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Symmetry-adapted wavefunctions and matrix elements: the general case

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Abstract. The method of symmetry adaptation of wavefunctions with respect to any semisimple symmetry chain originating from a $SU(l+1)$ algebra for completely symmetrical representations $[N]$ of $SU(l+1)$ is extended to the case of arbitrary representations $[N_1, N_2, \ldots, N_{l+1}]$ of $SU(l+1)$ with $N_1 \geqslant N_2 \geqslant \ldots \geqslant N_{l+1}$ and $N_1+N_2+\ldots+N_{l+1}=N$.

1. Introduction

In a previous paper [1] we discussed a method for the symmetry adaptation and the determination of matrix elements according to an arbitrary semisimple symmetry chain originating from a unitary algebra $SU(l+1)$. A computer implementation of this method is available meanwhile [2]. The method in [1] is, however, limited to the case of *completely symmetric* representations of $SU(l+1)$.

In the present paper we deal with the case of representations of $SU(l+1)$ which correspond to an *arbitrary* symmetry of the symmetric group S_N. That is, we consider representations whose states (wavefunctions) transform with respect to the pair $(SU(l+1), S_N)$, where $l+1$ equals the number of distinct quantum states of single particle states, while N is equal to the number of (independent) particles from which the composite state is formed. It turns out that only minor modifications of the method described in [1] are necessary for this general case. Since the method itself remains essentially unchanged, we concentrate on these modifications in the following.

In [1] then, given a set of $l+1$ single particle states and N particles, each state of the representation $SU(l+1)$ was completely symmetric with respect to an exchange of the N particles. In the present article we consider representations of $SU(l+1)$ for which each state transforms like a state of an *arbitrary*, but fixed, irreducible representation of S_N. This is equivalent to stating that we discuss the case of an arbitrary finite dimensional irreducible representation of $SU(l+1)$ in an independent wavefunction (independent particle) picture. Direct products $SU(l_1+1)\otimes SU(l_2+1)\otimes\ldots\mapsto\ldots$ are treated in an analogous manner.

It should be pointed out that the method presented in [1] and in this article is not restricted to the Gel'fand-Zetlin basis chains, which have already been discussed in great detail (e.g. [3, 4]), but is also valid for *any other* semisimple symmetry chain.

2. Definitions

In [1] the completely symmetrical representations of $SU(l+1)$ were discussed which are characterized by the partition

$$[N, 0, \ldots, 0] \equiv [N]$$

where the number N of single particle wavefunctions is followed by l zeros. An arbitrary state of $[N]$ is then (uniquely) characterized by the sequence of non-negative integers (a weight)

$$[n_1, n_2, \ldots, n_{l+1}] \qquad \sum_{i=1}^{l+1} n_i = N.$$

Now, an irreducible representation of $SU(l+1)$ is characterized by a partition of N into non-negative integers N_i such that

$$[N_1, N_2, \ldots, N_{l+1}] \qquad N_1 \geqslant N_2 \geqslant \ldots \geqslant N_{l+1} \qquad \sum_{i=1}^{l+1} N_i = N.$$

An arbitrary state of this representation is again characterized by weights of the type

$$[n_1, n_2, \ldots, n_{l+1}] \qquad \sum_{i=1}^{l+1} n_i = N$$

but now

(*a*) there are subsidiary conditions on the n_i, and

(*b*) a given partition (weight) can correspond to more than one state (i.e. uniqueness is lost).

We do not need to discuss (*a*) and (*b*), since our method resolves both problems in a natural and automatic manner.

The completely symmetrical representations of [1] form a special case of the representations considered in the present work, with multiplicity of weights equal to 1. The sets of weights (weight diagrams) of the representations considered here form subsets of the sets of weights of the completely symmetrical representations $[N]$ of [1], and their multiplicity is $\geqslant 1$.

3. Symmetry adaptation and matrix elements

Starting with the (unique) state which corresponds to a highest weight of a finite dimensional irreducible representation of $SU(l+1)$, which is either $[N]$ (for the case of completely symmetrical representations) or $[N_1, N_2, \ldots, N_{l+1}]$, with $N_2 > 0$ (for the not completely symmetrical representations), the action of the (simple) lowering operators of $SU(l+1)$ generates a state which corresponds to a lower weight (unless the state is mapped to zero). This state is uniquely characterized for representations $[N]$, while this is not the case for the not completely symmetrical representations with $N_2 > 0$. However, from the invariance and irreducibility of the representations it follows that the action of the (simple) lowering operators yields a set of states which spans the subspace associated with any given weight. (This is analogous to the problem encountered in [1] for the case of non-completely symmetrical representations of *sub*algebras of $SU(l+1)$.) Orthonormalization then yields an orthonormal basis for the weight subspace, as well as the matrix elements for the action of the lowering operators.

What needs to be determined is thus the unique state (weight function) which corresponds to the highest weight of an arbitrary representation $[N_1, N_2, \ldots, N_{l+1}]$ of SU($l+1$). This is achieved by constructing a N-particle wavefunction from N_1 wavefunctions of type 1, N_2 wavefunctions of type 2, etc., which obeys the symmetry $[N_1, N_2, \ldots, N_{l+1}]$ of the symmetric group S_N. The procedure used to construct such a wavefunction is standard and well known [3, 5–8]. Since the irreducible representations of S_N may have dimensionality greater than 1, one obtains in general different realizations of a given SU($l+1$) representation. A complete *set* of equivalent realizations of the same representation $[N_1, N_2, \ldots, N_{l+1}]$ of SU($l+1$) then forms a basis for the representation $[N_1, N_2, \ldots, N_{l+1}]$ of S_N.

For the case of the completely symmetrical representations $[N]$ of SU($l+1$) considered in [1] the limits of a weight diagram are always given by the vanishing of the matrix elements of the lowering (or raising) operators. For the general case of representations of arbitrary symmetry the limit of a weight diagram can also be given by the vanishing of a wavefunction, while the matrix element remains finite and non-zero. This is a consequence of the non-trivial symmetry of wavefunctions in this general case.

Due to the nature of the completely symmetrical representations $[N]$ of SU($l+1$) a boson operator calculus can be introduced. That is, boson creation operators b_i^+ and boson annihilator operators b_i with $i=1, 2, \ldots, l+1$ are introduced by means of which both the algebra SU($l+1$) and the states of its completely symmetrical representations can be realized:

$$E(e_j - e_i) \equiv b_j^+ b_i$$

$$[n_1, n_2, \ldots, n_{l+1}] \equiv \frac{1}{\sqrt{n_1!}}(b_1^+)^{n_1} \frac{1}{\sqrt{n_2!}}(b_2^+)^{n_2} \ldots \frac{1}{\sqrt{n_{l+1}!}}(b_{l+1}^+)^{n_{l+1}}$$

where the b_i^+, b_j satisfy the familiar commutation relations

$$[b_i, b_j] = 0 \qquad [b_i, b_j^+] = \delta_{ij}.$$

Moreover we assume that the b_i acting upon the vacuum state $|0\rangle$ (the identity **1** in the algebra) yield zero:

$$b_i|0\rangle \equiv b_i 1 = 0.$$

With this, the action of a boson creation and annihilation operator pair upon a state $[n_1, n_2, \ldots, n_{l+1}]$ is straightforward:

$$\begin{aligned} E(e_j - e_i)&\left\{\ldots \frac{1}{\sqrt{n_i!}}(b_i^+)^{n_i} \ldots \frac{1}{\sqrt{n_j!}}(b_j^+)^{n_j} \ldots\right\} \\ &= \left\{\ldots \frac{n_i}{\sqrt{n_i!}}(b_i^+)^{n_i-1} \ldots \frac{1}{\sqrt{n_j!}}(b_j^+)^{n_j+1} \ldots\right\} \\ &= \sqrt{n_i}\sqrt{n_j+1}\left\{\ldots \frac{1}{\sqrt{(n_i+1)!}}(b_i^+)^{n_i-1} \ldots \frac{1}{\sqrt{(n_j+1)!}}(b_j^+)^{n_j+1} \ldots\right\} \\ &= \sqrt{n_i}\sqrt{n_j+1}\,[n_1, \ldots, n_i - 1, \ldots, n_j + 1, \ldots, n_{l+1}]. \end{aligned}$$

Obviously the states $[n_1, n_2, \ldots, n_{l+1}]$ can never disappear, and it is the zero matrix elements which limit the representation.

For the general case of a representation $[N_1, N_2, \ldots, N_{l+1}]$ of SU($l+1$), which is the scope of this paper, this simple boson picture does not apply. In order to treat the general situation we consider the N bosons to be inequivalent, i.e. to be labelled:

$$b_i^+(k) \qquad k = 1, 2, \ldots, N.$$

Furthermore we assume the Lie products

$$[b_i(k), b_j(s)] = 0 \qquad [b_i(k), b_j^+(s)] = \delta_{ij}\delta_{ks}$$

and

$$b_i(k)|0\rangle \equiv b_i(k)1^{(k)} = 0.$$

That is, we are dealing with a direct product $b_i^+(k) \otimes b_j^+(s) \equiv b_i^+(k)b_j^+(s)$ of N *independent* and *inequivalent* bosons,

$$b_i^+(1)b_i^+(2)\ldots b_i^+(n_1)b_j^+(n_1+1)\ldots b_j^+(n_1+n_2)\ldots b_s^+(n_i+n_j+\ldots+n_s=N)$$

with $i<j<\ldots<s$, $i, j, \ldots, s = 1, 2, \ldots, l+1$, and the notation

$$b^+_{\text{state}}(\text{particle}).$$

For this direct product the shift operators are given as

$$E^{\otimes}(e_j-e_i) = E^{(1)}(e_j-e_i) + E^{(2)}(e_j-e_i) + \ldots + E^{(N)}(e_j-e_i)$$

with $E^{(k)}(e_j-e_i) = b_j^+(k)b_i(k)$, where we have used the simplifying standard notation of ignoring the identity operators $1^{(k)}$. Acting with a shift operator upon a properly symmetrized and normalized state $\{\ldots\}$ corresponding to the weight $m = (m_1, m_2, \ldots, m_{l+1})$, we obtain (with $r \geqslant n+n_i$ and $b_i(n+1)1^{(n+1)} = 0$):

$$\begin{aligned}
E^{\otimes}(e_j-e_i)&\{\ldots b_i^+(n+1)b_i^+(n+2)\ldots b_i^+(n+n_i)\ldots b_j^+(r+1)b_j^+(r+2)\ldots b_j^+(r+n_j)\ldots\} \\
&= \{\ldots[(b_i^+(n+1)b_i^+(n+2)1^{(n+1)} + 1^{(n+1)})b_j^+(n+1)b_i^+(n+2)\ldots b_i^+(n+n_i) \\
&\quad + b_i^+(n+1)b_j^+(n+2)\ldots b_i^+(n+n_i) \\
&\quad \vdots \\
&\quad + b_i^+(n+1)b_i^+(n+2)\ldots b_j^+(n+n_i)]\ldots \\
&\quad \ldots b_j^+(r+1)b_j^+(r+2)\ldots b_j^+(r+n_j)\ldots\} \qquad \text{for } n_i>0
\end{aligned}$$

and

$$\begin{aligned}
E^{\otimes}(e_j-e_i)&\{\ldots b_i^+(n+1)b_i^+(n+2)\ldots b_i^+(n+n_i)\ldots b_j^+(r+1)b_j^+(r+2)\ldots b_j^+(r+n_j)\ldots\} \\
&= 0 \qquad \text{for } n_i = 0.
\end{aligned}$$

The resultant state, if non-zero, belongs to weight $m+e_j-e_i$. Normalization of a, non-zero state of the above form yields the matrix element of the operator $E^{\otimes}(e_j-e_i)$ between the two states.

As pointed out before, the resultant state may in fact be the zero state. This will happen if the various terms of the linear combination which make up the state add up to zero. (In the general expression given above only one such term was considered.)

This generalization of the boson operator calculus yields all finite dimensional irreducible representations $[N_1, N_2, \ldots, N_{l+1}]$ with $N_1 \geqslant N_2 \geqslant \ldots \geqslant N_{l+1}$ and $N_1+N_2+\ldots+N_{l+1} = N$ for the algebras SU($l+1$). Having obtained the properly symmetrized states for the representations of SU($l+1$) with respect to S_N in this manner, the symmetrization according to a semisimple symmetry chain originating from SU($l+1$) follows the familiar pattern described in [1].

For the completely symmetrical representations $[N]$ of SU$(l+1)$ we obtain from the generalized boson calculus the familiar result by 'collapsing' the states, i.e. by making the bosons equivalent. This is achieved by dropping the labels k,

$$b_j^+(k) \mapsto b_j^+.$$

Inserting the numerical factors which are needed for the normalization (to 1) of the boson states [9], we then obtain the familiar result for the case of completely symmetrical representations $[N]$ of SU$(l+1)$; all other representations $[N_1, N_2, \ldots, N_{l+1}]$ with $N_2 > 0$ collapse to zero in this case.

A computer code for this general case of the arbitrary representations $[N_1, N_2, \ldots, N_{l+1}]$ of SU$(l+1)$ has been developed [10] and will be available soon [11].

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