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Exact solution for N-coupled symmetric rotors

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Abstract. The N-coupled symmetric rotor problem is solved exactly by using an infinite-dimensional algebra. A formalism for solving the corresponding Hamiltonian eigenvalue problem is also proposed. The system of equations that solves a special Hamiltonian eigenvalue problem is shown to yield coupling coefficients of the corresponding Lie algebra.

The quantum rotor has proven to be a very useful model for many physical applications, especially in the fields of molecular [1, 2] and nuclear physics [3, 4]. A summary can be found in a review paper by Draayer and Leschber [5]. In nuclear physics a connection between irreducible representations (irreps) of the $SU(3)$ shell model and eigenvalues of the principal moments of inertia of the rotor Hamiltonian has been established [6]. From this it follows that the dynamics of a quantum rotor can be realized in a $SU(3)$ shell-model framework. By exploiting this connection, a two-rotor picture can be realized via the coupling of two $SU(3)$ irreps [7]. This means that enhanced $M1$ transitions in heavy and well-deformed nuclei, predicted within the framework of the phenomenological two-rotor model (TRM) which considers the protons and neutrons as ellipsoidal distributions that perform rotational oscillations against one another, can be given a shell-model interpretation [8, 9]. Indeed, the scissors mode of the TRM, together with a novel twist mode that is realized when the parent proton and neutron distributions have triaxial shapes, has been given a microscopic interpretation within the framework of the pseudo-$SU(3)$ model [10, 11]. Likewise, N-coupled systems as found in Heisenberg spin chains [12], Hubbard models [13], and so on, are of general interest in other branches of physics.

Recently, it was shown that there may be a large class of many-body problems that can be solved exactly by introducing an infinite-dimensional algebra. The method was demonstrated for nuclear pairing problems [14, 15]. In these cases, the infinite-dimensional algebra is exactly, or similar to, the affine $SU(2)$ Lie algebra without central extension. In this paper, the N-coupled rotor Hamiltonian will be solved using a similar technique.

First, we introduce the following generators

$$I_{\pm}^{m} = \sum_{j=1}^{N} c_j^{2m+1} I_{\pm}(j) \qquad I_0^{m} = \sum_{j=1}^{N} c_j^{2m} I_0(j) \tag{1}$$

where c_j, with $j = 1, 2, \ldots, N$, are free parameters which for simplicity are taken to be real, $I_\mu(j)$ with $\mu = 0, +, -$, are generators of the intrinsic angular momentum for the jth

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rotor, and m can be taken to be a positive or negative integer, or zero. It is straightforward to verify that these generators satisfy

$$[I_+^m, I_-^n] = -2I_0^{m+n+1} \qquad [I_0^m, I_\pm^n] = -(\pm)I_\pm^{m+n}. \tag{2}$$

The algebra defined by these operators is therefore similar to the intrinsic $SU(2)$ affine Lie algebra without central extension [16]. Using the generators given in (1), one can write out the following N-coupled symmetric rotor Hamiltonian

$$\hat{H} = I_-^0 I_+^0 - I_0^1 + a\left(I_0^0\right)^2 + bI_0^0 I_0^1 \tag{3}$$

where a and b are additional parameters. Using (1), Hamiltonian (3) can be written as

$$\hat{H} = \hat{H}_0 + \hat{H}_{\mathrm{int}} = \sum_{j=1}^{N}(c_j^2(I_-(j)I_+(j) - I_0(j)) + (a + bc_j^2)(I_0(j))^2)$$
$$+ \sum_{j\neq j'}^{N}[(a + bc_{j'}^2)I_0(j)I_0(j') + c_j c_{j'} I_-(j)I_+(j')]. \tag{4}$$

By comparing expression (4) with the Hamiltonian of a symmetric rotor, the Hamiltonian of the jth subrotor can be identified as

$$\hat{H}_0(j) = c_j^2\left(I_x^2(j) + I_y^2(j)\right) + (a + bc_j^2)I_z^2(j). \tag{5}$$

Therefore, the moments of inertia of the jth subrotor are

$$\mathcal{J}_x = \mathcal{J}_y = \frac{1}{2c_j^2} \qquad \mathcal{J}_z = \frac{1}{2(a + bc_j^2)} \tag{6}$$

while

$$\hat{H}_{\mathrm{int}} = \sum_{j\neq j'}^{N}[(a + bc_{j'}^2)I_0(j)I_0(j') + c_j c_{j'} I_-(j)I_+(j')] \tag{7}$$

describes interactions among the N rotors. Specifically, for $N = 2$ the interaction term is

$$\hat{H}_{\mathrm{int}}^{N=2} = [2a + b(c_1^2 + c_2^2)]I_0(1)I_0(2) + c_1c_2[I_-(1)I_+(2) + I_-(2)I_+(1)]. \tag{8}$$

In this case, there are four parameters: c_j with $j = 1, 2$ and a and b. For the case of N rotors there are $N + 2$ parameters.

Depending upon the parametrization of the Hamiltonian, there are two types of lowest-weight state vectors. One, which is an eigenstate of the total angular momentum I, is achieved when $a = 1$ and all the c_j parameters are taken to be equal, $c_j = c \neq 0$ for $j = 1, 2, \ldots, N$. In this case the Hamiltonian can be written in terms of the total angular momentum operator,

$$\hat{H} = c^2 I^2 + bcI_0 \tag{9}$$

and lowest-weight state vectors are simply basis vectors of the total angular momentum and its third component, $|I, M_I\rangle$, with $M_I = -I$. A nontrivial case occurs when the c_j and the a and b are all different real numbers. In this case an exact solution of the corresponding eigenvalue problem can be achieved with the help of the infinite-dimensional algebra given in (2). The lowest-weight states for this case satisfy

$$I_+^m|0\rangle = 0 \qquad m = 0, \pm 1, \pm 2, \ldots \tag{10}$$

where

$$|0\rangle = |I_1, -I_1; I_2, -I_2; \ldots; I_N, -I_N\rangle \tag{11}$$

is an uncoupled lowest-weight state with fixed angular momenta $I_1, I_2, \ldots, I_N$, respectively, for each of the subrotor representations, and

$$I_0^m|0\rangle = \Lambda_0^m|0\rangle = \sum_{j=1}^{N}(-I_j)c_j^{2m}|0\rangle. \tag{12}$$

This lowest-weight state, which is the ground state of the N-coupled rotor problem, will be called the level 0 state. Excited states are classified according to the number of raising operators $I_-(j)$ that are applied on the level 0 state. If a state is constructed by applying $I_-(j)$ on the level 0 state k times, the state is called the level k state. It can be shown that up to a normalization factor the level k eigenvectors of the Hamiltonian (3) can be written in the form

$$|k\rangle = I_-^{x_1} I_-^{x_2} \ldots I_-^{x_k}|0\rangle \tag{13}$$

where

$$I_-^{x_i} = \sum_{j=1}^{N} \frac{c_j}{1 - x_i c_j^2} I_-(j). \tag{14}$$

To obtain the variables x_i for $i = 1, 2, \ldots, k$, we first expand (14) in terms of x_i around $x_i = 0$. Thus,

$$|k\rangle = \sum_{n_i} x_1^{n_1} x_2^{n_2} \ldots x_k^{n_k} I_-^{n_1} I_-^{n_2} \ldots I_-^{n_k}|0\rangle \tag{15}$$

where $I_-^{n_i}$ are Fourier–Laurent coefficients in the expansion of $I_-^{x_i}$, namely

$$I_-^{n_i} = \frac{1}{2\pi \mathrm{i}} \oint_0 \mathrm{d}x_i\, x_i^{n_i} I_-^{x_i}. \tag{16}$$

Using (15) and commutation relations (2), one can easily prove that the x_i with $i = 1, 2, \ldots, k$, satisfy the following relations

$$h^{(k)} = \sum_{i=1}^{N} \frac{b(\Lambda_0^0 + k) - 1}{x_i} \tag{17}$$

$$\frac{b(\Lambda_0^0 + k) - 1}{x_i} = \sum_{p=1}^{N} \frac{2I_p c_p^2}{1 - x_i c_p^2} - \sum_{j \neq i} \frac{2}{x_i - x_j} \qquad \text{for } i = 1, 2, \ldots, k \tag{18}$$

where

$$h^{(k)} = E_k - a\Lambda_0^0(\Lambda_0^0 + 2k) - b\Lambda_0^1(\Lambda_0^0 + k) - ak^2 + \Lambda_0^1 \tag{19}$$

and E_k is the energy eigenvalue for level k. Even though these relations are derived near $x_i = 0$, they are valid in the entire complex plane. Hence, the coefficients x_i and energy eigenvalues are simultaneously determined by the system of equations (17) and (18). Equations (17) and (18) give exact solutions for the energy spectrum and wavefunctions.

In general, total angular momentum is not a good quantum number for the N-coupled rotor Hamiltonian given by (3) with different c_j parameters. As a consequence, it cannot be used to solve coupling problems of $SU(2)$. However, this becomes feasible if one considers another type of Hamiltonian, namely

$$\hat{H} = J_-^1 J_+^1 - J_0^2 + a(J_0^1)^2 + bJ_0^0 J_0^1. \tag{20}$$

The generators J_μ^m with $m = 1, 2, \ldots,$ and $\mu = 0, \pm$, are defined by

$$J_\mu^m = \sum_{j=1}^{N} c_j^m I_\mu(j) \tag{21}$$

with the following commutation relations

$$[J_+^m, J_-^n] = -2J_0^{m+n} \qquad [J_0^m, J_\pm^n] = -(\pm)J_\pm^{m+n}. \tag{22}$$

In the following, the paramters c_j are assumed to be different real numbers. Using the same method as employed for diagonalizing (3), one can prove that exact solutions can only be obtained for the $a = 1$ case. The eigenvalues $E^{(k)}$ for the level k state

$$|k\rangle = J_-^{x_1} J_-^{x_2} \ldots J_-^{x_k} |0\rangle \tag{23}$$

where

$$J_-^{x_i} = \sum_{j=1}^{N} \frac{c_j x_i}{1 - x_i c_j} I_-(j) \tag{24}$$

are given by

$$h^{(k)} = \sum_{i \neq j} \frac{2}{x_i x_j} + \Delta_k \sum_{i=1}^{k} \frac{1}{x_i} \tag{25}$$

where

$$h^{(k)} = E^k - \lambda_0^2 - b\lambda_0^1\lambda_0^0 - (\lambda_0^1)^2 - kb\lambda_0^1 \tag{26}$$

$$\Delta_k = 2\lambda_0^1 + b(\lambda_0^0 + k) \tag{27}$$

$$\lambda_0^n = -\sum_{j=1}^{N} I_j c_j^n \tag{28}$$

with the x_i are determined by the following set of equations

$$\sum_{j=1}^{N} \frac{c_j^2 x_i I_j}{c_j x_i - 1} = \sum_{q \neq i} \frac{1}{x_i - x_q} - \Delta_k/2 \tag{29}$$

for $i = 1, 2, \ldots, k$.

It can be verified that whereas the third component of the total angular momentum, J_0^0, is a good quantum number for Hamiltonian (20), the total angular momentum itself is in general not a conserved quantity. An interesting case occurs when $N = 2$ with $b = 0$. In this special case, the total angular momentum is a good quantum number and the Hamiltonian (20) can be written as

$$\hat{H} = c_1^2 \boldsymbol{I}(1)^2 + c_2^2 \boldsymbol{I}(2)^2 + 2c_1c_2 \boldsymbol{I}(1) \cdot \boldsymbol{I}(2). \tag{30}$$

The general level k state can be recognized, up to a normalization factor, as

$$|k\rangle = \mathcal{N} \sum_{1 \leqslant j_1 j_2 \ldots j_k \leqslant 2} \prod_{i=1}^{k} \left(\frac{I_-(j_i) x_i c_{j_i}}{1 - x_i c_{j_i}} \right) |0\rangle = |(I_1 I_2) I M\rangle = \sum_{M_1 M_2} C_{I_1 M_1 I_2 M_2}^{IM} |I_1 M_1; I_2 M_2\rangle \tag{31}$$

where $\mathcal{N}$ is the normalization factor, $M = k - I_1 - I_2$, and $C_{I_1 M_1 I_2 M_2}^{IM}$ is the corresponding Clebsch–Gordan (CG) coefficients of SU(2). Therefore, (29) can be used to evaluate coupling coefficients of $SU(2)$ when $b = 0$ and $N = 2$, regardless of what c_j values are taken.

It can be verified that the level k states given by (23) have S_k symmetry with respect to permutations among different roots x_i for $i = 1, 2, \ldots, k$ determined by (29). It can also be shown that $\pm\infty$ are always solutions when $b = 0$. The basis vectors (31) and energy eigenvalues (25) also remain invariant under a sign change from $-\infty$ to $+\infty$ for some of the roots x_i. This means we can choose $+\infty$ for the roots x_i for some cases, which enables us to discuss the root systems systematically. For example, the roots can be arranged as $|x_1| < |x_2| < \cdots < |x_\mu| < x_{\mu+1} = x_{\mu+2} = \cdots = x_k = +\infty$ if the μth root is a finite complex number. If two roots x_i and x_{i+1} are conjugate to each other, $a_1 \pm \mathrm{i}a_2$, where the a_i with $i = 1, 2$ are real numbers, we always write $x_i = a_1 - \mathrm{i}a_2$, $x_{i+1} = a_1 + \mathrm{i}a_2$. The total angular momentum quantum number is written as

$$I = I_1 + I_2 - t \tag{32}$$

where $t = 0, 1, 2, \ldots, I_1 + I_2 - |I_1 - I_2|$. Thus, for a given level k, $t \leqslant k$. One can easily obtain the following solutions

$$x_i = \infty \qquad \text{with } i = 1, 2, \ldots, k \text{ for } t = 0 \tag{33}$$

$$x_1 = \frac{c_1 I_1 + c_2 I_2}{c_1 c_2 (I_1 + I_2)} \qquad x_2 = x_3 = \cdots = x_k = \infty \text{ for } t = 1 \tag{34}$$

$$x_1 = \frac{(2I_1 + 2I_2 - 1)(2c_1 I_1 + 2c_2 I_2 - c_1 c_2) + \mathrm{i}(c_1 - c_2)\sqrt{(2I_1 - 1)(2I_2 - 1)(2I_1 + 2I_2 - 1)}}{2c_1 c_2 (I_1 + I_2 - 1)(2I_1 + 2I_2 - 1)}$$

$$x_2 = \frac{(2I_1 + 2I_2 - 1)(2c_1 I_1 + 2c_2 I_2 - c_1 c_2) - \mathrm{i}(c_1 - c_2)\sqrt{(2I_1 - 1)(2I_2 - 1)(2I_1 + 2I_2 - 1)}}{2c_1 c_2 (I_1 + I_2 - 1)(2I_1 + 2I_2 - 1)}$$

$$x_3 = x_4 = \cdots = x_k = \infty \text{ for } t = 2 \tag{35}$$

$$\cdots \quad \cdots .$$

For $t = \mu$, μ finite roots should be obtained from (29) with $i = 1, 2, \ldots, \mu$, while other roots are all infinite. Finally, when $t = k$, the k roots are all finite different complex numbers $x_1 < x_2 < x_3 < \cdots < x_k$, which can be derived directly from (29).

As examples, we now derive CG coefficients using the proposed method. For the $k = 1$ case, only $t = 0$ or 1 is possible. For $t = 0$, the CG coefficients are very simply given, after normalization, by

$$C^{I_1+I_2, 1-I_1-I_2}_{I_1-I_1+1, I_2-I_2} = \sqrt{\frac{I_1}{I_1 + I_2}} \qquad C^{I_1+I_2, 1-I_1-I_2}_{I_1-I_1, I_2-I_2+1} = \sqrt{\frac{I_2}{I_1 + I_2}}. \tag{36}$$

For the $t = 1$ case, the basis vector can be written as

$$|I_1 + I_2 - 1, 1 - I_1 - I_2\rangle = \frac{c_1 x\sqrt{2I_1}}{1 - c_1 x}|I_1, 1 - I_1; I_2, -I_2\rangle + \frac{c_2 x\sqrt{2I_2}}{1 - x c_2}|I_1, -I_1; I_2, 1 - I_2\rangle \tag{37}$$

where

$$x = \frac{c_1 I_1 + c_2 I_2}{c_1 c_2 (I_1 + I_2)}. \tag{38}$$

After normalization, we obtain

$$C^{I_1+I_2-1, 1-I_1-I_2}_{I_1-I_1+1, I_2-I_2} = \sqrt{\frac{I_2}{I_1 + I_2}} \qquad C^{I_1+I_2-1, 1-I_1-I_2}_{I_1-I_1, I_2-I_2+1} = -\sqrt{\frac{I_1}{I_1 + I_2}}. \tag{39}$$

The phase has been set to the standard Condon–Shortley convention.

It should be pointed out that there is a correspondence between the Hamiltonians introduced in (3) and (20) with $N = 2$ and the Hamiltonian used to describe a two-rotor neutron–proton model for nuclei, which have recently been discussed in detail within an $SU(3)$ framework [10, 17] through the mapping from an intrinsic variable description to its algebraic $SU(3)$ realization [5, 6]. Such Hamiltonians may also be useful in the description of spin-glass systems [18, 19].

Actually, the approach presented in this paper follows the algebraic Bethe ansatz [20] for wavefunctions (13) and (23), which has become a standard procedure in exactly solvable models [13, 21, 22]. The difference between this method and other Bethe ansatz solutions is that an infinite Lie algebra is used instead of finite nonlinear algebras such as the Yang–Baxter or Zamolodchikov types. There should be a link between an infinite Lie algebra of the type discussed here and a corresponding nonlinear algebra. This will be studied in the near future.

The methodology introduced in this paper, when extended to higher-rank Lie algebras, is nontrivial. Nevertheless, coupling coefficients, including multiplicities, can be evaluated via equations similar to (29). This will be the topic of a future study.

We conclude that there are new classes of exactly sovable many-body problems that can be discovered by exploiting infinite-dimensional algebraic techniques. As this paper shows, it is also possible to use this technique for the evaluation of coupling coefficients of the corresponding Lie algebra. Applications of this method to other many-body problems, especially associated with higher-rank algebras, are in progress.

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