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1988 J. Phys. A: Math. Gen. 21 4471

(http://iopscience.iop.org/0305-4470/21/24/005)

J. Phys. A: Math. Gen. **21** (1988) 4471-4486. Printed in the UK

Symmetry adaptation of wavefunctions and matrix elements

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Received 5 December 1987

Abstract. We describe a method for the symmetrisation of basis states of representations of semisimple Lie algebras according to semisimple symmetry chains. This method also yields the matrix elements for the generators of all algebras of the symmetry chain, and thus also for the elements of their enveloping algebras. The symmetry adaptation coefficients, and the matrix elements, are obtained in the explicit form $\sqrt{p/q}$, p, $q \in \mathbb{Z}$.

The present paper describes the method for the case of su$(l+1)$, l being the rank, as the leading algebra of the chain, and for completely symmetric representations $[N]$ of su$(l+1)$. The semisimple symmetry chain with leading algebra su$(l+1)$ is arbitrary, and can be specified according to individual requirements.

The symmetry adaptation of states and the calculation of matrix elements, as outlined in this paper, has been implemented for computer evaluation. As a consequence of the method of evaluation all results are obtained in an exact manner.

1. Introduction

Semisimple symmetry chains have found frequent and highly successful applications in many fields of physics. Familiar examples are the atomic [1] and nuclear [2] shell models, both of which had far reaching consequences for a more fundamental understanding of the underlying phenomena. More recent applications of semisimple symmetry chains are found in particle physics [3], the Jahn-Teller effect [4], the interacting boson model of the nucleus [5] and in molecular physics [6]. Again, the results achieved in these areas by means of the application of symmetry chains have been profound, and at times truly astonishing.

With semisimple symmetry chains playing such an important role in physics, it is obvious that one tries to extract all the information which they can supply. A great deal has been achieved in this respect. However the calculation of the symmetry-adapted states, and the matrix elements for the generators of the subalgebras of a symmetry chain still pose problems, in particular if the dimensions of the representations become large.

In this paper we describe a method for the explicit computation of symmetry-adapted states according to a semisimple symmetry chain. The method to be described is very general and applies to any semisimple symmetry chain which starts out with an su$(l+1)$ algebra.

Apart from its generality, the method to be described permits the explicit calculation of the symmetry-adapted states with relative ease. Appropriate linear combinations of states of irreducible representations of su$(l+1)$ are formed which transform properly with respect to the subalgebras of su$(l+1)$. This is achieved by making use of Dynkin's theory for the embedding of semisimple Lie algebras in semisimple Lie algebras [7-9], and by making use of irreducibility of representations and the orthogonality of basis states of the representations.

The construction of the bases for the irreducible representations of the algebras of a symmetry chain resolves the weight subspace degeneracy automatically. A set of linear independent, but not orthogonal, vectors is obtained which spans a weight subspace. Orthonormalisation of the basis for a weight subspace is carried out in a separate step.

The degeneracy associated with the multiple occurrence of a given representation of a subalgebra, contained in the restriction of a representation of an algebra to a subalgebra, cannot be resolved naturally. Lacking a physical principle for a preferred choice of basis we introduce an orthonormal basis by arbitrary choice. Should a physical principle become available for a preferred choice of bases for the multiple copies of irreducible representations of the subalgebra, then a simple transformation will achieve the change to the desired basis.

The method for the calculation of the symmetry-adapted states described in this article also yields the matrix elements for the generators of all (sub)algebras of a symmetry chain, for all representations into which a given su$(l+1)$ representation decomposes under restriction to the (sub)algebra.

In this paper we limit our attention to completely symmetric representations of su$(l+1)$, characterised by the partition $[N]$, $N \in \mathbb{N}$. For these representations the matrix elements are of a particularly simple form, and have a simple closed form for the symmetrised basis which we use in our analysis. The case of an arbitrary (irreducible) representation of su$(l+1)$, characterised by a partition, $\lambda_1, \lambda_2, \ldots, \lambda_{l+1}$, will be discussed in a subsequent paper. The method described in this paper works for the general case of a representation of su$(l+1)$ in the same manner, except that for the general case the su$(l+1)$ matrix elements will be determined numerically.

In § 2 we define the notation used in this paper and establish the correspondence to other notations which are commonly encountered in the literature. We also define the symmetry-adapted states, following a sequence of maximally embedded algebras, in a general manner. The notation introduced here for the symmetry-adapted states will later be specialised to particular situations, and will be used in simplified form wherever this is possible without causing confusion.

In § 3 we present our method for the symmetry adaptation of states according to a given symmetry chain, as well as the determination of the matrix elements for the generators of all algebras of the chain, in all representations which occur.

In §§ 4 and 5 we apply our method to the familiar case of the su(6) interacting boson model of the nucleus (IBM) for the purpose of illustration. In § 4 we give the necessary definitions for the embeddings used for the three su(6) IBM symmetry chains. Moreover we illustrate the similarity transformation which relates the three chains. In § 5 we discuss the two-boson case of the su(6) IBM as an explicit example.

2. Definitions and notation

In the first part of this section we establish the notation used in this article. Then we briefly list various other notations used for certain groups and explain how they relate to our notation. In the second part of this section we define the symmetry-adapted states according to a symmetry chain.

Throughout the article we will use weight notation, except for the case of the algebra su$(l+1)$, as the leading algebra (model algebra) of a symmetry chain. For that case we use the partition notation. Since the partition notation is essentially the same as the weight notation we will frequently refer to a partition as a weight. For su$(l+1)$ we use the notation:

$$\text{weight:}\quad m=(m_1, m_2, \ldots, m_{l+1}) \qquad m_i=\frac{k}{l+1}$$

$$k\in\mathbb{Z} \qquad \sum_{i=1}^{l+1} m_i=0$$

$$\text{dominant weight:}\quad m_1\geqslant m_2\geqslant\cdots\geqslant m_{l+1}$$

$$\text{highest (dominant) weight:}\quad M=(M_1, M_2, \ldots, M_{l+1})$$

$$M_1\geqslant M_2\geqslant\cdots\geqslant M_{l+1}$$

$$\text{partition:}\quad [n]=[n_1, n_2, \ldots, n_{l+1}]$$

$$n_i\in\mathbb{N} \qquad \sum_{i=1}^{l+1} n_i=N\in\mathbb{N}$$

$$\text{dominant partition:}\quad n_1\geqslant n_2\geqslant\ldots\geqslant n_{l+1}$$

$$\text{highest (dominant) partition:}\quad [\lambda]=[\lambda_1, \lambda_2, \ldots, \lambda_l, \lambda_{l+1}=0]$$

$$\lambda_i\in\mathbb{N} \qquad \sum_{i=1}^{l} \lambda_i=N.$$

We have the relationships

$$m_i=n_i-N/(l+1) \qquad i=1,2,\ldots,l+1$$

$$\lambda_i=m_i-m_{l+1} \qquad i=1,2,\ldots,l+1.$$

For su(3) the following notations are frequently found in the literature:

(a) $[\lambda_1, \lambda_2, 0]\equiv[\lambda, \mu]$

(b) $m=(m_1, m_2, m_3) \qquad m_1+m_2+m_3=0 \qquad m_i=\frac{1}{3}k \qquad k\in\mathbb{Z}$

(c) $M=p\frac{1}{3}(2,-1,-1)+q\frac{1}{3}(1,1,-2) \qquad p, q\in\mathbb{N}$

$$\begin{matrix}\lambda=m_1-m_3\\ \mu=m_2-m_3\end{matrix} \quad \begin{cases} m_1=\frac{1}{3}(2\lambda-\mu)\\ m_2=\frac{1}{3}(-\lambda+2\mu)\\ m_3=\frac{1}{3}(-\lambda-\mu)\end{cases}$$

$$\begin{matrix}p=m_1-m_2\\ q=m_2-m_3\end{matrix} \quad \begin{cases} m_1=\frac{1}{3}(2p+q)\\ m_2=\frac{1}{3}(-p+q)\\ m_3=\frac{1}{3}(-p-2q).\end{cases}$$

For su(2) $\sim$ so(3) the notation employed is

$$j=\tfrac{1}{2}\lambda_1 \qquad \lambda_1\in\mathbb{N}$$

$$m\equiv m_1=\tfrac{1}{2}k \qquad k\in\mathbb{Z} \qquad m_1+m_2=0.$$

For so($2l+1$) we use the weight notation,

$$m=(m_1, m_2, \ldots, m_l) \qquad m_i=\tfrac{1}{2}k \qquad k \in \mathbb{Z}.$$

The irreducible representations are characterised by weights satisfying

$$m_1 \geqslant m_2 \geqslant \ldots \geqslant m_1 \geqslant 0 \qquad \text{(dominant weight condition).}$$

For so(21) we use the weight notation,

$$m=(m_1, m_2, \ldots m_1) \qquad m_i=\tfrac{1}{2}k \qquad k \in \mathbb{Z}.$$

The irreducible representations are characterised by weights satisfying

$$m_1 \geqslant m_2 \geqslant \ldots \geqslant |m_l|.$$

The algebra so(4) $\sim$ so(3) $\times$ so(3) is semisimple. We use the notation

$$\text{so(4):} \qquad m=(m_1, m_2) \qquad m_i=\tfrac{1}{2}k \qquad k \in \mathbb{Z}.$$

For highest weights

$$m_1 \geqslant |m_2|$$

$$\text{su(2)} \times \text{su(2):} \qquad m_1=\tfrac{1}{2}(m_1-m_2) \qquad m_2'=\tfrac{1}{2}(m_1+m_2).$$

For sp($2l$) we use the weight notation

$$m=[m_1, m_2, \ldots, m_1] \qquad m_i \in \mathbb{Z}.$$

The highest weights satisfy the dominant weight condition

$$m_1 \geqslant m_2 \geqslant \ldots \geqslant m_l \geqslant 0.$$

We call a weight m (partition $[n]$) larger than a weight m' (partition $[n']$) if for the first non-vanishing difference of components it holds that $m_k-m_k'>0$ ($n_k-n_k'>0$).

In the following we define a symmetry-adapted state, according to a given symmetry chain. Consider a symmetry chain consisting of a sequence of algebras

$$G \supset \tilde{G} \supset \ldots \supset G' \supset G'' \tag{2.1}$$

with the property that each subalgebra is a *maximal* subalgebra of the preceding algebra [8, 9]. A subalgebra $\tilde{\mathrm{G}}$ of an algebra G is called a maximal subalgebra if there exists no algebra G_s such that $\mathrm{G} \supset \mathrm{G}_s \supset \tilde{\mathrm{G}}$. The algebra G of the symmetry chain (2.1) is a consequence of the assumptions made for the model, and we will call G the 'model algebra'. The last algebra of a symmetry chain usually represents symmetry operations with respect to which the physical model is invariant. We therefore will refer to it as the 'invariance algebra'.

In this article we assume the model algebra to be of the type $\mathrm{A}_l \sim$ su($l+1$), l being the rank, or to be a direct sum of such algebras.

We will use the following notation.

(i) G (model algebra su($l+1$) of rank l):

$$\text{weight:} \quad m=(m, m_2, \ldots, m_{l+1})$$

highest weight of irreducible representation, highest weight of the set of dominant weights of an irreducible representation: $M=(M_1, M_2, \ldots, M_{l+1})$

irreducible representation of G corresponding to the highest weight M: $D(M)$

basis state for irreducible representation $D(M)$ which belongs to the weight subspace V_m, the label σ characterising the weight space degeneracy: $|M; m\sigma\rangle$. (2.2)

As mentioned before we will use the closely related partition notation interchangeably with the weight notation for the su$(l+1)$ algebras.

(ii) G′ (a subalgebra of G, not necessarily a maximal subalgebra of G):

weight: $m'=(m'_1, m'_2, \ldots, m'_{l'})$ $\quad l'\leqslant l$.

highest (dominant) weight of an irreducible representation: $M'=(M'_1, M'_2, \ldots, M'_{l'})$

irreducible representation of G′ corresponding to highest weight M': $D(M')$

basis sate of irreducible representation $D(M')$ of G′ belonging to weight subspace $V_{m'}$: $|M, \tilde{M}\tilde{\tau}, \ldots, M'\tau'; m'\sigma'\rangle$. (2.3)

The label σ' in (2.3) characterises the weight space degeneracy. The state (2, 3) consists of a linear combination of states $|M; m\sigma\rangle$ of $D(M)$ of G and has been symmetry adapted along the chain $\mathrm{G}\supset\tilde{\mathrm{G}}\supset\ldots\supset\mathrm{G}'$. That is, the state transforms according to the representation $D(M)$ of G, $D(\tilde{M})\tilde{\tau}$ of $\tilde{\mathrm{G}}, \ldots, D(M')\tau'$ of G′, and belongs to the weight $m'\sigma'$ of $D(M')\ \tau'$. The labels $\tilde{\tau}, \ldots, \tau'$ distinguish identical copies of irreducible representations $D\tilde{M}), \ldots, D(M')$. The label σ distinguishes basis states of the weight subspace $V_{m'}$ of $D(M')$. We have

$$|M, \tilde{M}\tilde{\tau}, \ldots, M'\tau'; m'\sigma'\rangle = \sum_{\substack{m\sigma\in D(M)\\ f(m)=m'}} d'(M, \tilde{M}\tilde{\tau}, \ldots, M'\tau'; m'\sigma'|m\sigma)|M; m\sigma\rangle \qquad d'(\ldots)\in\mathbb{C} \tag{2.4}$$

where the sum is over states $m\sigma$ of the representation $D(M)$ of G. In fact, the sum is only over those states $m\sigma$ of $D(M)$ for which the weight m is projected upon the weight m' by the embedding matrix f' of G′ in G, $f'(m)=m'$.

(iii) G″ (G″ maximal in G′). Following (ii) above we have

$$\begin{aligned}|M, \tilde{M}\tilde{\tau}, \ldots, M'\tau', M''\tau''; m''\sigma''\rangle &= \sum_{\substack{m\sigma\in D(M)\\ f''(m)=m''}} d''(M, \tilde{M}\tilde{\tau}, \ldots, M'\tau', M''\tau''; m''\sigma''|m\sigma)\\ &\quad\times|M, m\sigma\rangle \qquad d''\in\mathbb{C} &(2.5)\\ &= \sum_{\substack{m'\sigma'\in D(M')\\ g(m')=m''}} c(M, \tilde{M}\tilde{\tau}, \ldots, M'\tau', M''\tau''; m''\sigma''|m'\sigma')\\ &\quad\times|M, \tilde{M}\tilde{\tau}, \ldots, M'\tau'; m'\sigma'\rangle \qquad c\in\mathbb{C}. &(2.6)\end{aligned}$$

where g is the embedding matrix of G″ in G′. The first equality sign expresses the state in terms of states of the model algebra G. The second equality sign expresses the same state as a sum over states which have already been symmetry adapted along the chain $G \supset \tilde{G} \supset \ldots \supset G'$. Substitution of (2.4) carries this expression over into the first one, and yields relationships for the symmetry-adaptation coefficients.

3. Symmetry adaptation and matrix elements

Given a symmetry chain $G \supset \tilde{G} \supset \ldots \supset G'$, the model algebra G is, by assumption, of the type su$(l+1)$. All subalgebras $\tilde{G}, \ldots, G'$ of the symmetry chain are embedded in su$(l+1)$. Thus the generators of all algebras $G, \tilde{G}, \ldots, G'$ will act upon su$(l+1)$ states, and we need to study only the action of the su$(l+1)$ generators upon the su$(l+1)$ states.

Let $[\lambda]=[N, 0, \ldots, 0]$ denote a partition which labels a completely symmetrical su$(l+1)$ representation. Let $[n]=[n_1, n_2, \ldots, n_{l+1}]$, $\Sigma_{i=1}^{l+1} n_i = N$, $n_i \in \mathbb{N}$, $i = 1, 2, \ldots, l+1$, denote an arbitrary partition of the irreducible representation $[N]$. Moreover, let

$$|[N], [n]\rangle \tag{3.1}$$

denote a state of the representation $[N]$ labelled by $[n]$. We assume that this state is normalised to 1. Then we have for the action of the shift operator E_α, α being a root of su$(l+1)$,

$$\begin{aligned} &E_{e_i-e_j}|[N], [n_1, \ldots, n_i, \ldots, n_j, \ldots, n_{l+1}]\rangle \\ &\qquad = \sqrt{n_i+1}\,\sqrt{n_j}\,|[N], [n_1, \ldots, n_i+1, \ldots, n_j-1, \ldots, n_{l+1}]\rangle. \end{aligned} \tag{3.2}$$

Note that the matrix elements are those of a product of a boson creation and a boson annihilation operator.

In what follows it will be seen that for each given algebra of the symmetry chain we will only need to consider the action of the generators which correspond to the simple negative roots of that algebra. However, the embedding of these generators in su$(l+1)$ will, in general, also involve shift operators of su$(l+1)$ other than those which correspond to the simple negative roots.

Given a subalgebra G′ of the symmetry chain, its shift operators will act upon the symmetrised, and normalised, states of an su$(l+1)$ representation via their embedding in su$(l+1)$. In general it will require linear combinations of the symmetrised and normalised states of su$(l+1)$ to transform properly with respect to the subalgebra G′ of su$(l+1)$. We assume that we are given such a linear combination of su$(l+1)$ states which transforms according to a certain state of an irreducible representation of G′, and that this state is normalised to 1. Acting upon this state with a shift operator of G′, embedded in su$(l+1)$, we obtain another state of the same representation G′, unless the state is mapped to zero. The resultant state is in general no longer normalised to 1. Normalising the new state to 1 we obtain the matrix element for the action of the shift operator between the two normalised states. Thus, we not only have the matrix elements of the generators of su$(l+1)$ in the representation $[N]$, but obtain the matrix elements of all generators of all subalgebras of the symmetry chain as well, for all irreducible representations of the subalgebras into which the representation $[N]$ of su$(l+1)$ branches.

For a given algebra the action of the shift operators $E_{-\alpha}$, which correspond to the simple negative roots $-\alpha$, is sufficient to generate all states of an irreducible representation if they act upon the state which corresponds to the highest weight of the representation (i.e. $E_\alpha|M\rangle = 0$ for all positive simple roots α). Thus the multiplicity associated with the weight space degeneracy σ poses no problem and is solved automatically. The basis vectors for a given weight subspace will not, however, be orthonormal and need to be orthonormalised separately.

The multiplicity associated with the branching of a representation of a group under restriction to one of its subgroups has no natural solution if the multiplicity becomes $\geqslant 2$. Unless a physical principle is given for a particular choice of a basis for the multiple copies of representations of a subalgebra there is no criteria available for the choice of one basis over another. Thus, we arbitrarily introduce an orthonormal basis for multiple copies of identical representations.

In the following we denote by Σ the root system of an algebra and by $\pi_\pm$ the set of positive and negative simple roots of an algebra. By σ $(D(M'), m')$ we denote the dimension of the weight subspace of a weight $m' \in D(M')$ of G′. By $\tau(M, M')$ we denote the number of (identical) irreducible representations $D(M')$ of G′ which are obtained from a representation $D(M)$ of G under restriction of G to its subalgebra G′. By $S(M, m')$ we denote the total number of weights $m \in D(M)$ which are projected onto a given weight m' of G′ under the restriction of G to G′.

In the following we give a stepwise procedure for the determination of symmetry-adapted states, following a chain of maximally embedded subalgebras.

(1) $\mathrm{G}(\mathrm{su}(l+1)) \supset \mathrm{G}'$, maximally. Choose the desired $\mathrm{su}(l+1)$ representation $D([N])$. The vector of highest weight of $D([N])$ is $|[N]; [N, 0, \ldots, 0]\rangle$. This vector is unique. The shift operators $E_{-\alpha}$, $-\alpha \in \pi_-$, acting upon this vector generate all basis states of the representation $D([N])$.

(2) Let $f(E'_{\alpha'}) \in \mathrm{G}$ denote the shift operators $E'_{\alpha'}$, $\alpha' \in \pi_+$, of G′, embedded in the algebra G. Let $M'_{(1)}$ denote the *highest* weight of G′ which occurs in the projection $f([n])$ of the weights $[n] \in D([N])$ onto the weight space of G′, let $n([N], M'_{(1)})$ denote its multiplicity, and let $S([N], M'_{(1)}) = \{|[N]; [n]\rangle, f([n]) = M'_{(1)}\}$ denote the set of states of $D([N])$ for which $f([n]) = M'_{(1)}$. The state(s) satisfying

$$f(E'_{\alpha'})|[N], M'_{(1)}; M'_{(1)}\rangle = 0$$

$$|[N], M'_{(1)}; M'_{(1)}\rangle = \sum_{\substack{[n]\in D([N])\\ f([n])=M'_{(1)}}} C_{[n]}|[N]; [n]\rangle \qquad C_{[n]} \in \mathbb{C}$$

generate the basis states for the irreducible representation(s) $D(M'_{(1)})$ of G′. We call these vectors extremal vectors [10]. In the case where more than one extremal vector is obtained we have a non-trivial branching multiplicity, i.e. $\tau([N], M'_{(1)}) = S > 1$. In that case we have to introduce an additional label τ to distinguish otherwise identical copies $D(M'_{(1)})$. The extremal vectors $|[N], M'_{(1)}\tau; M'_{(1)}\rangle$, $\tau = 1, 2, 3, \ldots, S$, define an S-dimensional subspace since $\sigma = 1$ for any extremal vector. In this S-dimensional space we can choose an orthonormal basis at will, and each basis vector will define an identical representation $D(M'_{(1)})$. That is, acting with the $f(E'_{-\alpha'})$, $-\alpha' \in \pi_-$, upon each of these orthonormal vectors yields a basis for a copy $D(M'_{(1)})$. The weight space multiplicity $\sigma(M'_{(1)}, m')$ is resolved automatically (within each of the S copies $D(M'_{(1)})$), with the basis elements for the weight subspaces consisting of linear independent, but non-orthogonal, vectors (note, we use $f(E'_{-\alpha'})$ with *simple* negative roots only). Basis vectors which belong to different weight subspace are automatically orthogonal, while those which belong to the same weight of a given irreducible representation need to be orthonormalised in a separate step.

In general, the action of an operator $f(E'_{-\alpha})$ upon an orthonormalised state $|[N], M'_{(1)}; m'\rangle$ will result in a state which is no longer normalised to 1. Normalising the state obtained to 1, we obtain a normalised state $|[N], M'_{(1)}; m'-\alpha'\rangle$ multiplied by the matrix element for the generator $E'_{-\alpha'}$ of G′ connecting these two states of $D(M'_{(1)})$.

(3) The next highest dominant weight $M'_{(2)}$ is located in the sequence $M'_{(1)} \geqslant M'_{(2)} \geqslant \ldots$ of projected dominant weights. We have

$$S([N], M'_{(2)}) - \tau([N], M'_{(1)})\sigma(D(M'_{(1)}, M'_{(2)}) = k \geqslant 0.$$

If $k=0$, then there exists no representation $D(M'_{(2)})$ in the restriction of $D([N])$ to G′. If $k>0$, then there exist k copies of $D(M'_{(2)})$ in the restriction of $D([N])$ to G′. The associated extremal vectors

$$|[N], M'_{(2)}\tau; M'_{(2)}\rangle = \sum_{\substack{[n]\in D([N]) \\ f([n])=M'_{(2)}}} C_{[n]}|[N]; [n]\rangle$$

$$C_{[n]} \in \mathbb{C} \qquad \tau = 1, 2, \ldots, k$$

generate the representations $D(M'_{(2)}\ \tau)$ in accordance with (2).

The subspace spanned by the k extremal vectors is orthogonal to the weight subspace(s) of the weight $M'_{(2)}$ in the representation(s) $D(M'_{(1)})$. This subspace can thus be determined by orthogonalisation. It is the subspace of the space spanned by $S([N], M'_{(2)})$ which is orthogonal to the weight subspaces corresponding to the weights $M'_{(2)}$ in the representation(s) $D(M'_{(1)})$. For $k=1$ the orthogonalisation determines the (single) extremal vector uniquely, apart from its normalisation. If $k>1$ then the *subspace* is uniquely determined, for which an arbitrary orthonormal basis can be defined. Acting with the $f(E'_{-\alpha})$, $-\alpha' \in \pi_-$, upon the basis vector(s) (extremal vectors), a copy of $D(M'_{(2)})$ is generated.

(4) Assuming that, in sequence, the irreducible representations corresponding to highest weights $M'_{(1)} \geqslant M'_{(2)} \geqslant \ldots, M'_{(q-1)}$ have been determined,

$$D(M'_{(1)}, \tau'_1) \qquad D(M'_{(2)}, \tau'_2) \qquad \ldots \qquad D(M'_{(q-1)}, \tau'_{q-1})$$

we proceed to determine the representations associated with the next-highest weight $M'_{(q)}$. We have

$$S([N], M'_{(q)}) - \sum_{i=1}^{q-1} \tau([N], M'_{(i)})\sigma(M'_{(i)}, M'_{(q)}) = k \geqslant 0.$$

If $k=0$, there is no representation $D(M'_{(q)})$ in the restriction of $D([N])$ to G′. If $k \geqslant 1$, then there are k copies of $D(M'_{(q)})$ in the restriction of $D([N])$ to G′. We find the subspace orthogonal to all weight subspaces $M'_{(q)}$ in the representations $D(M'_{(i)})$, $i=1, 2, \ldots, q-1$. If $k=1$, then orthogonalisation *determines* the extremal vector (uniquely, apart from normalisation),

$$|[N]; M'_{(q)}, M'_{(q)}\rangle = \sum_{\substack{[n]\in D([N]) \\ f([n])=M'_{(q)}}} C_{[n]}|[N], [n]\rangle.$$

If $k>1$, then the subspace of the space spanned by

$$S([N], M'_{(q)}) = \{[n] \in D([N]); f([n]) = M'_{(q)}\}$$

which is orthogonal to the direct sum of all weight subspaces corresponding to the weight $M'_{(q)}$ in all representations $D(M'_{(i)})$, $i=1,2,\ldots,q-1$, is uniquely determined. The basis vectors of these weight subspaces are known, since they have already been found. The direct sum of the weight subspaces forms a subspace V of the space spanned by $S([N], M'_{(q)})$. The orthogonal complement of V in the space $S([N], M'_{(q)})$ is the subspace we are looking for. An orthonormal basis is introduced into this subspace in an arbitrary manner. Each basis vector is an extremal vector $|[N], M'_{(q)}\tau'; M'_{(q)}\rangle$, $\tau'=1,2,\ldots,k$. for each value $\tau'=1,2,\ldots,k$ the action of the shift operators $f(E'_{-\alpha'})$, $-\alpha'\in\pi_-$, generates a copy of $D(M'_{(q)})$.

(5) Having found all representations $D(M')$ contained in the representation $D(M)$ under the restriction of G(su($l+1$)) to G′, one proceeds to the next (maximal) subgroup G″, G ⊃ G′ ⊃ G″. All steps repeat themselves, with G″ replacing G′ *in* G, *except that the orthogonalisation proceedure has to be carried out in* G′ (and not in G). Only then is the orthogonalisation procedure unique—apart from the arbitrariness for the choice of basis for multiple copies of identical representations $D(M'')$ of G″ which occur in the restriction of a representation $D(M')$ of G′ to the subalgebra G″. In other words, while the basis states for the representations $D(M'')$ are calculated in the form of (2.5), the orthogonalisation procedure needs to be carried out with the basis states of $D(M'')$ expressed in the form of (2.6).

4. Example: su(6) IBM

The su(6) IBM has three symmetry chains which lead from the model algebra su(6) to its physical subalgebra so(3) ~ su(2) (locally) [5, 9]. They are: su(6) → su(5) → so(5) → so(3), su(6) → so(6) ~ su(4) → so(5) → so(3) and su(6) → su(3) → so(3). Boson creation and annihilation operators s^+, s and d^+_m, d_m, $m=2,1,0,-1,-2$, are introduced, for angular momentum $l=0$ and $l=2$ respectively. They satisfy the usual Lie products. From them the Lie algebra su(6) is built and the subalgebra chains are identified.

We need to introduce at this point a few concepts [8, 9]. An embedding of a (semisimple) Lie algebra G′ in a (semisimple) Lie algebra G is a linear map f of G′ into G,

$$f: X'_i \to f(X'_i)\in \mathrm{G} \qquad \forall X'_i\in \mathrm{G}' \tag{4.1}$$

such that

$$[f(X'_i), f(X'_j)] = c'^k_{ij} f(X'_k). \tag{4.2}$$

The X'_i denote basis elements of G′, the c' are the structure constants of G′, and the Lie product (4.2) is *in* G. The embedding has the property that

$$f(H'_i) = \sum_{j=1}^{l+1} f_{ij} H_j \qquad i=1,2,\ldots,l' \qquad f_{ij}\in\mathbb{R}. \tag{4.3}$$

The H'_i denote basis elements of the Cartan subalgebra of G′, the H_j basis elements of the Cartan subalgebra of G. The rank of G′ is l', the rank of G is l. The embedding of the raising operators $E'_{\alpha'}\in$ G′, $\alpha'>0$, in G is given as

$$f(E'_\alpha) = \sum_{\alpha\in\Gamma_{\alpha'}} C_{\alpha'\alpha} E_\alpha,\ E_\alpha\in G \qquad c_{\alpha'\alpha}\in\mathbb{C} \tag{4.4}$$

and the lowering operators $E'_{-\alpha'}\in$ G′ are given as

$$f(E'_{-\alpha'}) = f(E'_{\alpha'})^+. \tag{4.5}$$

The set $\Gamma_{\alpha'}$ of roots of G is defined as the subset of roots of the root system Σ of G,

$$\Gamma_{\alpha'} = \{\alpha \in \Sigma | f(\alpha) = \alpha'\} \tag{4.6}$$

with

$$[f(\alpha)]_i = \sum_{j=1}^{l+1} f_{ij}\alpha_j = \alpha'_i. \tag{4.7}$$

In general, the embedding matrix acts as a projection operator from the weight space of G into the weight space of G′.

$$[f(m)]_i = \sum_{j=1}^{l+1} f_{ij} m_j = m'_i. \tag{4.8}$$

We are now ready to discuss the su(6) IBM symmetry chains in the language of embeddings. The examples given below will illustrate the meaning of the concepts given above.

(A) The chain su(6)→su(5)→so(5)→so(3):
su(6)→su(5): the generators of su(5) are embedded in su(6) as:

$$\begin{aligned} &f(E'_{e_2-e_1}) = E_{e_6-e_1} \qquad f(E'_{e_3-e_2}) = E_{e_3-e_6} \\ &f(E'_{e_4-e_3}) = E_{e_2-e_3} \qquad f(E'_{e_5-e_4}) = E_{e_5-e_2} \\ &f(H'_1) = H_1 \qquad f(H'_2) = H_6 \qquad f(H'_3) = H_3 \\ &f(H'_4) = H_2 \qquad f(H'_5) = H_5. \end{aligned} \tag{4.9}$$

The $e_i - e_j$, $i \neq j$, denote the roots of G′ and G.
su(6)→su(5)→so(5): the generators of so(5) are embedded in su(6) as:

$$\begin{aligned} &f(E'_{e_2-e_1}) = E_{e_2-e_1} + E_{e_6-e_5} \qquad f(E'_{-e_2}) = E_{e_5-e_3} + E_{e_3-e_2} \\ &f(H'_1) = H_1 - H_6 \qquad f(H'_2) = H_2 - H_5. \end{aligned} \tag{4.10}$$

su(6)→su(5)→so(5)→so(3): the generators of so(3) are embedded in su(6) as:

$$\begin{aligned} &f(L_-) = \sqrt{2}(E_{e_2-e_1} + E_{e_6-e_5}) + \sqrt{3}(E_{e_5-e_3} + E_{e_3-e_2}) \\ &f(L_0) = 2H_1 + H_2 - H_5 - 2H_6. \end{aligned} \tag{4.11}$$

The correspondence of the notation used above to the boson operator description is the following. Let $[n]$, $\Sigma_{i=1}^6 n_i = N$, denote a partition (weight) of the representation $[N]$ of su(6). Then we have

$$[n_1, n_2, \ldots, n_6] = \frac{(d_2^+)^{n_1}}{\sqrt{n_1!}} \frac{(d_1^+)^{n_2}}{\sqrt{n_2!}} \frac{(d_0^+)^{n_3}}{\sqrt{n_3!}} \frac{(s^+)^{n_4}}{\sqrt{n_4!}} \frac{(d_{-1}^+)^{n_5}}{\sqrt{n_5!}} \frac{(d_{-2}^+)^{n_6}}{\sqrt{n_6!}}. \tag{4.12}$$

All boson creation operators commute and thus the particular ordering is of no relevance.

Introducing boson operators b_j^+, b_i such that

$$b_1^+ = d_2^+ \qquad b_2^+ = d_1^+ \qquad b_3^+ = d_0^+ \qquad b_4^+ = s^+ \qquad b_5^+ = d_{-1}^+ \qquad b_6^+ = d_{-2}^+ \tag{4.13}$$

we obtain

$$E_{e_j-e_i} = b_j^+ b_i \qquad H_i = b_i^+ b_i. \tag{4.14}$$

The angular momentum algebra embedded through chain (4.11) takes on the form

$$\begin{aligned} f(L_-) &= \sqrt{2}(d_1^+ d_2 + d_{-2}^+ d_{-1}) + \sqrt{3}(d_{-1}^+ d_0 + d_0^+ d_1) \\ f(L_0) &= 2d_2^+ d_2 + d_1^+ d_1 - d_{-1}^+ d_{-1} - 2d_{-2}^+ d_{-2}. \end{aligned} \tag{4.15}$$

(B) The chain su(6) → su(3) → so(3):
su(6) → su(3): the generators of su(3) in su(6) are:

$$\begin{aligned} f(E'_{e_2-e_1}) &= \sqrt{2}(E_{e_5-e_3} + E_{e_6-e_5}) + E_{e_4-e_2} \\ f(E'_{e_3-e_2}) &= \sqrt{2}(E_{e_2-e_1} + E_{e_3-e_2}) + E_{e_5-e_4} \\ f(H'_1) &= \tfrac{1}{3}(2H_1 + 2H_2 + 2H_3 - H_4 - H_5 - 4H_6) \\ f(H'_2) &= \tfrac{1}{3}(2H_1 - H_2 - 4H_3 + 2H_4 - H_5 + 2H_6) \\ f(H'_3) &= \tfrac{1}{3}(-4H_1 - H_2 + 2H_3 - H_4 + 2H_5 + 2H_6) \end{aligned} \tag{4.16}$$

su(6) → su(3) → so(3): the generators of so(3) in su(6) are:

$$\begin{aligned} f(L_-)' &= \sqrt{2}(E_{e_2-e_1} + E_{e_3-e_2} + E_{e_5-e_3} + E_{e_6-e_5}) + E_{e_4-e_2} + E_{e_5-e_4} \\ f(L_0)' &= 2H_1 + H_2 - H_5 - 2H_6. \end{aligned} \tag{4.17}$$

Comparing (4.17) and (4.11) it might appear that we are dealing with two distinct embeddings of so(3) in su(6). This is not the case. The two embeddings are mathematically equivalent and go over into each other under a suitable change of basis of the defining representation [1] of su(6). For the case of chain (A) we have defined a basis for the representation [1] of su(6):

$$\begin{aligned} d_2^+ &= [100000] = |[1], [1], (1,0), 2; 2\rangle \\ d_1^+ &= [010000] = |[1], [1], (1,0), 2; 1\rangle \\ d_0^+ &= [001000] = |[1], [1], (1,0), 2; 0\rangle \\ d_{-1}^+ &= [000010] = |[1], [1], (1,0), 2; -1\rangle \\ d_{-2}^+ &= [000001] = |[1], [1], (1,0), 2; -2\rangle \\ s^+ &= [000100] = |[1], [0], (0,0), 0; 0\rangle. \end{aligned} \tag{4.18}$$

This basis is trivially symmetry adapted according to chain (A). If we act upon this basis with the generator $f(L_-)'$ of so(3), embedded in su(6) via chain (B), we obtain

$$\begin{aligned} |[1], (2,0), 2; 2\rangle &= |[1], [1], (1,0), 2; 2\rangle = d_2^+ \\ |[1], (2,0), 2; 1\rangle &= |[1], [1], (1,0), 2; 1\rangle = d_1^+ \\ |[1], (2,0), 2; 0\rangle &= \sqrt{\tfrac{2}{3}}|[1], [1], (1,0), 2; 0\rangle + \sqrt{\tfrac{1}{3}}|[1], [0], (0,0), 0; 0\rangle \\ &= \sqrt{\tfrac{2}{3}}d_0^+ + \sqrt{\tfrac{1}{3}}s^+ \\ |[1], (2,0), 2; -1\rangle &= |[1], [1], (1,0), 2; -1\rangle = d_{-1}^+ \\ |[1], (2,0), 2; -2\rangle &= |[1], [1], (1,0), 2; -2\rangle = d_{-2}^+ \\ |[1], (2,0), 0; 0\rangle &= \sqrt{\tfrac{1}{3}}|[1], [1], (1,0), 2; 0\rangle - \sqrt{\tfrac{2}{3}}|[1], [0], (0,0), 0; 0\rangle \\ &= \sqrt{\tfrac{1}{3}}d_0^+ - \sqrt{\tfrac{2}{3}}s^+. \end{aligned} \tag{4.19}$$

Thus we have introduced new bosons, symmetry adapted according to chain (B),

$$d_2'^+ = d_2^+ \qquad d_1'^+ = d_1^+ \qquad d_0'^+ = \sqrt{\tfrac{2}{3}}d_0^+ + \sqrt{\tfrac{1}{3}}s^+$$
$$d_{-1}'^+ = d_{-1}^+ \qquad d_{-2}'^+ = d_{-2}^+ \qquad s'^+ = \sqrt{\tfrac{1}{3}}d_0^+ - \sqrt{\tfrac{2}{3}}s^+.$$

Ordering the primed and unprimed bosons in the sequence d_2^+, d_1^+, d_0^+, s^+, d_{-1}^+, d_{-2}^+ the similarity transformation

$$M = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{2}{3}} & \sqrt{\frac{1}{3}} & 0 & 0 \\ 0 & 0 & \sqrt{\frac{1}{3}} & -\sqrt{\frac{2}{3}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

carries the unprimed bosons into the primed bosons, and vice versa ($M^{-1} = M$). The similarity transformation

$$f(L_-) = M^{-1} f(L_-)' M \tag{4.20}$$

carries the generators $f(L_-)'$ over into the form $f(L_-)$.

The embedding (4.11) corresponds to orbital angular momentum. In order to have chain (B) also represent orbital angular momentum we must perform the similarity transformation (4.20). The original (mathematically equivalent) embeddings (4.11) and (4.17) have the property that the Cartan subalgebra H of su(6) remains the same for both embeddings. The similarity transformation M induces in su(6) a different choice for the Cartan subalgebra H for the two embeddings.

(C) The chain su(6) → su(4) ~ so(6) → so(5) → so(3).

su(6) → su(4): the generators of su(4) in su(6) are:

$$\begin{aligned} & f(E'_{e_2-e_1}) = E_{e_4-e_2} + E_{e_5-e_3} \qquad f(E'_{e_3-e_2}) = E_{e_2-e_1} + E_{e_6-e_5} \\ & f(E'_{e_4-e_3}) = E_{e_3-e_2} + E e_5 - e_4 \\ & f(H'_1) = \tfrac{1}{2}(H_1 + H_2 + H_3 - H_4 - H_5 - H_6) \\ & f(H'_2) = \tfrac{1}{2}(H_1 - H_2 - H_3 + H_4 + H_5 - H_6) \\ & f(H'_3) = \tfrac{1}{2}(-H_1 + H_2 - H_3 + H_4 - H_5 + H_6) \\ & f(H'_4) = \tfrac{1}{2}(-H_1 - H_2 + H_3 - H_4 + H_5 + H_6). \end{aligned} \tag{4.21}$$

su(6) → su(4) → so(5): the generators of so(5) in su(6) are:

$$\begin{aligned} & f(E'_{e_2-e_1}) = E_{e_2-e_1} + E_{e_6-e_5} \\ & f(E'_{-e_2}) = \sqrt{\tfrac{1}{2}}(E_{e_4-e_2} + E_{e_5-e_3} + E_{e_3-e_2} + E_{e_5-e_4}) \\ & f(H'_1) = H_1 - H_6 \qquad f(H'_2) = H_2 - H_5. \end{aligned} \tag{4.22}$$

su(6) → su(4) → so(5) → so(3): the generators of so(3) in su(6) are:

$$\begin{aligned} & f(L_-)'' = \sqrt{2}(E_{e_2-e_1} + E_{e_6-e_5}) + \sqrt{\tfrac{3}{2}}(E_{e_4-e_2} + E_{e_5-e_3} + E_{e_3-e_2} + E_{e_5-e_4}) \\ & f(L_0)'' = 2H_1 + H_2 - H_5 - 2H_6. \end{aligned} \tag{4.23}$$

The change of basis of the representation [1] of su(6) which brings $f(L_-)''$ into the form $f(L_-)$ is given by the matrix M''

$$M''=\begin{vmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} & 0 & 0 \\ 0 & 0 & -\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{vmatrix}. \tag{4.24}$$

The symmetry-adapted bosons for this chain are thus expressed in terms of the bosons of chain (A) as

$$d_2''^+ = d_2^+ \qquad d_1''^+ = d_1^+ \qquad d_0''^+ = \sqrt{\tfrac{1}{2}}d_0^+ + \sqrt{\tfrac{1}{2}}s_0^+$$
$$d_{-1}''^+ = d_{-1}^+ \qquad d_{-2}''^+ = d_{-2}^+ \qquad s''^+ = -\sqrt{\tfrac{1}{2}}d_0^+ + \sqrt{\tfrac{1}{2}}s^+.$$

5. Example: the representation [2]

In this section we choose the representation [2] of su(6) as an example. We will discuss the two boson states which transform at the so(3) level like $l=4$, $m=1$, 0. The states will be given in the notation which we use for the purpose of computer evaluation, as well as in the boson operator notation. The action of shift operators upon these states will be illustrated. Finally we will show the equivalence of the three states $l=4$, $m=0$ which are obtained through symmetry adaptation according to the three symmetry chains.

(A) Chain su(6)→su(5)→so(5)→so(3).

The symmetry adapted state for $l=4$, $m=1$, is obtained as

$$|[2],[2],(2,0),4;1\rangle = \sqrt{\tfrac{6}{7}}[011000]+\sqrt{\tfrac{1}{7}}[100010] = \sqrt{\tfrac{6}{7}}d_1^+d_0^+ + \sqrt{\tfrac{1}{7}}d_2^+d_{-1}^+$$

The operator $f(L_-)$ acts upon this state, in the form (4.11) with (3.2) or in the form (4.15),

$$\begin{aligned} f(L_-)|[2],[2],(2,0),4;1\rangle &= \sqrt{10}(4\sqrt{\tfrac{2}{70}}[010010]+\sqrt{\tfrac{2}{70}}[100001]+6\sqrt{\tfrac{1}{70}}[002000]) \\ &= \sqrt{10}(4\sqrt{\tfrac{2}{70}}d_1^+d_{-1}^+ + \sqrt{\tfrac{2}{70}}d_2^+d_{-2}^+ + 6\sqrt{\tfrac{1}{70}}(d_0^+)^2/\sqrt{2!}) \\ &= \sqrt{10}|[2],[2],(2,0),4;0\rangle. \end{aligned}$$

The $\sqrt{10}$ is the matrix element of $f(L_-)$ between the two states.

(B) Chain su(6)→su(3)→so(3).

The symmetry-adapted state for $l=4$, $m=1$, is obtained as

$$\begin{aligned} |[2],(0,4),4;1\rangle &= \sqrt{\tfrac{2}{7}}[010100]+\sqrt{\tfrac{1}{7}}[100010]+2\sqrt{\tfrac{1}{7}}[011000] \\ &= \sqrt{\tfrac{2}{7}}d_1^+s^+ + \sqrt{\tfrac{1}{7}}d_2^+d_{-1}^+ + 2\sqrt{\tfrac{1}{7}}d_1^+d_0^+. \end{aligned}$$

The operator $f(L_-)'$ acts upon this state in its form (4.17), or in the transcribed boson operator form,

$$\begin{aligned} f(L_-)'|[2],(0,4),4;1\rangle &= \sqrt{10}(4\sqrt{\tfrac{1}{70}}[002000]+2\sqrt{\tfrac{1}{70}}[000200]+4\sqrt{\tfrac{1}{70}}[001100]+4\sqrt{\tfrac{2}{70}}[010010] \\ &\quad +\sqrt{\tfrac{2}{70}}[100001]) \\ &= \sqrt{10}(4\sqrt{\tfrac{1}{70}}\frac{(d_0^+)^2}{\sqrt{2}}+2\sqrt{\tfrac{1}{70}}\frac{(s^+)^2}{\sqrt{2}}+4\sqrt{\tfrac{1}{70}}d_0^+s^++4\sqrt{\tfrac{2}{70}}d_1^+d_{-1}^++\sqrt{\tfrac{2}{70}}d_2^+d_{-2}^+) \\ &= \sqrt{10}|[2],(0,4),4;0\rangle. \end{aligned}$$

In obtaining this result we have used the same basis states, i.e. the same bosons, as for chain (A). If instead we introduce a new basis, i.e. primed bosons, defined by symmetry adaptation of the old basis according to chain (B) equation (4.19), then simple substitution yields

$$\begin{aligned} |[2],(0,4),4;0\rangle &= 4\sqrt{\tfrac{2}{70}}[010010]'+\sqrt{\tfrac{2}{70}}[100001]'+6\sqrt{\tfrac{1}{70}}[002000]' \\ &= 4\sqrt{\tfrac{2}{70}}d_1'^+d_{-1}'^++\sqrt{\tfrac{2}{70}}d_2'^+d_{-2}'^++6\sqrt{\tfrac{1}{70}}\sqrt{\tfrac{1}{2}}(d_0'^+)^2. \end{aligned}$$

(C) Chain $su(6)\to su(4)\sim so(6)\to so(5)\to so(3)$.

The symmetry adapted state for $l=4$, $m=1$ is obtained as

$$\begin{aligned} |[2],(11\text{—}1\text{—}1),(2,0),4;1\rangle &= \sqrt{\tfrac{3}{7}}[010100]+\sqrt{\tfrac{3}{7}}[011000]+\sqrt{\tfrac{1}{7}}[100010] \\ &= \sqrt{\tfrac{3}{7}}d_1^+s^++\sqrt{\tfrac{3}{7}}d_1^+d_0^++\sqrt{\tfrac{1}{7}}d_2^+d_{-1}^+. \end{aligned}$$

The operator $f(L_-)''$ acts upon this state in its form (4.23), or in the transcribed boson operator form,

$$\begin{aligned} f(L_-)''|[2],(11\text{—}1\text{—}1),(2,0),4;1\rangle &= \sqrt{10}\{3\sqrt{\tfrac{1}{70}}[002000]+3\sqrt{\tfrac{1}{70}}[000200]+3\sqrt{\tfrac{2}{70}}[001100] \\ &\quad +4\sqrt{\tfrac{2}{70}}[010010]+\sqrt{\tfrac{2}{70}}[100001] \\ &= \sqrt{10}(3\sqrt{\tfrac{1}{70}}\sqrt{\tfrac{1}{2}}(d_0^+)^2+3\sqrt{\tfrac{1}{70}}\sqrt{\tfrac{1}{2}}(s^+)^2+3\sqrt{\tfrac{2}{70}}d_0^+s^++4\sqrt{\tfrac{2}{70}}d_1^+d_{-1}^++\sqrt{\tfrac{2}{70}}d_2^+d_{-2}^+ \\ &= \sqrt{10}|[2],(11\text{—}1\text{—}1),(2,0),4;0\rangle. \end{aligned}$$

These states are given in the basis which is symmetry adapted through chain (A), represented by unprimed states and boson operators. Introducing a new basis, i.e. new boson operators, symmetry adapted through chain (C), and defined by (4.24), then simple substitution yields

$$\begin{aligned} |[2],(11\text{—}1\text{—}1),(2,0),4;0\rangle &= 4\sqrt{\tfrac{2}{70}}[010010]''+\sqrt{\tfrac{2}{70}}[100001]''+6\sqrt{\tfrac{1}{70}}[002000]'' \\ &= 4\sqrt{\tfrac{2}{70}}d_1''^+d_{-1}''^++\sqrt{\tfrac{2}{70}}d_2''^+d_{-2}''^++6\sqrt{\tfrac{1}{70}}\sqrt{\tfrac{1}{2}}(d_0''^+)^2. \end{aligned}$$

6. Final remarks

The method for the calculation for the symmetry adaptation of wavefunctions described in this article is valid for *any* semisimple symmetry chain. It is based upon *integer calculus*, and thus the results are *exact*.

Three problems, often considered as separate problems, are treated in a unified manner, namely:

(a) the construction of bases for the irreducible representations of semisimple Lie algebras L;

(b) the construction of bases for irreducible representations $D(M')$ for any semisimple Lie algebra L′ of L in terms of the basis $D(M)$ of the Lie algebra L;

(c) the direct product of representations of a semisimple Lie algebra L.

Thus, our definition of symmetry adaptations coefficients is very general and implies:

(i) the coefficients for the linear combinations of the originally chosen basis states which need to be formed in order that the algebra takes on its standard form (diagonal Cartan subalgebra raising and lowering operators);

(ii) the coefficients of the linear combinations of basis states $|M, m\rangle$ of the algebra L, which need to be formed in order to obtain the appropriate basis $D(M')$, for any of its semisimple Lie subalgebras L′;

(iii) the familiar Clebsch-Gordan coefficients. With (i), (ii) and (iii) are associated multiplicity problems, namely; for (i), the 'inner multiplicity', i.e. the dimension of the weight subspaces of an (irreducible) representation space; for (ii), the 'branching multiplicity', i.e. the multiple occurrence of identical representations of a subalgebra L′ of L under restriction of L to L′; and for (iii) the 'outer multiplicity', i.e. the multiple occurrence of identical representations in the reduction of the direct product of representations.

These multiplicity problems are automatically resolved by our method. However for (ii) and (iii) we make an arbitrary choice of basis for multiplicities $\geqslant 2$, due to the lack of a physical principle for a preferred choice of basis. Any other desired choice of basis is then obtained as a linear combination over the bases which we obtain for identical representations.

The symmetry adaptation of states and the calculation of matrix elements, as outlined in this article, has been implemented for computer evaluation. A computer code for symmetry adaptation coefficients has been worked out by two of the authors [11-13]; as an example a systematic and complete tabulation has been obtained for *all* semisimple symmetry chains of su(4) ~ so(6), for all irreducible representations of su(4) up to, and including, four particles (i.e. $[N_1, N_2, N_3, N_4]$, $N = \Sigma_{i=1}^4 N_i$, $N_i \leqslant 4$). The representation [3, 1, 1, 1] is also included as an example for a larger value of N. Direct products will be discussed in volumes 3 and 4 of [13].

Acknowledgment

One of the authors (BG) wishes to thank Professor F Zaccaria for hospitality at the Dipartimento di Fisica Teorica of the Università di Napoli.

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