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Dynamic multi-coupling coefficients

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Abstract. Dynamic multi-coupling coefficients are introduced to describe $SU(2)$ couplings in quantum many-body systems in which the coupling coefficients of N angular momenta are parameter-dependent. It is shown that these dynamic multi-coupling coefficients in a spin-interaction system for arbitrary spin can be determined by solving a set of nonlinear algebraic equations using an algebraic Bethe ansatz.

Coupling coefficients are important in various quantum many-body problems. The concept of coupling two angular momenta is well known through standard texts [1–4]. In this case the coefficients are called either Clebsch–Gordan (CG) coefficients, $3j$ symbols or Wigner coefficients—all of which are related to one another by simple phase and/or normalization factors.

Coefficients for coupling N angular momenta are multi-coupling coefficients. Assume, for example, that there are N particles in a system. One can easily construct an N-particle state with good total angular momentum by sequentially coupling, using two-particle coupling (CG) coefficients, the angular momentum of each particle to the angular momentum of the previously coupled set. The process starts with two particles and keeps track of all intermediate angular momentum values. For example, if there are three particles with angular momenta I_1, I_2 and I_3, respectively, one has

$$|(I_1I_2)I_{12}, I_3; IM_I\rangle = \sum_{m_1m_2m_3m_{12}} \langle I_1m_1, I_2m_2|I_{12}m_{12}\rangle\langle I_{12}m_{12}, I_3m_3|IM_I\rangle|I_1m_1, I_2m_2, I_3m_3\rangle \tag{1}$$

where $\langle I_1m_1, I_2m_2|I_{12}m_{12}\rangle$ is an $SU(2)$ CG coefficient. In this case the intermediate quantum number I_{12} can serve as an additional quantum number to distinguish multiple occurrences of the total angular momentum I. Alternatively, one may change the order of couplings by first coupling I_2 with I_3, or I_1 with I_3. In the latter two cases, I_{23} or I_{13}, respectively, play the same role as I_{12} does in the former case. It is well known that these three distinct couplings schemes can be transformed into one another using Racah coefficients or, equivalently, $6j$ symbols. There is an extensive literature dealing with this problem. The projection technique of Löwdin has been one of the most popular [5]. In [4], Biedenharn and Louck provide a Wigner operator method that combines CG couplings with results from the theory of the symmetric groups.

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Other methods can be found in the literature [6–12]. It is important to note, however, that for arbitrary N and angular momenta $I(j)$ $(j = 1, 2, \ldots, N)$, a unique scheme for the construction of basis vectors with good total angular momentum has not been given, principally because of unsolved problems relating to the additional labels that are required to specify a basis uniquely. This challenge is related to the multiplicity of occurrences of irreps of $SU(2) \times S_N$ in coupled representations. The only case that has been treated explicitly [4] is N particles with spin $\frac{1}{2}$.

There are some quantum many-body systems for which all intermediate angular momenta $\vec{I}(ij) = \vec{I}(i) + \vec{I}(j)$ with $1 \leqslant i, j \leqslant N$ are broken, while the total angular momentum $\vec{I} = \sum_i \vec{I}(i)$ is conserved. In such cases, straightforward coupling methods are not useful. As an example, let us consider the N-spin interaction system [13] for which the Hamiltonian may be written as

$$\hat{H} = \sum_{ij} c_i c_j \left(I_+(i) I_-(j) + I_0(i) I_0(j)\right) - \sum_j c_j^2 I_0(j) \tag{2}$$

where c_i $(i = 1, 2, \ldots, N)$ are assumed to be real but unequal parameters, and $I_\mu(j)$ with $\mu = 0, +, -$ are generators of the jth spin. It can be proven that the total spin operators $I_\mu = \sum_i I_\mu(i)$ commute with the Hamiltonian $\hat{H}$,

$$[\hat{H}, I_\mu] = 0 \qquad \text{for} \quad \mu = 0, +, -. \tag{3}$$

Therefore, the total spin I and the quantum number of its third component M_I are good quantum numbers. On the other hand, one can also verify that all the intermediate spins $I_\mu(ij) = I_\mu(i) + I_\mu(j)$ with $i \neq j$ for $N > 2$ are not conserved:

$$[\hat{H}, I_\mu(ij)] \neq 0 \qquad \text{for} \quad N > 2. \tag{4}$$

In the latter case, one cannot use elementary $SU(2)$ pair couplings to obtain final states with total spin I and projection M_I as described in equation (1).

To diagonalize the Hamiltonian (2) and obtain the corresponding eigenstates, we introduce the $SU(2)$ Kac–Moody algebra with generators J_μ^m $(m = 0, 1, 2, \ldots)$ defined by

$$J_\mu^m = \sum_{j=1}^{N} c_j^m I_\mu(j) \tag{5}$$

which satisfy the following commutation relations:

$$[J_+^m, J_-^n] = 2J_0^{m+n} \qquad [J_0^m, J_\pm^n] = \pm J_\pm^{m+n}. \tag{6}$$

Then, Hamiltonian (2) can be rewritten in terms of the generators of the $SU(2)$ Kac–Moody algebra as follows:

$$\hat{H} = J_+^1 J_-^1 + (J_0^1)^2 - J_0^2. \tag{7}$$

The lowest-weight state satisfies

$$J_-^m |0\rangle = 0 \qquad \text{for} \quad m = 0, \pm 1, \pm 2, \ldots \tag{8}$$

where

$$|0\rangle = |I_1, -I_1; I_2, -I_2; \cdots; I_N, -I_N\rangle \tag{9}$$

is the uncoupled lowest-weight state with angular momenta $I_1, I_2, \ldots, I_N$. For convenience, the lowest-weight state defined in (8) is called the level zero state. Excited states are classified according to the number of raising operators $I_+(j)$ that are applied to the level zero state. If a state is constructed by applying $I_+(j)$ on the level zero state k times, the state is called a level k state. It can be proven [13] that up to a normalization constant the level k states of the Hamiltonian (7) can be written as

$$|k;\eta\rangle = J_+(x_1^{(\eta)})J_+(x_2^{(\eta)})\cdots J_+(x_k^{(\eta)})|0\rangle \tag{10}$$

where

$$J_+(x_i^{(\eta)}) = \sum_{j=1}^{N}\frac{c_j x_i^{(\eta)}}{1-x_i^{(\eta)}c_j}I_+(j) \tag{11}$$

and η is used to distinguish different eigenstates of (7) with the same k. The eigenvalues $E^{(k)}$ of (7) for the level k states are given by

$$E^{(k)} = \left(\sum_{j=1}^{N} I_j c_j\right)^2 - \sum_{j=1}^{N} I_j c_j^2 - 2\sum_{j=1}^{N} I_j c_j \sum_{i=1}^{k}\frac{1}{x_i^{(\eta)}} + \sum_{1\leqslant r\neq q\leqslant k}\frac{2}{x_r^{(\eta)}x_q^{(\eta)}} \tag{12}$$

where $x_i^{(\eta)}$ are determined by the following set of equations:

$$\sum_{j=1}^{N}\frac{c_j^2 x_i^{(\eta)} I_j}{c_j x_i^{(\eta)}-1} = \sum_{q\neq i}\frac{1}{x_i^{(\eta)}-x_q^{(\eta)}} + \sum_{j=1}^{N} c_j I_j \tag{13}$$

for $i = 1, 2, \ldots, k$. It should be clear that η is used to denote the ηth set of solutions $\{x_i^{(\eta)}\}$ of equation (13).

Hence, the general level k states can be recognized, up to a normalization constant, as

$$|k;\eta\rangle = \mathcal{N}\sum_{1\leqslant j_1 j_2\cdots j_k\leqslant N}\prod_{i=1}^{k}\left(\frac{I_+(j_i)x_i^{(\eta)}c_{j_i}}{1-x_i^{(\eta)}c_{j_i}}\right)|0\rangle$$
$$= \sum_{m_1 m_2\cdots m_N} W^{I_1 I_2\cdots I_N;\eta\ I}_{m_1 m_2\cdots m_N}(c_1, c_2, \ldots, c_N)|I_1 m_1; I_2 m_2; \cdots; I_N m_N\rangle \tag{14}$$

where $W^{I_1 I_2\cdots I_N;\eta\ I}_{m_1 m_2\cdots m_N}(c_1, c_2, \ldots, c_N)$ are defined as dynamic multi-coupling coefficients (DMCC) that depend on the dynamic parameters c_j ($j = 1, 2, \ldots, N$) for $N > 2$. These DMCCs reduce to the ordinary multi-coupling coefficients when all dynamic parameters c_j are the same, and to the CG coefficients of $SU(2)$ for $N = 2$. As has been stated, the intermediate spins $I(ij)$ for $N > 2$ are not good quantum numbers when the parameters c_j are unequal. Hence, these quantum numbers cannot be used to distinguish multiple occurrences of the final spin I in the coupling. However, one can verify that η can serve as a natural additional quantum number for distinguishing multiple occurrences of a final spin I in this case.

It can be shown that $\pm\infty$ are always solutions of equation (13). Furthermore, the basis vectors (14) and energy eigenvalues remain invariant under a sign change from $-\infty$ to $+\infty$. One can therefore choose $+\infty$ for the roots $x_i^{(\eta)}$ and arrange other roots systematically. For example, the roots can be arranged as $|x_1^{(\eta)}| < |x_2^{(\eta)}| < \cdots < |x_\mu^{(\eta)}| < x_{\mu+1}^{(\eta)} = x_{\mu+2}^{(\eta)} = \cdots = x_k^{(\eta)} = +\infty$ if the μth root is a finite complex number. If two roots $x_i^{(\eta)}$, $x_{i+1}^{(\eta)}$ are conjugate to each other with $a_1 \pm \mathrm{i}a_2$, where a_1 and a_2 are real numbers, we always set $x_i^{(\eta)} = a_1 - \mathrm{i}a_2$, $x_{i+1}^{(\eta)} = a_1 + \mathrm{i}a_2$.

The total spin quantum number is written as

$$I = I_1 + I_2 + \cdots + I_N - t \tag{15}$$

where $t = 0, 1, 2, \ldots, p$. The maximum integer value of t when $t = p$ should keep the spin quantum number I a positive integer or half-integer. For $t = 0$, there is only one set of solutions with $x_i = \infty$ ($i = 1, 2, \ldots, k$), which corresponds to the highest weight of the

Kronecker product of $SU(2)$ $I_1 \otimes I_2 \otimes \cdots \otimes I_N \downarrow I$ with $I = \sum_{i=1}^{N} I_i$. This coincides with the fact that the highest-weight configuration is always simple. For $t = 1$, the roots $x_2^{(\eta)} = x_3^{(\eta)} = \cdots = x_k^{(\eta)} = +\infty$. While $x_1^{(\eta)}$ should be determined by equation (13), in this case there are $N - 1$ sets of solutions with $x_1^{(\eta)}$ ($\eta = 1, 2, \ldots, N - 1$), which gives multiple occurrences of the weight $I_1 + I_2 + \cdots + I_N - 1$. For $t = p$, p finite roots should be obtained from (13) with $x_{p+\mu}^{(\eta)} = \infty$, $\mu = 1, 2, \ldots, k - p$. Using this procedure, one obtains the final state $|I; \eta; M_I\rangle$ with total angular momentum $I = I_1 + I_2 + \cdots + I_N - p$ and projection (third component) $M_I = k - I_1 - I_2 - \cdots - I_N$.

As an example, let us consider the $N = 3$ case. Eigenstates with $I = I_1 + I_2 + I_3 - 1$ and $M_I = 1 - I_1 - I_2 - I_3$ can be written as

$$\begin{aligned}|I; \eta; M_I\rangle = \mathcal{N}\big(&c_1\sqrt{2I_1}(1 - c_2x^{(\eta)})(1 - c_3x^{(\eta)})|I_1, 1 - I_1; I_2, -I_2; I_3, -I_3\rangle \\ &+c_2\sqrt{2I_2}(1 - c_1x^{(\eta)})(1 - c_3x^{(\eta)})|I_1, -I_1; I_2, 1 - I_2; I_3, -I_3\rangle \\ &+c_3\sqrt{2I_3}(1 - c_1x^{(\eta)})(1 - c_2x^{(\eta)})|I_1, -I_1; I_2, -I_2; I_3, 1 - I_3\rangle\big)\end{aligned} \tag{16}$$

where $\mathcal{N}$ is a normalization factor given by

$$\begin{aligned}\mathcal{N} = \big\{&c_1^2(1 - c_2x^{(\eta)})^2(1 - c_3x^{(\eta)})^2 2I_1 + c_2^2(1 - c_1x^{(\eta)})^2(1 - c_3x^{(\eta)})^2 2I_2 \\ &+c_3^2(1 - c_1x^{(\eta)})^2(1 - c_2x^{(\eta)})^2 2I_3\big\}^{-\frac{1}{2}}.\end{aligned} \tag{17}$$

One can read the multi-coupling coefficients from (16) as

$$\begin{aligned}W^{I_1,I_2,I_3;\eta,I}_{1-I_1,-I_2,-I_3} &= \mathcal{N}c_1\sqrt{2I_1}(1 - c_2x^{(\eta)})(1 - c_3x^{(\eta)}) \\ W^{I_1,I_2,I_3;\eta,I}_{-I_1,1-I_2,-I_3} &= \mathcal{N}c_2\sqrt{2I_2}(1 - c_1x^{(\eta)})(1 - c_3x^{(\eta)}) \\ W^{I_1,I_2,I_3;\eta,I}_{-I_1,-I_2,1-I_3} &= \mathcal{N}c_3\sqrt{2I_3}(1 - c_1x^{(\eta)})(1 - c_2x^{(\eta)})\end{aligned} \tag{18}$$

where the two different roots $x^{(\eta)}$ with $\eta = 1, 2$ of equation (13) are given by

$$x^{(1)} = \frac{c_1I_1(c_2 + c_3) + c_2I_2(c_1 + c_3) + c_3I_3(c_1 + c_2) - \mathcal{A}}{2c_1c_2c_3(I_1 + I_2 + I_3)} \tag{19a}$$

$$x^{(2)} = \frac{c_1I_1(c_2 + c_3) + c_2I_2(c_1 + c_3) + c_3I_3(c_1 + c_2) + \mathcal{A}}{2c_1c_2c_3(I_1 + I_2 + I_3)} \tag{19b}$$

where

$$\begin{aligned}\mathcal{A} = \{&c_1^2(c_2 - c_3)^2I_1^2 + 2c_1c_2(c_1 - c_3)(c_2 - c_3)I_1I_2 \\ &+c_2^2(c_1 - c_3)^2I_2^2 + 2c_1c_3(c_1 - c_2)(c_3 - c_2)I_1I_3 \\ &+2c_2c_3(c_2 - c_1)(c_3 - c_1)I_2I_3 + c_3^2(c_2 - c_1)^2I_3^2\}^{\frac{1}{2}}\end{aligned} \tag{20}$$

which is invariant under permutation of the indices 1, 2, 3.

Furthermore, one can verify that the number of sets of non-trivial roots $x_i^{(\eta)} \neq \infty$ of equation (13) with $k = t$ and $c_1 \neq c_2 \neq \cdots \neq c_N \neq 0$ is exactly equal to the number of occurrence of $I = \sum_{j=1}^{N} I_j - t$ in the decomposition of the Kronecker product $I_1 \otimes I_2 \otimes \cdots \otimes I_N \downarrow I$. For example, because there are $N - 1$ non-trivial roots $x_1^{(\eta)}$ when $k = t = 1$, one can conclude that $\sum_{j=1}^{N} I_j - 1$ occurs $N - 1$ times in the decomposition of the Kronecker product $I_1 \otimes I_2 \otimes \cdots \otimes I_N \downarrow \sum_{j=1}^{N} I_j - 1$ for $I_j \neq 0$ ($j = 1, 2, \ldots, N$). This result is also valid when c_j ($j = 1, 2, \ldots, N$) are all the same, which is consistent with the results of branching rules of $I_1 \otimes I_2 \otimes \cdots \otimes I_N \downarrow I$ in the angular momentum theory

Table 1. The number of occurrences ξ of $I = \frac{5}{2} - t$ for $t = 0, 1, 2$, and the corresponding roots of equation (13) with $c_1 = 1,\ c_2 = 2,\ c_3 = 3,\ c_4 = 4,\ c_5 = 5$ for the decomposition $\left(\frac{1}{2}\otimes\right)^4 \frac{1}{2} \downarrow I$.

$(I)^\xi$	t	Roots
$\frac{5}{2}$	0	—
$\left(\frac{3}{2}\right)^4$	1	$x_1^{(1)} = 0.220\,82,\ x_1^{(2)} = 0.295\,28$
		$x_1^{(3)} = 0.440\,84,\ x_1^{(4)} = 0.869\,72$
$\left(\frac{1}{2}\right)^5$	2	$x_1^{(1)} = 0.221\,78,\ x_2^{(1)} = 0.811\,99$
		$x_1^{(2)} = 0.223\,94,\ x_2^{(2)} = 0.411\,67$
		$x_1^{(3)} = 0.298\,26,\ x_2^{(3)} = 0.799\,35$
		$x_1^{(4)} = 0.455\,77,\ x_2^{(4)} = 0.722\,12$
		$x_1^{(5)} = 0.310\,89 - 0.0322\mathrm{i},\ x_2^{(5)} = 0.310\,89 + 0.0322\mathrm{i}$

Table 2. The number of occurrences ξ of $I = \frac{7}{2} - t$ for $t = 0, 1, 2$, and the corresponding roots of equation (13) with $c_1 = 1, c_2 = 2, c_3 = 3, c_4 = 4, c_5 = 5$ for the decomposition $\left(\frac{1}{2}\otimes\right)^4 \frac{3}{2} \downarrow I$.

$(I)^\xi$	t	Roots
$\frac{7}{2}$	0	—
$\left(\frac{5}{2}\right)^4$	1	$x_1^{(1)} = 0.235\,53,\ x_1^{(2)} = 0.307\,48$
		$x_1^{(3)} = 0.456\,24,\ x_1^{(4)} = 0.900\,75$
$\left(\frac{3}{2}\right)^6$	2	$x_1^{(1)} = 0.235\,96,\ x_2^{(1)} = 0.867\,40$
		$x_1^{(2)} = 0.236\,84,\ x_2^{(2)} = 0.437\,03$
		$x_1^{(3)} = 0.242\,28,\ x_2^{(3)} = 0.269\,01$
		$x_1^{(4)} = 0.309\,14,\ x_2^{(4)} = 0.861\,33$
		$x_1^{(5)} = 0.315\,49,\ x_2^{(5)} = 0.407\,82$
		$x_1^{(6)} = 0.463\,37,\ x_2^{(6)} = 0.834\,34$
$\left(\frac{1}{2}\right)^4$	3	$x_1^{(1)} = 0.237\,26,\ x_2^{(1)} = 0.454\,09,\ x_3^{(1)} = 0.708\,85$
		$x_1^{(2)} = 0.239\,73,\ x_2^{(2)} = 0.287\,74 - 0.0528\mathrm{i},\ x_3^{(2)} = 0.287\,74 + 0.0528\mathrm{i}$
		$x_1^{(3)} = 0.241\,38,\ x_2^{(3)} = 0.277\,12,\ x_3^{(3)} = 0.797\,11$
		$x_1^{(4)} = 0.315\,34,\ x_2^{(4)} = 0.443\,63,\ x_3^{(4)} = 0.676\,68$

[1–4]. Although it is not easy to prove this conclusion for $t > 1$ cases, it can be verified for any specific case. In tables 1–3 we report three non-trivial examples for decompositions of $\left(\frac{1}{2}\otimes\right)^4 \frac{1}{2}$, $\left(\frac{1}{2}\otimes\right)^4 \frac{3}{2}$ and $1\otimes 2\otimes 3$, respectively, and the corresponding roots, which are obtained by solving equation (13) with $c_i = i$ $(i = 1, 2, \ldots \leqslant 5)$. These examples show that the number of sets of non-trivial roots $x_i^{(\eta)} \neq \infty$ of equation (13) with $k = t$ and $c_1 \neq c_2 \neq \cdots \neq c_N \neq 0$ is indeed exactly equal to the number of occurrence of $I = \sum_{j=1}^{N} I_j - t$ in the decomposition of the Kronecker product $I_1 \otimes I_2 \otimes \cdots \otimes I_N \downarrow I$. It should also be stated that the DMCCs derived by equations (13) and (14) are mutually orthogonal with respect to different η values.

In summary, the concept of the dynamic multi-coupling coefficients is introduced to describe $SU(2)$ dynamic couplings in some quantum many-body systems, in which the coupling coefficients for N angular momenta are dynamic parameter-dependent and the intermediate angular momenta are not conserved. We provide an example for evaluation

Table 3. The number of occurrences ξ of $I = 6 - t$ for $t = 0, 1, 2, 3, 4, 5, 6$ and the corresponding roots of equation (13) with $c_1 = 1,\ c_2 = 2,\ c_3 = 3$ for the decomposition $1 \otimes 2 \otimes 3 \downarrow I$.

$(I)^\xi$	t	Roots
6	0	—
$(5)^2$	1	$x_1^{(1)} = 0.430\,96,\ x_1^{(2)} = 0.902\,37$
$(4)^3$	2	$x_1^{(1)} = 0.433\,95,\ x_2^{(1)} = 0.881\,96$
		$x_1^{(2)} = 0.434\,23 - 0.0273\mathrm{i},\ x_2^{(2)} = 0.434\,23 + 0.0273\mathrm{i}$
		$x_1^{(3)} = 0.941\,15 - 0.0531\mathrm{i},\ x_2^{(3)} = 0.941\,15 + 0.0531\mathrm{i}$
$(3)^3$	3	$x_1^{(1)} = 0.435\,91,\ x_2^{(1)} = 0.441\,21 - 0.053\mathrm{i},\ x_3^{(1)} = 0.441\,21 + 0.053\mathrm{i}$
		$x_1^{(2)} = 0.436\,28,\ x_2^{(2)} = 0.925\,59 - 0.0653\mathrm{i},\ x_3^{(2)} = 0.925\,59 + 0.0653\mathrm{i}$
		$x_1^{(3)} = 0.438\,67 - 0.026\,77\mathrm{i},\ x_2^{(3)} = 0.438\,67 + 0.026\,77\mathrm{i},\ x_3^{(3)} = 0.850\,20$
$(2)^3$	4	$x_1^{(1)} = 0.425\,45,\ x_2^{(1)} = 0.430\,62 - 0.410\,17\mathrm{i}$
		$x_3^{(1)} = 0.430\,62 + 0.410\,17\mathrm{i},\ x_4^{(1)} = 0.660\,65$
		$x_1^{(2)} = 0.441\,81 - 0.026\mathrm{i},\ x_2^{(2)} = 0.441\,81 + 0.026\mathrm{i}$
		$x_3^{(2)} = 0.898\,19 - 0.0853\mathrm{i},\ x_4^{(2)} = 0.898\,19 + 0.0853\mathrm{i}$
		$x_1^{(3)} = 0.442\,2,\ x_2^{(3)} = 0.449\,96 - 0.051\mathrm{i}$
		$x_3^{(3)} = 0.449\,96 + 0.051\mathrm{i},\ x_4^{(3)} = 0.792\,06$
$(1)^2$	5	$x_1^{(1)} = 0.445\,76,\ x_2^{(1)} = 0.4547 - 0.0486\mathrm{i}$
		$x_3^{(1)} = 0.454\,7 + 0.0486\mathrm{i},\ x_4^{(1)} = 0.833\,89 - 0.1248\mathrm{i}$
		$x_5^{(1)} = 0.833\,89 + 0.1248\mathrm{i}$
		$x_1^{(2)} = 0.449\,6,\ x_2^{(2)} = 0.457\,86 - 0.043\mathrm{i}$
		$x_3^{(2)} = 0.457\,86 + 0.043\mathrm{i},\ x_4^{(2)} = 0.514\,23 - 0.12\mathrm{i}$
		$x_5^{(2)} = 0.514\,23 + 0.12\mathrm{i}$
0	6	$x_1^{(1)} = 0.449\,1 - 0.02\mathrm{i},\ x_2^{(1)} = 0.4491 + 0.02\mathrm{i}$
		$x_3^{(1)} = 0.468\,2 - 0.074\mathrm{i},\ x_4^{(1)} = 0.4682 + 0.074\mathrm{i}$
		$x_5^{(1)} = 0.582\,71 - 0.2965\mathrm{i},\ x_6^{(1)} = 0.582\,71 + 0.2965\mathrm{i}$

of the DMCCs in a spin-interaction system for arbitrary spin value. In this case, the DMCCs can be determined by solving a set of nonlinear algebraic equations using an algebraic Bethe ansatz. It may be possible to extend this procedure to higher-rank Lie algebras.

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