ALGEBRAIC REALIZATION OF ROTATIONAL DYNAMICS

Yorick LESCHBER and J.P. DRAAYER
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4001, USA.

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It is shown that the dynamics of a quantum rotor can be realized in terms of the SU(2)\(\otimes\)SO(3) group algebra. Specifically, an analytic result is given for mapping from the hamiltonian of a rotating rotor to its algebraic image. Under the mapping invariants of the rotor are carried into Casimir invariants of the algebraic theory. Results for specific transition rates and various states are given to demonstrate the effectiveness of the mapping. The theory gives physical significance to operators that were first introduced by Racah as a means for resolving the SU(2)\(\otimes\)SO(3) state labelling problem. As the SU(2)\(\otimes\)SO(3) structure is common to the rotational limit of several nuclear models, the theory also offers an opportunity to explore in a new way the microscopic underpinnings of rotational phenomena in nuclei.

The rotor is one of the earliest and most thoroughly studied problems in quantum mechanics [1]. The hamiltonian is given by

\[
H^{ro}\ =\ A_1 I_1^2 \ +\ A_2 I_2^2 \ +\ A_I I_I^2 ,
\]

where \(I_k\) is the projection of the angular momentum on the \(k\)-th body-fixed principal axis and \(A_k = 1/2\ I_k\) is the corresponding inertia parameter. To select one of the 3N equivalent rotor geometries, let \(A_1 < A_2 < A_3\). It is then convenient to introduce an asymmetric parameter \(\kappa = (A_2 - A_1)/(A_2 - A_3)\) with range \(-1 < \kappa < 1\). The \(\kappa = -1\) limit corresponds to a prolate rotor \((A_3 = A_1)\) while \(\kappa = +1\) specifies an oblate geometry \((A_3 = A_2)\) and \(\kappa = 0\) is the most asymmetric case \((A_3 = A_2 - A_1)/2\).

The rotor hamiltonian is invariant under rotations by \(\pi\) about the principal axes. This set of transformations, \(\{E_{I}\}\), where \(E\) is the identity and \(E_{I} = \exp(i\xi I_{I})\), generates the Wigner group \((D_{3})\). As a consequence the hamiltonian matrix, which has dimension \(2I + 1\) for angular momentum \(I\), can be brought into block diagonal form with the submatrices labelled by the symmetry classes of \(D_{3}\) of table 1. A convenient representation for the eigenstates is given by

\[
y_{L}(x,\theta) = \sum_{\lambda=0}^{L} C^{L}(x,\theta) P^{L}(x,\theta) \phi_{\lambda},
\]

where \(\phi_{\lambda}\) is an eigenstate of \(H^{ro}\) with eigenvalue \(\lambda\), that is, \(\phi_{\lambda} = \lambda \phi_{\lambda} \). Note that

\[
\phi_{\lambda} = \frac{2I + 1}{(I + \alpha)(I + \beta)} \phi_{\lambda}.
\]

\[
\left[D_{3}\phi_{\lambda} = (-1)^{x+y+z} D_{3}\phi_{\lambda}\right],
\]

where \(D_{3}\phi_{\lambda}\) are standard SO(3) rotation matrices. For the axially symmetric case \((\kappa = 1)\) the magnitude of \(\kappa\) which is the eigenvalue of \(I_{1}\) is a good quantum number but, as indicated, eigenstates of the asymmetric rotor \((\kappa = -1)\) involve a linear combination of states with different \(\kappa\) values. The prime on the summation indicates either all even or all odd values for \(\kappa\). The parameterization of the phase in (2) in terms of \(\lambda\) which can be even or odd, and \(\mu\), which is even for \(\kappa\) even and odd for \(\kappa\) odd, is done in anticipation of the corresponding algebraic result that is given below. The traditional choice replaces the \(\lambda = 0\) \(\phi^{\lambda}\) expression by a single quantity \(\gamma\) and it rather cumbersome rule for assigning it a value. Note how simply \(\lambda\) and \(\mu\) specify the symmetry class of \(D_{3}\) to which the eigenstates belong, see table 1.

The rotor hamiltonian can be rewritten in a frame-independent form by introducing and using the mass quadrupole tensor,

\[
Q_{\mu\nu} = \frac{1}{2}(3xz - z^2 - \delta_{\mu\nu} d^2) d^2 r,
\]

In the principal axis system \(Q_{\mu\nu}\) is diagonal with eigenvalues \(\lambda_{\mu}\) that is, \(Q_{\mu\nu} = \lambda_{\mu} \delta_{\mu\nu}\). Note that

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\[ \lambda_1 + \lambda_2 + \lambda_3 = 0. \]

It follows from this definition that

\[ X_1 = \sum_{\alpha} \lambda_\alpha^{(1)} X_\alpha + \lambda_\alpha^{(2)} X_\alpha, \]

\[ X_2 = \sum_{\alpha} \lambda_\alpha^{(3)} X_\alpha. \]

The superindex "a" is appended to denote collective model operators. This set of equations (4), can be solved to yield the \( I_1, I_2, I_3 \) as functions of \( I_1, X_1, \) and \( X_2 \):

\[ I_1 = (\lambda_1 I_1 + \lambda_2 I_2 + \lambda_3 I_3) (2 I_2^2 + 2 \lambda_2 I_3). \]

Substituting (5) into (1) one finds that

\[ A_1 I_1^2 + A_2 I_2^2 + A_3 I_3^2 = H_{\text{rot}} \]

\[ = a I_1^2 + b X_1^2 + c X_2. \]

Note that no assumption is made regarding a relationship between the \( X_1 \) and the \( I_1, I_2, I_3 \). For example, an asymmetric shape can be mapped onto a symmetric inertia ellipsoid.

The rotor Hamiltonian is rewritten in a frame-independent form, even though the principal-axis expression is simpler, because it that form its SU(3) \( \rightarrow \text{SO}(3) \) image follows as a trivial corollary [2]. To see this, recall that the eight generators of SU(3) can be realized as five components of a second rank quadrupole tensor, \( Q^\mu \) \( (\mu = -2, -1, 0, +1, \)

+2), and the three components of the rank one angular momentum operator, \( L_\alpha \) \( (\alpha = 1, 2, 3). \) The \( L_\alpha \) generate the SO(3) subgroup of SU(3). The superindex "a" is appended to distinguish the algebraic \( Q^\alpha \) which are symmetric in the coordinate and momentum variables from the collective model \( Q^\alpha \) which are not. One consequence of this difference is that the \( Q^\alpha \) have no matrix elements coupling different major shells of the oscillator whereas the \( Q^\alpha \) do. More precisely, the \( [L_\alpha, Q^\alpha] \) generate a semidirect product, noncompact structure \( T_S \times \text{SO}(3) \) which is the symmetry group of the rotor and has infinite dimensional representations while the \( [L_\alpha, Q^\alpha] \) generate a semidirect product, noncompact structure \( T_S \times \text{SO}(3) \) which is a compact group with finite dimensional representations. This difference and consequences of it will be discussed in greater depth elsewhere.

If one ignores differences between the algebraic and the collective model \( Q^\alpha \) one is driven to postulate the following form for the SU(3) \( \rightarrow \text{SO}(3) \) image of the rotor Hamiltonian:

\[ H_{\text{rot}} \approx a I_1^2 + b X_1^2 + c X_2. \]

Here the \( L_1^2, X_1, \) and \( X_2 \) operators are given by (4) with \( I = -L \) and \( Q^\alpha \rightarrow Q^\alpha. \) Apart from an additive constant factor and an \( L_1^2 \) term, this form for \( H_{\text{rot}} \) is in the most general so-called invariant interaction one can form that is of order four or less in the generators of SU(3). Of course if \( H_{\text{rot}} \) included an \( L_1^2 \) term, which introduces a centrifugal stretching or antisymmetric "correction" to the rotor dynamics, it would be required in \( H_{\text{rot}} \) too.

The constants \( (a, b, c) \) of \( H_{\text{rot}} \) depend on the iner-
ria parameters of the rotor and the eigenvalues of $Q_r$, see (6). For a consistent picture, the constants ($\lambda$, $\beta$, $\epsilon$) of $H_{\text{rot}}$ should have the same functional form as those for $H_{\text{rot}}$, but with the eigenvalues of $Q_r$ replaced by those of $Q_0$. But what are these eigenvalues? The Hill-Wheeler projection prescription used by Elliott provides an answer [3]. Basis states of the SU(1) × SO(3) type can be generated by projecting from an SU(3) × SU(2) × U(1) intrinsic state of highest weight. The highest weight state is defined to be that commutant configuration of the oscillator with the largest number of quanta in the 3 direction, the next greatest number in the 1 direction, and the least number of quanta in the 2 direction, $|\sigma_1\rangle > |\sigma_2\rangle > |\sigma_3\rangle$. Since the number of quanta in any direction is directly proportional to the expectation value of the square of the corresponding coordinate which, in turn, is proportional to the eigenvalue of that component of the mass quadrupole operator, one has the following:

$$
\lambda_0 \sim \langle \lambda_0 | = \langle \sigma_1 | = \langle \sigma_2 | = \langle \sigma_3 | = \langle \sigma_1 - \sigma_2 | = \langle \sigma_2 - \sigma_3 | = \langle \sigma_3 - \sigma_1 |
$$

$$
\lambda_1 \sim \langle \sigma_1 | = \langle \sigma_1 + \sigma_2 | = \langle \sigma_2 + \sigma_3 | = \langle \sigma_3 + \sigma_1 |
$$

$$
\lambda_2 \sim \langle \sigma_2 | = \langle \sigma_2 + \sigma_3 | = \langle \sigma_3 + \sigma_2 | = \langle \sigma_1 + \sigma_2 |
$$

In (8), $\lambda$ and $\mu$ are irreducible representation labels of SU(1) × SO(3) and the $\sigma_i$ are additive constants satisfying the commutation relations $\sigma_i \sigma_j + \sigma_j \sigma_i = 6$. They can be fixed by requiring the collective model invariants to map onto Casimir invariants of the algebraic theory. The choice $\sigma_1 = 0$, $\sigma_2 = -1$, $\sigma_3 = 1$ yields

$$
\text{Tr}(Q_r^2) = \lambda_0^2 + \lambda_1^2 + \lambda_2^2
$$

$$
\text{Tr}(Q_r^3) = \lambda_0^3 + \lambda_1^3 + \lambda_2^3
$$

$$
\text{Tr}(Q_r^4) = \lambda_0^4 + \lambda_1^4 + \lambda_2^4
$$

$$
\lambda_0 = \frac{1}{2} (\lambda_1 + \lambda_2 + \lambda_3)
$$

$$
\lambda_1 = \frac{1}{2} (\lambda_1 - \lambda_2 + \lambda_3)
$$

$$
\lambda_2 = \frac{1}{2} (\lambda_1 + \lambda_2 - \lambda_3)
$$

(9)

So given the representation labels $\lambda$ and $\mu$ of SU(3), and the inertia parameters of the rotor, $H_{\text{rot}}$ can be determined. But does this algebraic hamiltonian reproduce the roto dynamic? The results that follow may be of interest. We see that for $\epsilon > 0$ there are several cases. One involves the dimensionality of the model space and the $D_2$ symmetry. In ref. [4] the symmetry properties of the SU(1) × SO(3) basis states are given. From these it follows that for projection from the highest weight state

$$
\lambda_0 = - \lambda_1 = - \lambda_2 = - \lambda_3
$$

(10)

This is the relation that is satisfied by the eigenstates of $H_{\text{rot}}$, see (2). This suggests that the even or odd character of the representation label $\lambda$ and $\mu$ determine the symmetry class of $D_2$ to which the eigenstates of $H_{\text{rot}}$ belong. If dimensionality check reinforces this conjecture. The number of occurrences of a given value $\lambda$ in the representation $\lambda \lambda \lambda$ is given by

$$
\text{d}(\lambda, \mu, \nu) = \frac{1}{2} \left( \delta_{\lambda, \mu} + \delta_{\lambda, \mu} \right)
$$

(11)

The square bracket denotes the integer function. For the rotor the $2 \times 1$ states of angular momentum $I$ divide up under $D_2$ as shown in table 1, (1+2)2 for an $E$ and $A$-type symmetry, etc. It is a simple exercise to verify that for $L = \min (\lambda, \mu, \nu) + 1$ the two results agree. But for $L > \min (\lambda, \mu, \nu) + 1$, the two do not agree. This is because SU(3) is a complex group and $\lambda_0 \times \lambda_1 \times \lambda_2$ is noncomposable. For example, the $(\lambda_0 = 0, \lambda_1 = 1, \lambda_2 = 0)$ representation of SU(3) has three $L = 6$ states whereas the rotor has four. As will now be shown, the eigenstates of $H_{\text{rot}}$ correspond to the eigenstates of $H_{\text{rot}}$.

Eigensystems of the rotor are known to satisfy various sum rules. The most familiar of these, which applies for A-type symmetry, is $E_{\lambda_0} + E_{\lambda_1} = E_{\lambda_2}$, that is, the sum of the eigenenergies for $I = 3$ is equal to the sum of the eigenenergies for $I = 1$. The general result is

$$
\text{Tr}(H_{\text{rot}}) = \text{Tr}(H_{\text{rot}}), \gamma = 1.
$$

(12)

Similar relations hold for the other symmetry types. From these results analytic expressions for traces of $H_{\text{rot}}$ can be deduced, see table 2. Since the sums are different ($\epsilon = 1$) for each of the four classes of $D_2$, they can be used to demonstrate that the representation labels $\lambda$ and $\mu$ do indeed specify the symmetry
Table 2
Algebraic expression for traces of $H_{\alpha\beta}$ with $E_A = 2/3$ and $E_C = 2/3$.

<table>
<thead>
<tr>
<th>Symmetry type</th>
<th>Trace expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T(\alpha\beta)$</td>
<td>$T(\text{even})$ or $T(\text{odd})$</td>
</tr>
<tr>
<td>$A_1$</td>
<td>$T(2J+1)$ for $E_A = 2/3$</td>
</tr>
<tr>
<td>$B_1$</td>
<td>$T(2J+1)$ for $E_A = 2/3$</td>
</tr>
<tr>
<td>$B_2$</td>
<td>$T(2J+1)$ for $E_A = 2/3$</td>
</tr>
<tr>
<td>$A_2$</td>
<td>$T(2J+1)$ for $E_A = 2/3$</td>
</tr>
<tr>
<td>$T$</td>
<td>$T(2J+1)$ for $E_A = 2/3$</td>
</tr>
</tbody>
</table>

The class of the eigenstates of $H_{\alpha\beta}$. This is done in Fig. 1 for the $(2,2)$ $(20,8)$ representation, which is the leading one in a shell-model description of $^{136}$Xe, and its even-odd, odd-odd, and odd-odd neighbors.

The correspondence extends beyond traces of the matrices to the eigenvalues themselves. An unfavorable situation, chosen because it is only in such cases that one can really see differences between the eigenvalue spectrum of the rotor and its algebraic image, is shown in Fig. 2. The spectrum of $H_{\alpha\beta}$ for a $\pi = 0$ geometry is compared with the corresponding results for $H_{\alpha\beta}$ in the $(2,2)$ $(8,4)$ representation. The latter is the leading one in a shell-model description of $^{24}$Mg. In this case the rotor has more eigenstates for $I > 5$ than its algebraic image. Nonetheless, note that in the ground-state band the agreement is excellent, even up to the maximum angular momentum value ($L = 12$) found in the $(8,4)$ representation. Though the agreement is not quite as spectacular in other bands, it leaves little doubt concerning the validity of the mapping procedure. For larger representations such as those encountered in a shell-model description of rare-earth and actinide nuclear species, the agreement is much better than this, so good in fact that differences in the spectra of the two Hamiltonians cannot be detected for the states of physical interest.

As a final demonstration of the effectiveness of the mapping prescription, results for intra-band $E2$ transition rates are compared in Fig. 3 for the A-type symmetry and a $\pi = -1$ geometry. Though the corresponding curves have a similar form, note that the algebraic results for stretched transitions, $J_i - J_f = 2$, fall off compared to those for the rotor for higher values of the angular momentum. This can be traced to the compactness versus the noncompact nature of the underlying symmetry groups. A comparison of inter-band transition rates tells the same story, and likewise for transition rates for B-type symmetries and other geometries.

The operators $X_3$ and $X_4$ were first introduced by Racah and his students in their search for a canonical resolution of the $SU(3)$ state labelling problem [5]. The goal was to find an operator with...
simple eigenvalues that yielded a complete and orthonormal labelling of the basis states. The hope was that such an operator, if it could be found, would be associated with a constant of the motion such as the Runge-Lenz vector is for the $SO(4) \rightarrow SO(3)$ algebra of the hydrogen atom. The results presented here can be used to address that question for in the prolate limit of the rotor the magnitude of $K$ is a good quantum number. The operator of interest is therefore the algebraic image of $J^z$. For any $\lambda$ and $\mu$ this is given by

$$K^2 = (\lambda_1 \lambda_2 L^2 + \lambda_2 \lambda_3 X^2 + \lambda_3 \lambda_1 Y^2) / (2 \lambda + \lambda_2 - \lambda_3),$$

$$\lambda_1 = (-\lambda + \mu)/3, \quad \lambda_2 = (-\lambda - 2\mu - 3)/3, \quad \lambda_3 = (2\lambda + \mu + 3)/3. \quad (13)$$

Finally it seems important to note that since $SU(3) \rightarrow SO(3)$ is a root symmetry in shell-model descriptions of nuclear rotational phenomena, the theory offers an opportunity to explore in a new way the microscopic underpinnings of this collective motion. The picture that emerges is a relatively simple one: the shell model can be thought of as a collection of interacting rotors. Work on this is in progress.

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References


Fig. 3. Intramolecular $B(E2)$ rates of the methyl model for $\kappa = 1$ geometry are compared with the corresponding $SO(3)$ results in the $(l_0 \mu) = (10,8)$ representation.