the elements of crystal tensors, and discuss some illustrative problems.

1. Introduction

Lagrange boasted that his *Mécanique Analytique* did not contain a single diagram (Ziman 1960, preface). The opposite extreme is equally possible: one may develop physical theory using graphical operations to the exclusion of algebraic equations. The ubiquitous Feynman diagram and graphical techniques in angular momentum theory are adequate illustrations. They have obvious value in conciseness, structural clarity and as a mnemonic and book-keeping aid; this is enhanced by depolymerization theorems which permit the replacement of a diagram by a simpler structure. For Feynman diagrams, factorization (or indeed any associative combination rule) of separate diagrams or of their component parts leads to such important results as the linked cluster theorem, the Dyson equation, the Bethe–Salpeter equation (Mattuck 1967). In group theory a set of graphical reduction theorems exist which cover the theorems conventionally known as the great orthogonality theorem, Schur's lemma, Wigner–Eckart theorem, etc (Stedman 1975, to be referred to as I)†. These reduction theorems have been used extensively in discussing complicated problems in Jahn–Teller systems (Stedman 1976).

We develop a generalization of this group-theoretic example. Consider diagrams in which the set of labels L on any leg represents an invariant space under the operations

† These reduction theorems were enunciated for the case of the rotation group in three dimensions by Jucys and collaborators. They were first published in English under the names of Yutsis, Levinson and Vanagas (1962) and have been referred to subsequently as YLVn by several authors. We shall now refer to the generalized reduction theorems as JLVn in conformity with the original (Lithuanian) spelling of Jucys.

of a compact group G. (That is, L spans a representation of G. This is a much less stringent requirement than that of having irreducible labels, as in I.) We define a standard choice for subdiagrams (§ 3) which permits the Jucys reduction theorems to be generalized to all bipartite networks (§ 6). This allows the standardization of basis transformations, a deeper understanding and unification of many known results, and a general approach to group-theoretic restrictions on elements of physical tensors, such as crystal properties.

A glossary of definitions is provided in appendix 1.

2. General principles of the technique

The interpretation of a diagram is not affected by deformations within the plane that do not change the topology of interconnections or the rotational sequence of connections at a subdiagram.

Legs in a diagram correspond to algebraic labels† (e.g. matrix or tensor suffices, quantum numbers, irreducible group-theoretic labels, spatial coordinates). Different labels require different legs.

Joining legs corresponds to equating labels; labels omitted on internal legs are automatically summed over the relevant complete set. In general it is necessary to ensure the paired suffices have dual properties (e.g. annihilation and creation operators, covariant and contravariant labels) which we shall distinguish by the terms positive and negative parity (§ 3.1).

Two or more different labels may be joined, or one may be terminated, at subdiagrams which represent the tensors or matrices of the theory. The order of labels in the algebraic expression is reproduced in the diagram by working anticlockwise from a conventional point.

It is possible to cast many sections of undergraduate-level theoretical physics completely in diagram notation in accordance with the above principles, particularly where tensors or matrices are used. As an example of the manipulation of unitary matrices, see § 2 of I. A simple use of such techniques in exhibiting recursion relations has recently been given by Stone (1976). For an example in tensor calculus, see Penrose (1971), who lists the properties of the Levi-Civita tensor $\epsilon_{\alpha\beta\gamma}$ in diagram form. There is a striking resemblance between his diagrams and the Jucys reduction theorems, also Clebsch–Gordan orthogonality relations etc. In view of § 6 of this paper the resemblance is certainly not accidental (see appendix 2).

3. Network theorems for invariant, self-conjugate subdiagrams

3.1. *Introduction*

The applicability of the Jucys reduction theorems to a given network is conditional upon an invariance property for all the nodes in the network. Two diagram forms of this

† Alternative mappings are of course possible. By dualizing in the plane, labels could correspond to nodes, as in the projective geometric approach to 6-j symbols (Fano and Racah 1959, Robinson 1970), and one can have more abstract mappings based on simplex theory (Smorodinskii and Shelepin 1972) etc. In these three approaches a 3-j symbol is represented respectively by three lines at a point, three points on a line, and a triangle. We think the first to be more natural and useful to the physicist, as confirmed by the success of Feynman and group coupling diagrams.

invariance property are given in equation (4), and after the latter an algebraic transcription is given. In words, the quantity represented by each node should be unaffected by a simultaneous transformation (appropriate to any group operation) of all the labels on that node. In I, the Jucys reduction theorems were proved for the case of irrep labels on each leg. To extend this to reducible representation labels, we shall introduce the reduction transformation which block diagonalizes the representation into its irreducible components (§ 5). Since this transformation is unique for all group operations, it corresponds to an invariant node in the sense of equation (4). It follows that a subdiagram carrying reducible labels may be represented as a network of invariant nodes, some giving the irreducible parts and others the reduction transformations. At this point the applicability of the JLVn theorems becomes obvious (§ 6).

Since invariance may be defined in one of two senses (equations ($4a, b$)—in our jargon, nodes may have either even or odd parity) it is important to examine the connection between these two types of invariance. An invertible matrix may be defined for any set of labels so as to generate a parity transformation of those labels. It follows that a parity conjugate of a given node may be constructed by applying the appropriate parity transformation to each leg. Alternatively one may define the parity conjugate for a node representing an invertible matrix as the node representing the inverse matrix; it is straightforward to show that either definition produces a node with the opposite invariance property to the original node (e.g. theorem 1). We prove in § 3.3 that these two definitions of parity-conjugate nodes can be made to coincide for a certain class of nodes. We term these nodes self-conjugate. The theorems of § 3.3 give sufficient (though perhaps not necessary) conditions for a node to be self-conjugate. Roughly speaking (there may be exceptions) a unitary matrix element may be represented by a self-conjugate node. Our theorems cover the case of certain non-unitary matrices as well. Our prototype for an invariant, self-conjugate node is the 3-jm symbol, and that for a parity transformation, is the 2-jm symbol (cf I).

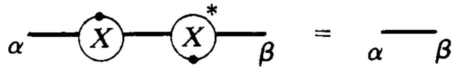
The proof that a 3-jm node is self-conjugate has previously been known as the Derome–Sharp lemma (Butler 1975); theorems 4 and 5 were obtained by generalizing the proof of this lemma. The concepts of parity transformation matrices and of self-conjugate nodes generalize and unify the discussion of particular cases by other authors (§ 5). For example, requiring the reduction transformation node (mentioned above) to be self-conjugate is equivalent, by theorem 5, to an appropriate definition of the parity transformation of a repetition index (§ 5). This generalizes the definitions given in the literature for special cases (e.g. a multiplicity index).

Much of the ambiguity in graphical construction can be avoided by explicit recognition of the parity of the component nodes, and insisting on a bipartite construction (in which each leg joins nodes of opposite parity). This restriction eliminates the sort of problem, familiar in the algebraic formalism, as to whether one should pre- or post-multiply a matrix by its transformation matrix, for example. From the viewpoint of § 6, our generalization of the Derome–Sharp lemma simplifies the definition of the reduced matrix elements associated with the Jucys reduction theorems.

The parity transformation may correspond to an asymmetric matrix; if so, its graphical representation must violate reflection symmetry. Both arrows and stubs have been used (cf I); we shall use stubs.

3.2. Basic definitions and theorems

Consider a diagram X which represents an invertible (i.e. square and non-singular) matrix; it may be a network composed of similar diagrams Z, which we denote by $X=\{Z\}$. We define the *adjoint* diagram X^* as that representing the transpose of the inverse matrix. Thus



(1)

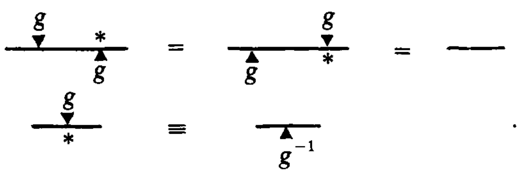
i.e. $\Sigma_\gamma X_{\alpha\gamma}X^*_{\beta\gamma}=\delta_{\alpha\beta}$. In the special case of unitary matrices, the asterisk therefore represents complex conjugation, as in I.

We take this definition of adjoint diagrams to apply to diagrams of degree greater than two when it is possible to identify an invertible matrix by suitable combinations of labels. For example, a 3-*jm* node has four legs corresponding to three sets of irreducible representation labels $\{\lambda_i l_i\}$, $i=1, 2, 3$ (l_i = component of irrep λ_i); and to a multiplicity index r. On grouping labels in the form $\alpha\equiv(\lambda_1 l_1, \lambda_2 l_2)$, $\beta=(\lambda_3 l_3, r)$ we have an invertible and indeed unitary matrix. If we assume that paired labels are arranged sequentially, starting from the conventional point of origin (cf § 2), this definition of adjoint is unaffected by rotation of the diagram, as required in § 2. For example, equation (1) for a 3-*jm* node has the expanded form

(2)

The adjoint operation is readily shown, from matrix manipulation, to obey $(X^*)^*=X$, and, for those linear networks in which paired labels join the same subdiagrams, $X^*=\{Z^*\}$, i.e. the adjoint of such a network of subdiagrams is the network obtained on replacing each subdiagram by its adjoint. Note that to ensure this result, it is necessary to transpose the inverse matrix in defining the adjoint.

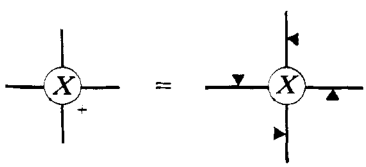
Since the space of labels L is invariant under a compact group G, we may define a *group operation node* as a transformation of labels within L. We denote this by a triangle (cf equation (3) of I), and define its adjoint in accordance with equation (1):



(3)

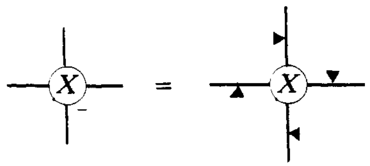
The asterisk does not now necessarily represent complex conjugation since, for general L, a group operation need not be unitary.

We define a *right invariant diagram* X (invariant under G, to be explicit) by the equation (taking a diagram of degree 4 for example):



(4a)

for all g in G, and a left invariant diagram by the same expression, but with a clockwise sense of rotation:



(4b)

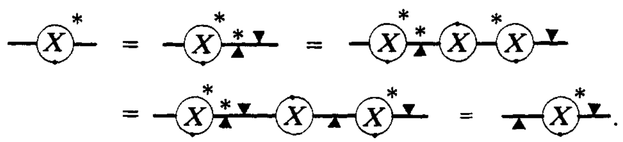
i.e.

$$X_{\alpha\beta\gamma\delta} = (\mathrm{O}_g)_{\alpha'\alpha}(\mathrm{O}_g)_{\beta'\beta}(\mathrm{O}_g)_{\gamma'\gamma}(\mathrm{O}_g)_{\delta'\delta}X_{\alpha'\beta'\gamma'\delta'}.$$

A sign indicating the relevant parity has been added on the left sides.

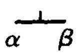
Theorem 1. If a diagram is right (left) invariant then its adjoint as defined by equation (2) is left (right) invariant.

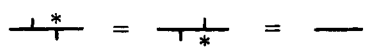
Proof. Suppose X has positive parity and degree 2. Then, using all above equations,



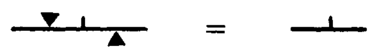
A similar proof may be written out for an X of higher degree.

We suppose that a *parity transformation node* for the labels L may be defined with the following properties. It represents an invertible matrix $\pi_{\alpha\beta}$,

$\pi_{\alpha\beta} \leftrightarrow$  (5)

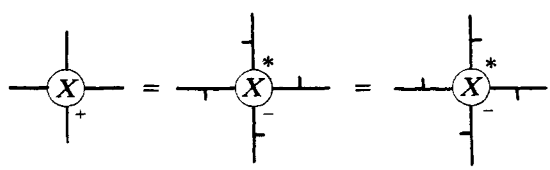
 (6)

which is right invariant:



i.e. $\pi_{\alpha\beta} = (\mathrm{O}_g)_{\alpha\alpha'}(\mathrm{O}_g)_{\beta\beta'}\pi_{\alpha'\beta'}$. To fix ideas, we may identify $\pi_{\alpha\beta}$ as the complex conjugate of the 2-*jm* symbol for irreducible representation labels L (§ 4) or the contravariant metric tensor in relativity (cf appendix 2). As the first example shows, $\pi_{\alpha\beta}$ is not necessarily a symmetric tensor, hence the need for a symbol which is not invariant under reflection.

We define a *right conjugate* diagram as one which obeys both the equations

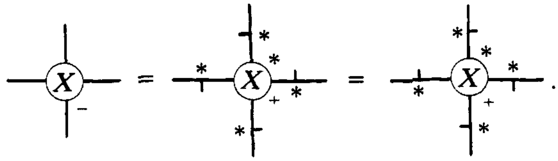


(7a)

e.g.

$$X_{\alpha\beta,\gamma\delta} = \pi_{\alpha\alpha'}\pi_{\beta\beta'}\pi_{\gamma\gamma'}\pi_{\delta\delta'}(X^{-1})_{\gamma'\delta',\alpha'\beta'}$$

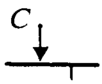
$((X^{-1})_{\gamma'\delta',\alpha'\beta'} = X^*_{\alpha'\beta',\gamma'\delta'})$ and a left conjugate diagram by the equations



(7*b*)

Collectively, such diagrams will be called self-conjugate.

If a diagram is right (left) invariant *and* right (left) conjugate, it will be called a *fundamental* diagram of positive (negative) parity. Two simple examples are the parity transformation itself, and the operation



(8)

where the group element is summed over at least a class C of G. Such diagrams, we suggest, should be our basic building blocks.

Theorem 2. If X is a self-conjugate diagram, X^* is also a self-conjugate diagram of opposite parity.

The proof is trivial; theorems 1 and 2 together imply a similar statement for fundamental diagrams.

Theorem 3. If the closure of a network (by which we mean the diagram obtained on bringing any external legs of a network to a new, common node) is bipartite, and if the network is composed of invariant, self-conjugate or fundamental diagrams, the network is an invariant, self-conjugate or fundamental diagram respectively of appropriate parity.

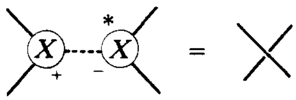
The proof is similar to those in theorems 1 and 2. Theorem 3 may be regarded as a generalization of the basic theorem in § 4.1 of I, itself the foundation of the Jucys reduction theorems. Theorem 3 is amply illustrated in the diagrams of I, of Stedman (1976) and of this paper. An obvious special case of a bipartite diagram is when each subdiagram has negative parity and each leg has a parity transformation node.

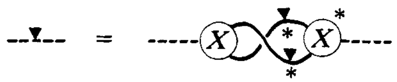
3.3. General theorems for self-conjugate nodes

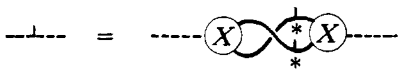
It is recommended that the details of this subsection be skipped at a first reading. We prove that a node representing an invertible matrix may be constructed to be self-conjugate, provided we are free to define the parity transformation on one leg L_1 in an appropriate manner, and provided certain other, relatively unimportant, conditions hold. In theorem 4, the other condition is that L_1 represent *all* the row *or* column labels for the matrix. In theorem 5, the other condition is that L_1 and say L_2 together cover the row *or* column labels, and that L_2 be irrep labels. Other generalizations may be possible but the above will be quite adequate for our purposes.

Theorem 4. If a diagram X of degree n where $n \geqslant 2$ represents an invertible matrix $X_{\alpha\beta}$ on defining labels by $\alpha \equiv L_1, \beta \equiv \{L_2, \ldots, L_n\}$ (L_i represents the labels in the ith leg), and if invertible group and parity operations are defined for $L_2, \ldots, L_n$, then group and parity operations on L_1 which obey equations (3) and (6) within bipartite networks may be constructed so that X is a fundamental diagram of either parity.

Proof. Choose X to be of degree 3 and of positive parity for definiteness. We make the definitions:


(9)


(10)


(11)

and their adjoints by the rule $X^* = \{Z^*\}$ in the above constructions. (Were X chosen to be of negative parity, one would interchange X and X^* in equations (10) and (11).) One may then verify the statements in the theorem by straightforward manipulations. To save space, we exhibit similar manipulations only in theorem 5.

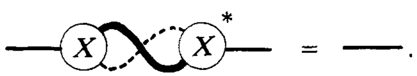
It is necessary to check the compatibility of these constructions with previous assumptions when applying these theorems otherwise, for example, identifying X as a group operator would lead to inconsistency. A simple triangle is not a fundamental node.

Theorem 5. If a diagram X of degree n where $n \geqslant 3$ satisfies the conditions:

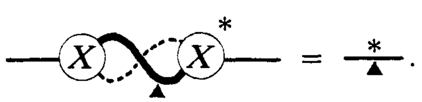
X represents an invertible matrix $X_{\alpha\beta}$ in the labels $\alpha = (L_1, L_2), \beta = (L_3, \ldots, L_n)$;
$L_1 = \{r\}$ where r is unaffected by group operation;
$L_2 = \{\lambda l\}$ where these are irreducible labels for G;
invertible group and parity operations are defined for $L_2, \ldots, L_n$;
X is right (left) invariant;

then a parity transformation on L_2 labels may be constructed so that X is a fundamental diagram of positive (negative) parity.

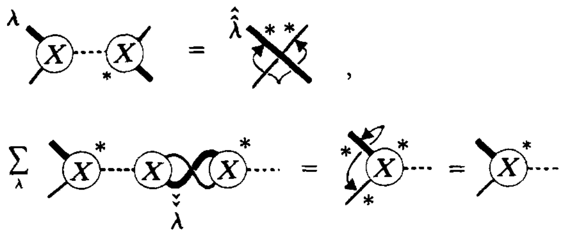
Proof. Let $n = 3$ and X be right invariant for definiteness. Then


(12)

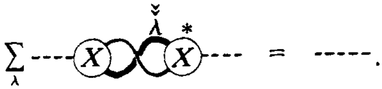
On using equation $(7a)$ for X and equation (3) we have



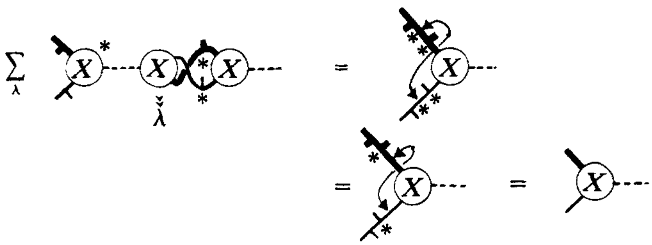
We project out the internal group-theoretic node by introducing another group operation and summing over G, using equation (5) of I($\hat{\hat{\lambda}} = (\hat{\lambda})^2 = (\check{\lambda})^{-1}$ = the dimension of irrep λ):



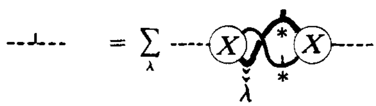
so that, at least for bipartite connections to X, we may make the identification

 (13)

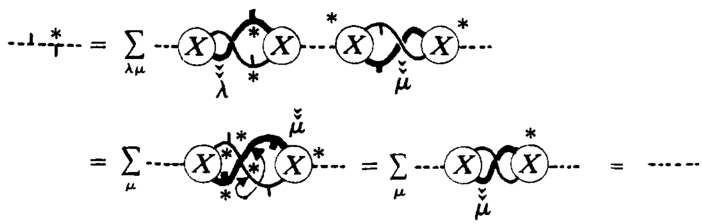
Hence also



so that under the same restriction we may make the identification

 (14)

since from the above equations this guarantees that X is right conjugate (equation (7a)). Finally we verify that the adjoint of this parity transformation obeys the rule $X^* = \{Z^*\}$



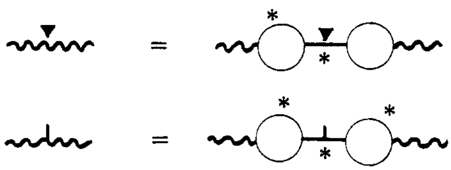
so that equation (7b) holds for X^*.

4. Kets, operators and basis transformations in quantum mechanics

We represent a *ket* $|xL\rangle$ where x represents the parentage labels and L is a set of quantum numbers, by

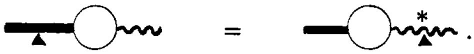
$|xL\rangle \leftrightarrow$  . (15)

This has some points in common with the El-Baz and Castel (1972) representation of spherical harmonics. The wavy ('spatial') leg symbolizes rays in the Hilbert subspace associated with x. We may define a *bra* as the adjoint diagram since orthogonality and completeness then reduce to equation (1). We now construct the group action and the parity transformation on the Hilbert space using theorem 4. If we follow the parity convention of equation (2.4) of Butler (1975) a ket (bra) is a fundamental node of negative (positive) parity. The constructions then become



(16)

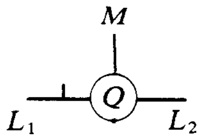
and equation (2.4) of Butler (1975) for a rotated ket becomes



(17)

Operators in the Hilbert space may be constructed via bra, ket and matrix elements. The last named are denoted (cf I):

$\langle xL_1|Q_M|xL_2\rangle \quad \leftrightarrow$

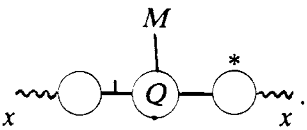


(18)

so that

$$Q_M = \sum_{L_1L_2} |xL_1\rangle\langle xL_1|Q_M|xL_2\rangle\langle xL_2|$$

$\leftrightarrow$

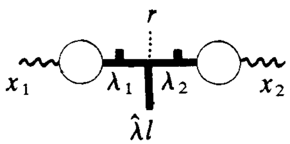


(19)

A generalized tensor operator then corresponds to choosing Q_M to be a left invariant node (usually of degree three).

As an example, we consider the unit tensor operators of § 17 of Butler (1975). Following the above definitions we write these as

$(r\lambda l(x_1\lambda_1, x_2\lambda_2)) \quad \leftrightarrow$

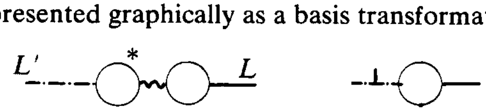


(20)

Note that in equation (20) while the internal construction is bipartite, the diagram does not yield bipartite graphs on closure because of the different parities of externally linked diagrams. In fact, these operators are not unitary.

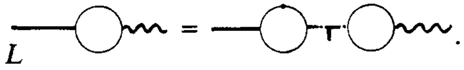
Now consider a basis transformation of our kets, in which $L \to L'$. The square matrix of inner products may be represented graphically as a basis transformation node:

$\langle xL'|xL\rangle \quad \leftrightarrow$



(21)

so that (cf equation (11.3) of Butler 1975):

 (22)

We have added a stub or parity transformation to ensure a bipartite construction. The transformation is of course invertible; from theorem 4 the basis transformation node is fundamental with negative parity. When $L = L'$ the basis transformation reduces to the adjoint of the parity transformation:

 (23)

Similarly, one may think of our representation of a ket (equation (15)) as a basis transformation from Hilbert space to quantum state labels.

We will be analysing physical problems in which the labels of such basis transformations are compounded of other labels, e.g. of irrep labels and repetition indices which specify the duplications or omissions of irreps of G necessary to give a complete mapping of the two label spaces. For example a Clebsch–Gordan coefficient may be regarded as a basis transformation. One label space is that of uncoupled states $\alpha = \{\lambda_1 l_1, \lambda_2 l_2\}$ and the other is that of a coupled state $\lambda_3 l_3$ together with a product multiplicity index r signifying the different occurrences of λ_3 in the Kronecker product $\lambda_1 \otimes \lambda_2$. This multiplicity label was given graphical representation in I, and is our prototype of a repetition label. It is invariant under group operations. We adopt the convention that wherever it is necessary to exhibit repetition labels, they will be associated with an extra, broken line, standing in an anticlockwise position to the legs representing the repeated labels. Theorem 5 (§ 3.3) is relevant, for example, to the situation in which the repeated labels are irrep labels and the diagrams in that theorem are in conformity with the above conventions.

5. Group-theoretic applications

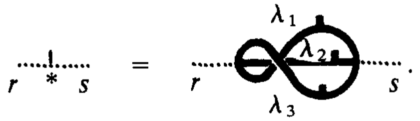
As mentioned in § 4, a 3-*jm* node (or Wigner or Clebsch–Gordan coefficient) is essentially a basis transformation from coupled to uncoupled kets. The transformation is unitary, and the adjoint is the complex conjugate expression. The 3-*jm* node of I is *left* invariant (this corrects an error in equation (12) of I). The 2-*jm* symbol is the parity transformation for group-theoretic labels; in R_3, it is the parity transformation for group-theoretic labels; in R_3, it has matrix elements $\pi_{mm'} = (-1)^{j-m}\,\delta_{-m,m'}$ for example. Again it is a unitary matrix with a trivial adjoint. Butler's (1975) definition of the 2-*jm* symbol in fact gives a left invariant node, so that its complex conjugate should be identified with our parity transformation stub. In I, the 2-*jm* symbol was taken to be real orthogonal, and thus self-adjoint. It is helpful not to assume reality of the 2-*jm* symbol and to exhibit the bipartite structure of the theory wherever possible. The 2-*jm* symbol can often be chosen to have a very simple value (Butler and Wybourne 1976).

The lemma of Derome and Sharp (1965) states that it is possible to find a unitary (parity) transformation of the multiplicity label in the 3-*jm* symbol such that, in our jargon, the 3-*jm* node is left conjugate and thus fundamental (cf equation (17) of I and equation (7) of this paper). The algebraic proofs of the Derome–Sharp lemma are isomorphic to the diagram proof rendered by theorem 5 where an orthogonality relationship for 3-*jm* coefficients (equation (11) of I):

(24)

is used for equation (12) of this paper. The construction of equation (14) then gives an explicit representation of the unitary transformation $A_{rs}(\lambda_1\lambda_2\lambda_3)$ of product multiplicity required by the lemma:

$A_{sr}(\lambda_1\lambda_2\lambda_3) \leftrightarrow$

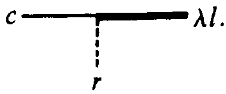


(25)

The diagram notation exhibits the structure of the theory and the significance of the lemma in an especially helpful manner, and suggests the generalizations we now present.

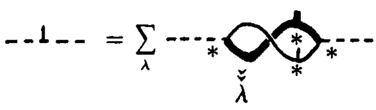
We now take any set of labels $L = \{c, c', \ldots, \}$ which form an invariant space under a compact group G, as in § 1. The group operation O_g has a representation in the basis L given by a square matrix $M_{cc'}(g)$. From elementary group theory, there exists an invertible matrix transformation $B_{c,r\lambda l}$ which will reduce the representation into block diagonal form, for all g in G, so that each block will be a unitary matrix appropriate to some irrep λ. If λ occurs $R_\lambda (= 0, 1, \ldots,)$ times in this reduction, we may obtain R_λ from character theory since $\chi(M) = \Sigma_\lambda R_\lambda \chi^\lambda$. We define a repetition index r running from 1 to R_λ for each λ. Following the convention for the diagram representation of repetition indices given in § 4, we depict the matrix $B_{c,r\lambda l}$ as a node in the form

$B_{c,r\lambda l} \leftrightarrow$



(26)

Since this node represents an invertible invariant matrix and since r is invariant, theorem 5 may be applied. In conformity with the standard conventions for the parity of a ket and a 3-*jm* symbol we choose the node to have negative parity. It follows that the node is fundamental given the construction

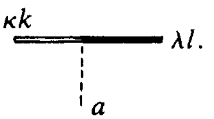


(27)

for the parity transformation on the repetition index r. The Derome–Sharp lemma is a special case of this result, with $L = \{\lambda_1 l_1, \lambda_2 l_2\}$.

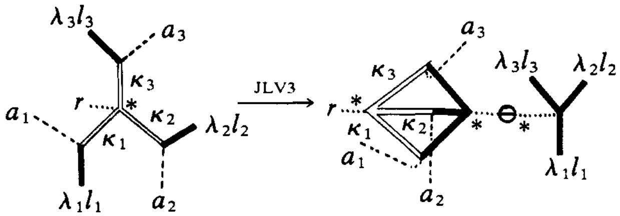
Another special case, which has not previously been discussed from this viewpoint, is that of group–subgroup reduction (Butler 1975). Let L now represent the irreducible labels κk of the irreps of a group $\hat{G}$, where $\hat{G} \supset G$. We use the symbol a for the repetition index in this case, also known as a branching multiplicity index or parentage label. We use a double line for the irrep labels of $\hat{G}$. Hence the group reduction transformation becomes denoted by

$B_{\kappa k, a\lambda l} \leftrightarrow$

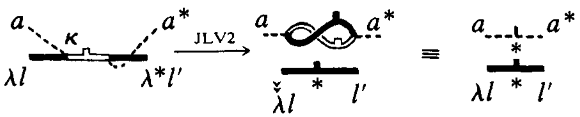


(28)

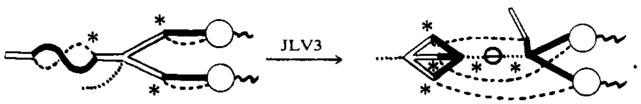
The properties of the corresponding parity transformation (resulting from an application of theorem 5) on the branching multiplicity index (cf equation (27)) have been discussed by Butler and Wybourne (1976), using the notation $(\lambda)_{a\mu,a'\mu'}$. Their derivation is quite different to ours. Analogues of their arguments are obtained by using the Jucys reduction theorems for G to G-invariant diagrams. For example:



(29)



(30)



(31)

The small figures on the multiplicity lines indicate 3-*jm* permutation matrices (table 1 of I) and equal a sum over two 3-*jm* coefficients as indicated by the figure. The equations (29)–(31) are counterparts of equations (13.2), (13.10) and the inverse of (12.9) of Butler (1975), respectively. Equation (29) is a general diagram form of the *Racah factorization lemma.* This representation of an isoscalar factor generalizes and renders unambiguous that of El-Baz and Castel (1972) for SU(2). These examples should suffice to illustrate how all the standard results (unitarity of isoscalar factors, group–subgroup reduction of 6-*j* symbols etc) may be written and used in diagram form. One may write the isoscalar factor as a fundamental node by suppressing the 3-*jm* nodes in its construction (§ 6), in which case the unitarity condition is of the form of equation (1). Note that if the parity transformation is not necessarily real we should add an asterisk to one stub in the reduction theorems YLV2, YLV4 in I and in Stedman (1976); which stub we conjugate is defined by the requirement of a bipartite construction (see § 6.5).

6. Generalized diagram reduction theorems with application to lattice dynamics

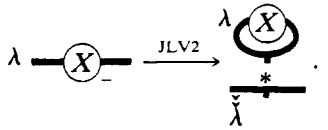
6.1. General

If a diagram X of degree n is invariant under some compact group, analogues of the Jucys reduction theorems JLVn exist even when external legs do not have irrep labels. It is merely necessary to introduce *invariant* basis transformations to irrep labels preserving a *bipartite* structure, then apply the standard JLVn theorem. Examples are given in the following theorem, which epitomises our conclusions.

Theorem 6. An invariant diagram X is uniquely defined by the coupling constants of the invariance group and by the choice of certain matrices ('reduced matrix elements') which act only on the repetition labels associated with the decomposition to irrep labels.

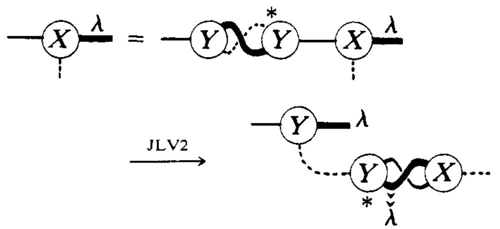
This choice may include an overall factor; for unitary basis transformations this factor can be only a phase. We prove the theorem for several representative cases.

Case 1. A diagram of degree two with irrep labels. The standard JLV2 theorem applies, giving a result equivalent to Schur's lemma. The transformation node is a parity transformation, or its adjoint (depending on its parity), with a multiplicative factor:



(32)

Case 2. A basis transformation with one irrep-labelled leg, as in equation (26). Let X, Y be two such diagrams of the same parity (say negative). Then



(33)

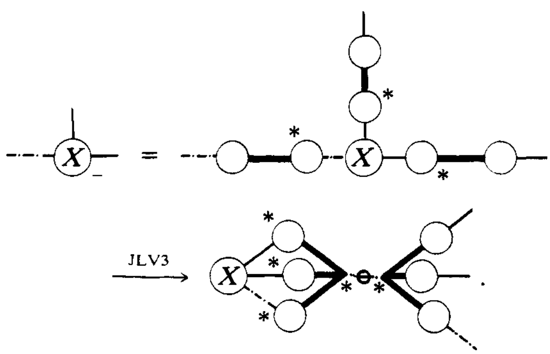
i.e. $X = Y$ apart from a matrix operation on the repetition index.

Case 3. A basis transformation linking two sets of labels L_1, L_2 of equal dimension, but neither of which are irrep labels. We introduce basis transformations taking both L_1 and L_2 to group-theoretic labels:

(34)

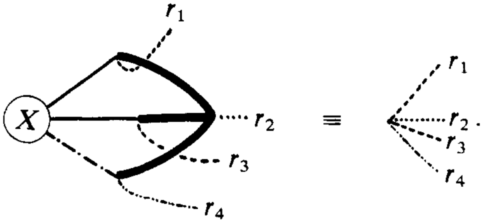
The basis transformations linked to external legs are unique to within a repetition index transformation by the result of case 2. The remaining part of the above network is unique to within a factor by the result of case 1. Hence the whole network has the stated property.

Case 4. A diagram of degree three with reducible labels. For clarity we omit repetition labels in the basis transformations required:



(35)

Since the basis transformations in equation (35) are unique to within a phase by the previous theorem, X is arbitrary only to the extent of choosing the 'reduced matrix elements' (we now exhibit repetition labels):



(36)

Hence it is scarcely necessary to label basis transformation diagrams; they are essentially determined by the nature of their legs. We called such diagrams nodes (cf appendix 1).

The physical significance of this theorem may be clarified by a few examples.

A spherical harmonic is a realization of a ket for $G = R_3$ and with spherical polar angles for spatial labels:

$Y^l_m(\theta, \phi) \leftrightarrow$ 

(37)

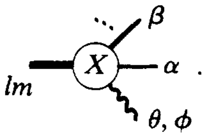
From the general point of view suggested in § 4, we may regard this as a basis transformation from spherical polar angles to R_3 (irrep) labels. With suitable normalization, Y^l_m is unitary. By theorem 6, it is unique to within a phase (there are no repetition labels), the ambiguity of which is well known.

Second, a lattice mode eigenvector for zero wavevector modes is essentially a basis transformation from the factor group (of the space group) labels to lattice site labels. That it is unique, up to a choice of phase and labelling convention, simply means that given a lattice one may immediately compute the appropriate eigenvectors within the same range of ambiguity; the problem is sufficiently defined.

Case 4 of the above theorem provides some rather less obvious conclusions. We shall illustrate these in two different fields.

6.2. *Tensor harmonics*

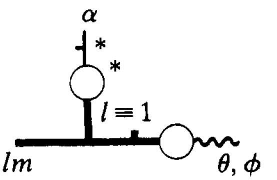
A tensor harmonic for R_3 (Jackson 1962, Campbell 1971) may be defined as a fundamental node $\mathbf{X}_{lm}(\theta, \phi)$ with more than two legs; one leg carries R_3 labels, one carries angular labels, and the remaining legs, Cartesian labels:



(38)

For a vector harmonic, with one Cartesian leg, it follows from theorem 6 that $\boldsymbol{X}_{lm}(\theta, \phi)$

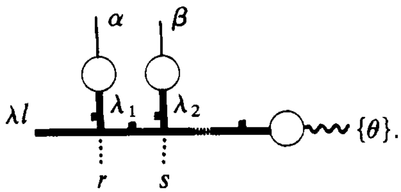
is essentially unique. The construction

$X^{\alpha}_{lm}(\theta, \phi) \leftrightarrow$  (39)

has the appropriate properties (when appropriately normalized) and by uniqueness may be taken to be the vector harmonic. This corresponds to the conventional definition:

$$\boldsymbol{X}_{lm}(\theta, \phi) \propto \boldsymbol{L} Y^{l}_{m}(\theta, \phi).$$

The generalization of tensor harmonics to an arbitrary group is now obvious; we form a bipartite construction of fundamental nodes with the desired character of external legs:

 (40)

Different choices of $\lambda_1, \lambda_2 \ldots, r, s, \ldots$ give different harmonics in general.

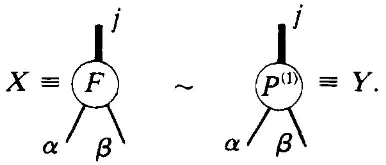
We mention that a fundamental node with either invariant or spatial (say Cartesian) leg labels is a member of the *integrity basis* of the group. We may derive such by realising the kets via Cartesian functions and coupling in a bipartite manner.

6.3. *Crystal tensors*

Theorem 6 illustrates the importance of group coupling coefficients in determining the structure of physically important tensors, invariant under some symmetry group. While plausible, this result has not previously been written down in full generality, nor has it been exploited greatly in physical applications, some of which are potentially important. Consider for example a crystal tensor, i.e. a tensor whose components may be determined by macroscopic measurements and which is therefore invariant under the operations of the factor group G of the crystal space group (Lax 1974). A special case (X having two Cartesian and one irrep-labelled leg) is discussed *de novo* by Birman and Berenson (1974) and Birman (1974a); they mention the possibility of other applications. This and other related topics have been reviewed by Birman (1974b) in a very comprehensive article. Particular attention has been paid to morphic effects by Anastassakis and Burstein (1971). We now relate our work to theirs, and in particular discuss one consequence of theorem 6: if two crystal tensors have the same indices and if all repetition indices are trivial (i.e. zero or one) the components of the two tensors are proportional.

As a simple example, consider the internal strain tensor $F_{\alpha\beta}(j)$ of Miller and Axe (1967). α, β, are Cartesian labels and j is a label for a zero wavevector lattice mode and thus is essentially an irrep label for the factor group of the crystal space group. Let

$P^{(1)}_{\alpha\beta}(j)$ be the first-order Raman scattering tensor (e.g. Birman and Berenson 1974). Then the tensors F and $P^{(1)}$ satisfy the requirements of tneorem 6:



(41)

On checking all character tables for the crystallographic point groups we find that in no case does $[\Gamma_\nu \otimes \Gamma_\nu]$ contain any irrep more than once, where Γ_ν is the vector rep. Hence repetition indices occurring in the reduction of F (or $P^{(1)}$) are trivial. It follows that the components of these tensors are proportional. Miller and Axe (1967) noted only that they were zero together, which did not include the above generalization or indeed the necessary step of checking on the absence of repeated representations.

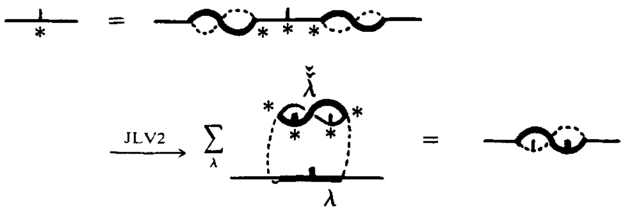
If we ignore questions of symmetrization of the Cartesian suffices, these two tensors can be related to the tensor $\mu^{(1,1)}$ describing electric-field-induced infrared absorption (Birman 1974b); if the field is static, only long-wavelength modes will be excited, and again the crystallographic point group is the relevant symmetry group. The lack of repeated representations is illustrated in the example Birman (1974b) gives of this effect, when discussing electric-field-induced infrared absorption in diamond.

By way of contrast, we take Birman's other example of a morphic effect: field-modulated Raman scattering in diamond. The components of the relevant tensor $\mathbf{P}^{(2,1)}$ multiply not only polarization vectors for the radiation but two powers of the electric field and the normal mode coordinate. On decomposing these with respect to the irreps of the space group for a typical case, a number of repetitions appear. Hence a corresponding number of reduced matrix elements are required to specify the appropriate tensor completely.

This is sometimes expressed by saying (Anastassakis and Burstein 1971, Lax 1974) that the number of repeated irreps in the relevant reduction gives the number of independent components of the tensor. This is rather misleading in general, since a given component may be a linear combination of the reduced matrix elements, which are the genuinely independent quantities. In simple cases, the reduced matrix elements contribute to disjoint sets of components, and the standard methods (Lax 1974) of direct inspection and of invariants are easily used. In more complex cases, particularly for the higher-order morphic effects of Anastassakis and Burstein (1971) in general crystal symmetries, our approach using the group coupling coefficients will be preferable, because of the mixing of reduced matrix elements and because of the systematic character of the method. This will be greatly facilitated by the soon-expected availability of tables of coupling coefficients for all crystallographic point groups (cf Butler and Wybourne 1976), and, following Berenson and Birman (1975), for space groups also. Even where direct inspection methods may be retained for their simplicity, it seems helpful to recognize that it is essentially the Wigner–Eckart theorem (more generally, JLVn) which underlies the restriction of choice of invariant tensor elements. Even the formal incorporation of such symmetry restrictions results in a considerable economy in the theory of lattice dynamics.

6.4. *Reduced matrix elements and the Derome–Sharp lemma*

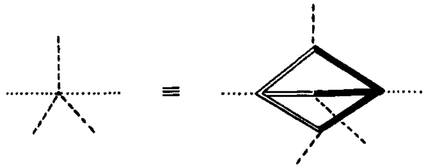
We have emphasized the interpretation of the generalized Derome–Sharp lemma (theorem 5) as a special relation between a node and its adjoint (§ 3). We now mention another useful viewpoint. Consider a parity transformation on labels L, and perform basis transformation to irrep labels as in § 5,



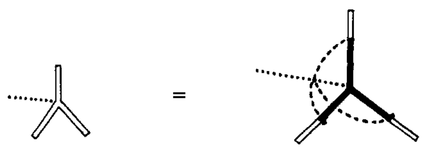
(42)

where in equation (42) we have used theorem 5 to construct the parity transformation on the repetition labels r (equation (25)). On examining equation (42), we note that this parity transformation is essentially the *reduced matrix element* of the original parity transformation for labels L. Note the reciprocal appearance of the labels L and r in equations (27) and (42).

This suggests that in general one may identify any reduced matrix element as a new, fundamental node in which all legs carry repetition labels. For example, we may introduce a condensed notation for the isoscalar factor of § 5:



(43)

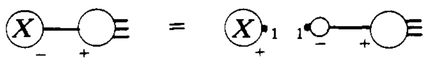


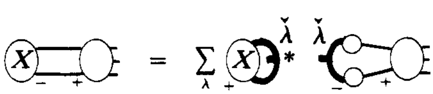
(44)

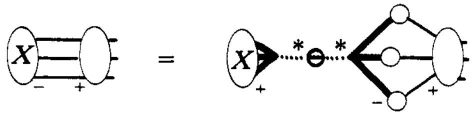
Again we have two equations with reciprocal appearance in that each of two nodes may be expressed in terms of the other. The left sides of equations (43) and (44) suppress the information contained on the right-hand side, just as in equation (25) (related to the original Derome–Sharp lemma). There is no ambiguity here, as a repetition label r when properly defined relates to a unique set of labels $(c\lambda l)$.

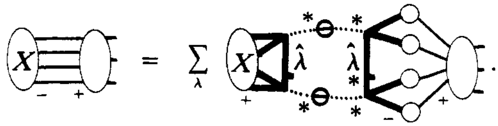
6.5. *Generalized reduction theorems*

Finally we give explicit forms for the extended JLVn theorems, $n = 1, \ldots, 4$ for nodes X of degree n which are left invariant under G. These may be compared with the relations in I and in Stedman (1976) for quasi-ambivalent G with real 2-jm symbols. The following forms are largely dictated by the requirement of bipartite construction. We choose to suppress all repetition labels, apart from product multiplicity, and also all basis transformations for X, while exhibiting those for Y, in the following:

JLV1 

JLV2 

JLV3 

JLV4 

7. Conclusions

From a graph-theoretic viewpoint, our main conclusion is that the diagrams of theoretical physics may be standardized as in § 3 (or with some necessary changes as in appendix 2 for example) by a definite parity assignment with respect to group operations and parity transformations. Further, the reduction theorems of compact group theory then imply the existence of severe restrictions on the possible internal structure of such diagrams (§ 6). This justifies the approach of this paper (which was really dictated by consistency with the work of Jucys *et al*, cf I) of putting all labels on legs wherever possible, and minimizing the internal structure of subdiagrams.

From a theoretical physics viewpoint, the Derome–Sharp lemma possesses an elegance which has not previously been exploited. The principles that go into its proof may be applied usefully in very different situations. This gives a standardized formulation of group-theoretic restrictions on physical tensors. For complicated symmetry-related problems (e.g. morphic effects in low symmetries) this promises to be the best framework for computations. Some novel results have been discussed by way of illustration in § 6; extended computations will be greatly facilitated by the availability of tables of coupling coefficients for crystallographic point and space groups.

Acknowledgments

I am grateful to Dr D J Newman, Dr P H Butler and Professor B G Wybourne for useful comments.

Appendix 1. Glossary of terms

Leg A line (edge) joining two subdiagrams

Degree (of subdiagram) The number of legs meeting at the subdiagram

Node A diagram with minimal internal structure, essentially defined by its leg labels

Network A diagram whose internal structure has been made explicit

Parity A conventional signature associated with a diagram, based on its invariance and/or conjugacy properties

Bipartite diagram A network in which each leg joins subdiagrams of opposite parity

Subdiagram Component of a network

Graph in the sense of Harary (1969): the figure obtained on replacing each sub-diagram by a point (with no structure). Hence each network has a unique graph, and a bipartite network has a bipartite graph

Invariant diagram A diagram unaffected by joint group operations on all labels in an appropriate sense (equation (4)); an invariant or irreducible tensor

Transformable diagram A diagram whose transform under a group operation is given by joint group operations on all legs in an appropriate sense (appendix 2)

Right (left, self-) conjugate diagram A diagram whose adjoint (equation (2)) is equal to its parity transform (equation (7), § 5)

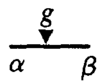
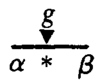
Fundamental diagram An invariant and self-conjugate diagram

Repetition index An invariant scalar label used to classify repetitions in the reduction of general labels to irrep labels

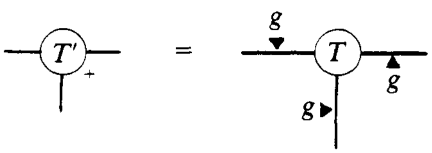
Appendix 2. Graphical manipulation of tensors in relativity

This section is illustrative, and shows how the formalism of this paper may be adapted to describe a well known theory. Consider the label space $L = \{x^\mu\} = \{x, y, z, ct\}$ with a flat-space metric $g^0_{\alpha\beta} = \mathrm{diag}(1, 1, 1, -1)$ together with the invariance group $G = \mathrm{SO}(3, 1)$.

Two major adaptations of the formalism are required. First, Cartesian, as opposed to irreducible, tensors are not invariant under group operations, but rather transform among their indices according to standard index operations. We define the group operations as follows: $\{x^\mu\} \xrightarrow{g} \{x'^\mu\}$:

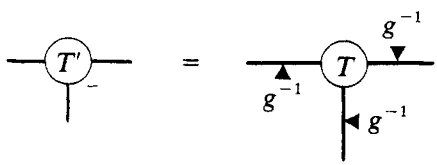
$\dfrac{\partial x'^\alpha}{\partial x^\beta} \leftrightarrow$  , $\dfrac{\partial x^\beta}{\partial x'^\alpha} \leftrightarrow$  . (A.1)

This preserves equation (3). A contravariant tensor T is then right transformable; i.e., under a group operation $T \to T'$ where



(A.2)

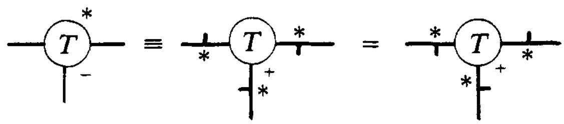
A covariant tensor is left transformable, i.e.:



(A.3)

The definitions of right and left invariance in § 3 are special cases of these definitions, for $T = T'$.

The second major change is that we no longer have square matrices. We must define the adjoint of a subgraph by the condition for self-conjugacy:



(A.4)

and similarly (following equation (7*b*)) for left conjugacy. The parity transformation, which converts left conjugate diagrams to right conjugate diagrams, must therefore be identified as the contravariant metric ($\pi_{\alpha\beta} \equiv g^{\alpha\beta}$) in equation (5). Thus right transformable, right conjugate diagrams correspond to *contravariant tensors* and are analogous to the fundamental (positive parity) diagrams of § 3.

Since the metric $g^{\alpha\beta}$ is right transformable and invertible, the definition of equation (A.4) is consistent with the old definition of adjoint in equation (1), and corresponds to the covariant metric; equation (6) reads $g^{\alpha\beta}g_{\beta\gamma} = \delta^{\alpha}{}_{\gamma}$. Therefore the adjoint of (the components of) a contravariant tensor is just the corresponding covariant tensor (components). All the standard formulation of relativity can then be carried over into graphical notation on this basis, the requirement that a covariant index be summed with a contravariant index being the analogue of our restriction to bipartite networks.

The extent to which the JLV*n* theorems are applicable for non-compact groups is unknown at present. Therefore the similarity between the diagram rules for the Levi-Civita tensor density $\epsilon_{\alpha\beta\gamma}$ given by Penrose (1971) and JLV*n* theorems (which was mentioned in § 2), must be ascribed to the invariance of $\epsilon_{\alpha\beta\gamma}$ under the compact group SO(3).

The above formalism ignores the possibility of mixed tensors. Once these are allowed, each leg-node junction (rather than each node) is invested with a parity (Penrose 1971 distinguishes 'arms' and 'legs'); also, graphs need not be bipartite. While mixed tensors are standard in tensor calculus, mixing parities at a node are unhelpful in our applications, since we think of a transformation matrix, or its reciprocal, as a single entity (cf § 3.1).

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