Structure constants of $su(2S + 1)$ algebra and the decomplexification of the Liouville-von Neumann equation

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Abstract. The analytic formulas for structure constants of $su(2S + 1)$ algebra in terms of $3jm$ and $6j$ symbols of $su(2)$ have been derived for the decomplexification of the Liouville-von Neumann equation.

1. Introduction

Let $\{C^S_i, C^S_j, \ldots, C^S_n\}$ be a base of $su(2S+1)$ algebra, where $S = 1/2, 1, 3/2, \ldots$ is the spin quantum number, $n = (2S + 1)^2 - 1$. We have according to [1]

\[
C^S_i C^S_j = \frac{c}{d} E \delta_{ij} + z^S_{ijk} C^S_k, \quad \text{Tr} C^S_i = 0, \quad \text{Tr} C^S_i C^S_j = c \delta_{ij},
\]

(1)

\[
z^S_{ijk} = g^S_{ijk} + ic^S_{ijk},
\]

(2)

hence

\[-i[C^S_i, C^S_j] = 2c^S_{ijk} C^S_k, \quad \{C^S_i, C^S_j\} = \frac{c}{d} E \delta_{ij} + 2g^S_{ijk} C^S_k,
\]

(3)

\[c^S_{ijk} = \frac{1}{2ic} \text{Tr} [C^S_i, C^S_j] C^S_k,
\]

(4)

\[g^S_{ijk} = \frac{1}{2c} \text{Tr} \{C^S_i, C^S_j\} C^S_k,
\]

(5)

where $d = 2S + 1$, $E$ is the unit matrix in dimension $d \times d$, $c$ is a constant, $\text{Tr}$ is a symbol for trace. It is easy to see that the structure constants $c^S_{ijk}$ and $g^S_{ijk}$ are completely antisymmetric and symmetric in the displacement of any pair of indices.

2. Hermitian basis

In order to calculate the structure constants we have to choose the basis. The basis is based on linear combinations of irreducible tensor operators.

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The matrix representations of irreducible tensor operators \( T^S_{k,q} \) can be calculated using the Wigner 3\( j \)m symbols:

\[
T^S_{k,q} = \sqrt{(2S + 1)(2k + 1)} \sum_{m,m'=-S}^S (-1)^{S-m} \left( \begin{array}{ccc}
S & k & m \\
-m & q & m'
\end{array} \right) |S,m><S,m'|,
\]

where \( 0 \leq k \leq 2S \), and \(-k \leq q \leq k\) in steps of 1. The normalization is such that \( T^S_{0,0} = E \). It is known that the Cartesian product operators \( S_x, S_y, \) and \( S_z \) for spin \( S = \frac{1}{2} \) are Hermitian and can be calculated from irreducible tensor operators [3]

\[
S^x_{\frac{1}{2}} = \frac{1}{2\sqrt{2}} (T^\frac{1}{2}_{1,-1} - T^\frac{1}{2}_{1,1}) = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},
\]

\[
S^y_{\frac{1}{2}} = \frac{i}{2\sqrt{2}} (T^\frac{1}{2}_{1,-1} + T^\frac{1}{2}_{1,1}) = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},
\]

\[
S^z_{\frac{1}{2}} = \frac{1}{2} T^{\frac{1}{2}}_{1,0} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

Allard and H"ard [4] have formed linear combinations of the irreducible tensor operators not only for single-quantum coherences, but also for all coherences according to

\[
C^S_{k,qx} = \sqrt{\frac{S(S+1)}{6}} (T^S_{k,-q} + (-1)^q T^S_{k,q}), \quad q \neq 0,
\]

\[
C^S_{k,gy} = i \sqrt{\frac{S(S+1)}{6}} (T^S_{k,-q} - (-1)^q T^S_{k,q}), \quad q \neq 0,
\]

\[
C^S_{k,z} = \sqrt{\frac{S(S+1)}{3}} T^S_{k,0}, \quad q = 0, k \geq 1,
\]

\[
C^S_{0,z} = \sqrt{\frac{S(S+1)}{3}} E,
\]

where \( 1 \leq k \leq 2S \), and \( 1 \leq q \leq k \) in \( C^S_{k,qx}, C^S_{k,gy} \) and \( 1 \leq k \leq 2S \), in \( C^S_{k,z} \) in steps of 1. The matrices \([10][11][12]\) are traceless and their number is equal to \((2S + 1)^2 - 1\). Using the well-known relations for the irreducible tensor operators

\[
(T^S_{k,q})^+ = (-1)^q T^S_{k,-q},
\]

we can see that matrices \([10][11][12]\) are Hermitian. Using the formula from [2]

\[
\text{Tr} T^S_{k,q} T^S_{k',q'} = (-1)^q (2S + 1) \delta_{k,k'} \delta_{q,-q'}
\]
it is easy to show that the basis is normalized so that \( S_x = C^S_{1,x}, S_y = C^S_{1,y}, S_z = C^S_{1,z} \), irrespective of the spin quantum number \( S \), i.e.

\[
(C_r, C_s) = \text{Tr} C_r C_s = \delta_{r,s} \frac{S(S + 1)(2S + 1)}{3}.
\] (16)

The set \( (10-13) \) is complete. The matrices \( C_{k,z} \) are diagonal

\[
[C^S_{k,z}, C^S_{k',z}] = 0.
\] (17)

There also exist the other useful bases \([5]\). From the physical point of view, for some applications the basis \([4]\) is preferred.

3. Analytic formulas for structure constants

There are 27 combinations in threes including the repetitions: \( XX'X'' \), \( XX'Y'' \), \( XX'Z'' \), where \( X = C^S_{k,q}, X' = C^S_{k',q'}, Y'' = C^S_{k'',q''}, Z'' = C^S_{k'',z} \) and so on. The use of the symmetrical properties of the Wigner 3\( j \)m symbols and the formula

\[
\text{Tr} T^S_{k,q} T^S_{k',q'} T^S_{k'',q''} = (-1)^{2S+k+k'+k''}(2S+1) \frac{3!}{2!} \{ k\ k'\ k'' \ q\ q'\ q'' \},
\]

where \( \{ k\ k'\ k'' \ q\ q'\ q'' \} \) is the 6\( j \) symbol, allows us after substitution of \( (10,11,12) \) in \( (4,5) \), to calculate all structure constants of \( su(2S + 1) \) algebra. Let us introduce the function

\[
F(k, k', k'', S) = \frac{(-1)^{2S}}{\sqrt{3}} \sqrt{S(S + 1)(2S + 1)(2k + 1)(2k' + 1)(2k'' + 1)} \{ k\ k'\ k'' \ S\ S\ S \}.
\] (19)

All antisymmetric structure constants are zero for \( K = k + k' + k'' \) even and nonvanishing antisymmetric structure constants in terms of 3\( jm \) and 6\( j \) symbols have the explicit form are presented by formulas \( (20,21,22) \) for \( K \) odd:

\[
\epsilon^S_{XX'Y''} = -F \sqrt{3} [(-1)^q \left( \frac{k\ k'\ k''}{q-q'-q''} \right) + (-1)^{q'} \left( \frac{k\ k'\ k''}{-q\ q'-q''} \right) + (-1)^{q''} \left( \frac{k\ k'\ k''}{q\ q'-q''} \right)],
\] (20)

\[
\epsilon^S_{YY'Y''} = \frac{F}{\sqrt{2}} [(-1)^q \left( \frac{k\ k'\ k''}{q-q'-q''} \right) + (-1)^{q'} \left( \frac{k\ k'\ k''}{-q\ q'-q''} \right) + (-1)^{q''} \left( \frac{k\ k'\ k''}{q\ q'-q''} \right)],
\] (21)

\[
\epsilon^S_{XY'Z''} = -F \left[ (-1)^q \left( \frac{k\ k'\ k''}{q-q'-q''} \right) \right].
\] (22)
All symmetric structure constants are zero for \( K = k + k' + k'' \) odd and nonvanishing symmetric structure constants in terms of \( 3jm \) and \( 6j \) symbols have the explicit form are presented by formulas (23,24,25) for \( K \) even:

\[
g_{XX'X''}^S = \frac{F}{\sqrt{2}} (-1)^q \left( \frac{k' k''}{q - q' - q''} \right) + (-1)^{q'} \left( \frac{k' k''}{-q' q' - q''} \right) + (-1)^{q''} \left( \frac{k' k''}{-q q' - q''} \right),
\]

(23)

\[
g_{XY'Y''}^S = \frac{F}{\sqrt{2}} (-1)^q \left( \frac{k k' k''}{q - q' - q''} \right) + (-1)^{q'} \left( \frac{k k' k''}{-q' q' - q''} \right) + (-1)^{q''} \left( \frac{k k' k''}{-q q' - q''} \right),
\]

(24)

\[
g_{XZ'Z''}^S = g_{YX'Y''}^S = F(-1)^q \left( \frac{k' k''}{q - q' - q''} \right), \quad g_{ZZ'Z''}^S = F(-1)^q \left( \frac{k k' k''}{0 0 0} \right).
\]

(25)

We have in \( X, Y \leq k, k', k'' \leq 2S, 1 \leq q \leq k, 1 \leq q' \leq k', 1 \leq q'' \leq k'' \) and in \( Z \leq k, k', k'' \leq 2S \) in steps of 1.

The direct calculation confirms that the structure constants \( e_{ijk}^S \) and \( g_{ijk}^S \) are completely antisymmetric and symmetric in the displacement of any pair of operators. In other words it is \( e_{XX'Y''}^S = -e_{XY'Y''}^S, g_{XX'Z''}^S = g_{YY'Z''}^S \) and so on.

4. Decomplexification of the Liouville-von Neumann equation

The structure constants of \( su(2S + 1) \) algebra have wide physical applications. Let us consider the Liouville-von Neumann equation for the density matrix \( \rho \), describing the dynamics of a system. It has the form

\[
i \partial_t \rho = [\hat{H}, \rho], \quad \rho(t = 0) = \rho_0, \quad \rho^+ = \rho, \quad Tr \rho = 1,
\]

(26)

where \( \hat{H} \) is the Hamiltonian of the system.

The state of a \( d \)-dimensional quantum system (qudit) is usually described by the \( d \times d \) density matrix \( \rho \). Let us present the solution of the equation (26) for one qudit as \( \rho = \frac{1}{(2S_1 + 1)!} \sqrt{\frac{S_1(S_1 + 1)}{2}} R_{0} C_{0}^{S_1}, \quad R_{0} = 1, \quad \hat{H} = \frac{1}{2} h_{\beta} C_{\beta}^{S_1}. \) We multiply (26) by \( C_{0}^{S_1} \) and execute the operation \( Tr \), where by definition

\[
Tr \rho C_{0}^{S_1} = \sqrt{\frac{S_1(S_1 + 1)}{2}} R_{0}, \quad C_{0}^{S_1} \in \{C_{0}^{S_1}, \ C_{k,q}^{S_1}, \ C_{k,q}^{S_1}, \ C_{k,z}^{S_1}, \ C_{0,z}^{S_1} \}. \quad \text{Hereinafter, the summation is made over the repeating Greek indices on the set (10,13), and over Latin indices on the set (10,11,12) and then on } k, \text{ and then on } q. \quad \text{The Liouville-von Neumann equation takes on the real form in terms of the functions } R_j \text{ as a closed system of differential equations for the set of initial conditions (9):}
\]

\[
\partial_t R_t = e_{ij}^{S_1} h_i R_j.
\]

(27)
The length of the generalized Bloch vector $b^{S_1}$ is conserved under unitary evolution

$$b^{S_1} = \sqrt{R_{m0}^2}. \quad (28)$$

For two different coupled qudits we have $\hat{H} = \frac{1}{2} h_{\alpha\beta} C^{S_1}_\alpha \otimes C^{S_2}_\beta$, 

$$\rho = \frac{3}{(2S_1 + 1)(2S_2 + 1)\sqrt{S_1(S_1 + 1)S_2(S_2 + 1)}} R_{\gamma\delta} C^{S_1}_\gamma \otimes C^{S_2}_\delta, \quad (29)$$

$R_{00} = 1$, where $\otimes$ is the symbol of direct product.

The dynamic equation (26) for two different qudits takes on the real form in terms of the functions $R_{m0}, R_{0m}, R_{mn}$ as a closed system of differential equations (30, 31, 32) for the set of initial conditions:

$$\partial_t R_{m0} = \frac{S_2(S_2 + 1)}{3} e^{S_1}_{pm} (h_{p0} R_{00} + h_{p1} R_{01}), \quad (30)$$

$$\partial_t R_{0m} = \frac{S_1(S_1 + 1)}{3} e^{S_2}_{pm} (h_{0p} R_{00} + h_{1p} R_{11}), \quad (31)$$

$$\partial_t R_{mn} = e^{S_1}_{pm} \left[ \frac{S_2(S_2 + 1)}{3} (h_{pm} R_{00} + h_{p0} R_{mi}) + g_{rln}^{S_2} h_{rn} R_{il} \right] +$$

$$+ e^{S_2}_{pm} \left[ \frac{S_1(S_1 + 1)}{3} (h_{mp} R_{00} + h_{0p} R_{mi}) + g_{rln}^{S_1} h_{rp} R_{il} \right], \quad (32)$$

where by definition

$$\text{Tr} \rho C^{S_1}_\alpha \otimes C^{S_2}_\beta = \frac{1}{3} \sqrt{S_1(S_1 + 1)S_2(S_2 + 1)} R_{\alpha\beta}, \quad (33)$$

and $C^{S_2}_\beta \in \{C^{S_2}_{k,0}, C^{S_2}_{k,qx}, C^{S_2}_{k,qy}, C^{S_2}_{k,z}, C^{S_2}_{0,z}\}$ . The functions $R_{m0}, R_{0m}$ describe the individual qudits and the functions $R_{mn}$ define their correlations.

The length of the generalized Bloch vector $b^{S_1S_2}$ is conserved under unitary evolution

$$b^{S_1S_2} = \sqrt{R_{m0}^2 + R_{0m}^2 + R_{mn}^2}. \quad (34)$$

The set of equations for 3 qubits has been obtained in [7]. The dynamic equations for 3 different qudits will be presented elsewhere.

5. Conclusion

It is not necessary for the basis to be Hermitian since the results of calculations are independent of the choice of base, but there is the main advantage with the Hermitian basis. It is that the Liouville-von Neuman equation not
involve any complex numbers and can be solved using real algebra. This is not true for non-Hermitian bases. Real algebra makes numerical calculations faster and simplifies the interpretation of the equation system. This basis forms a natural basis for calculations on coupled spin systems (multipartite systems) because all the single-spin operators are part of the complete basis when the unit operator is part of the single-spin basis. The convolutions of structure constants can give rise to the additional relations between 3jm and 6j symbols. The relationship between the basis and the Gell-Mann basis for spin 1 has been presented in the appendix.

Appendix

The matrix representation of the complete set of the Hermitian operators for spin 1 (for qudit) has the form

\[
C_{0,z} = C_0 = \sqrt{2/3} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad C_{1,x} = C_1 = 1/\sqrt{2} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \\
C_{1,y} = C_2 = i/\sqrt{2} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad C_{1,z} = C_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \\
C_{2,y} = C_4 = i \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix}, \quad C_{1,2y} = C_5 = i/\sqrt{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \\
C_{2,z} = C_6 = 1/\sqrt{3} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad C_{2,x} = C_7 = 1/\sqrt{2} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}, \\
C_{2,2x} = C_8 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}.
\]

These matrices are traceless \(\text{Tr} C_a = 0\) and orthogonal \(\text{Tr} C_a C_b = 2\delta_{ab}\), \(1 \leq a, b \leq 8\). The relationship between the basis \(C_a\) and the Gell-Mann basis \(\lambda_a\) is the following:

\[
C_1 = 1/\sqrt{2} (\lambda_1 + \lambda_6), C_2 = 1/\sqrt{2} (\lambda_2 + \lambda_7), C_3 = 1/2 \lambda_3 + \sqrt{3}/2 \lambda_8, C_4 = \lambda_5, C_5 = 1/\sqrt{2} (\lambda_2 - \lambda_7), C_6 = \sqrt{3}/2 \lambda_3 - 1/2 \lambda_8, C_7 = 1/\sqrt{2} (\lambda_1 - \lambda_6), C_8 = \lambda_4.
\]

The antisymmetric (symmetric) structure constants \(e_{abc}\) \(g_{abc}\) are correspondingly equal to: \(e_{123} = e_{158} = e_{254} = e_{278} = e_{375} = e_{471} = 1/2\), \(e_{156} = e_{672} = \sqrt{3}/2\), \(e_{348} = -1\); \(g_{336} = g_{446} = -g_{666} = g_{688} = 1/\sqrt{3}\), \(g_{556} = g_{116} = g_{226} = g_{677} = -1/2\sqrt{3}\), \(g_{235} = g_{118} = g_{558} = g_{124} = g_{137} = -g_{228} = -g_{778} = -g_{475} = 1/2\). Hence, we have \(C_a C_b = 2/3\delta_{ab} + g_{abc} C_c + i e_{abc} C_c\).
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