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Representation matrices for U(4)

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We propose an algorithm for the numerical calculation of matrix elements of general U(4) group elements, applicable to large totally symmetric representations of U(4). A possible generalization to the U(6) case is pointed out.

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I. INTRODUCTION

The application of an algebraic model in which a U(4) group structure is proposed to describe rotation-vibrational degrees of freedom of diatomic molecules[1] stimulated our interest in the properties of this group. In particular, to calculate transition probabilities,[2] we found it necessary to calculate representation matrices $\langle|e^{i\epsilon\hat{G}}|\rangle$ of this group for totally symmetric representations $[N]$ with large N. In this paper we present an algorithm to calculate these matrix elements numerically using the concept of coherent states. In Sec. II we give an outline of the problem, and in Sec. III we describe the algorithm. In the Sec. IV we summarize the merits of the proposed formulation, and indicate how it can be generalized to the case of U(6), the symmetry group of the interacting boson model,[3] which has been applied to describe collective properties of nuclei.

II. OUTLINE OF THE PROBLEM

We will use a Fock representation of the U(4) structure in terms of identical bosons that can occupy a scalar s state and a vector p state. All unitary transformations on these four single-boson states define the U(4) group of interest here. All states formed by distributing N bosons among these four single boson states constitute the completely symmetric representation $[N]$ of U(4). Such states can be explicitly constructed by creating N bosons in the vacuum $|0\rangle$. The creation and annihilation operators are

$$s^\dagger, p^\dagger_\mu \quad \text{and} \quad s, \tilde{p}_\mu \equiv (-)^\mu p_{-\mu} \quad (\mu = -1,0,1), \tag{1}$$

respectively. They satisfy the usual commutation rules. The 16 generators $\hat{G}_i$, of the U(4) group can be expressed in terms of these operators:

$$\{\hat{G}_j, j = 1\cdots 16\} = \{(s^\dagger s)^{(0)}_0, (p^\dagger \tilde{p})^{(0)}_0, (p^\dagger \tilde{p})^{(1)}_\mu,$$
$$(p^\dagger \tilde{p})^{(2)}_\mu, (p^\dagger s + s^\dagger \tilde{p})^{(1)}_\mu, i(p^\dagger s - s^\dagger \tilde{p})^{(1)}_\mu\}, \tag{2}$$

where the brackets denote angular momentum coupling. Since we have assigned, to the single-boson states, definite transformation properties under the rotation group O(3), there are only two group chains according to which we can label the N-boson states:

$$\mathrm{U}(4) \supset \mathrm{U}(3) \supset \mathrm{O}(3) \supset \mathrm{O}(2), \tag{3a}$$

$$\mathrm{U}(4) \supset \mathrm{O}(4) \supset \mathrm{O}(3) \supset \mathrm{O}(2). \tag{3b}$$

While the chain (3b) is appropriate for the description of molecular spectra[1] in practice it is more convenient to use the basis of the chain (3a) since the U(3) group consists of the transformations among the p-bosons and has n (the number of p-bosons) as an invariant. The quantum labels related to the chain (3a) are: $[N]$, n, l, m, and the corresponding states [the so-called U(3) basis]

$$|[N]nlm\rangle = A_{nl}(s^\dagger)^{N-n}(p^\dagger \cdot p^\dagger)^{(n-l)/2}\mathscr{Y}_{lm}(p^\dagger). \tag{4}$$

(The dot product is defined as $a\cdot b = \Sigma_\mu (-)^\mu a_\mu b_{-\mu}$). The coefficients A_{nl} are derived in Ref. 4:

$$A_{nl} = (-)^{(n-l)/2}[4\pi/(n+l+1)!!(n-l)!!(N-n)!]^{1/2} \tag{5}$$

and the $\mathscr{Y}_{lm}(p^\dagger)$ are solid harmonics in the p-boson creation operators.

A general element of the U(4) group can be expressed in terms of the generators

$$\hat{U}(\epsilon_j) = \exp\left(i\sum_j \epsilon_j \hat{G}_j\right). \tag{6}$$

We are interested in the evaluation of the following matrix elements:

$$\langle[N]nlm|\hat{U}(\epsilon_j)|[N]n'l'm'\rangle. \tag{7}$$

A 4×4 matrix representation for the generators can be obtained by considering their action on the four states $s^\dagger|0\rangle$ and $p^\dagger_\mu|0\rangle$. The unitary operator $\hat{U}$ can then be expressed simply as a 4×4 matrix $U^{(1)}$ by diagonalizing $\Sigma_j \epsilon_j \hat{G}_j$, exponentiating and transforming back to the original basis.

III. THE ALGORITHM

The procedure is based on three important properties of so-called coherent states,[5] which are product wavefunctions of the form

$$|[N]\alpha_\mu\rangle = \frac{1}{\sqrt{N!}}(\sqrt{1-\alpha\cdot\tilde{\alpha}^*}s^\dagger + \tilde{\alpha}\cdot p^\dagger)^N|0\rangle. \tag{8}$$

First, they have a simple behavior under the action of a group element (6),

$$\hat{U}(\epsilon_j)|[N]\alpha_\mu\rangle = \exp(i\beta N)|[N]\alpha'_\mu\rangle, \tag{9}$$

where β (real) and α'_μ can be determined from

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$$U^f\begin{pmatrix}\alpha_1\\ \alpha_0\\ \alpha_{-1}\\ (1-\alpha\cdot\tilde{\alpha}^*)^{1/2}\end{pmatrix}=e^{i\beta}\begin{pmatrix}\alpha'_1\\ \alpha'_0\\ \alpha'_{-1}\\ (1-\alpha'\cdot\tilde{\alpha}'^*)^{1/2}\end{pmatrix} \tag{10}$$

Secondly, the overlap of such a state with a U(3) basis state is given by [compare with Eq. (4)]

$$\langle[N]nlm|[N]\alpha_\mu\rangle = (N!)^{1/2}A_{nl}(1-\alpha\cdot\tilde{\alpha}^*)^{(N-n)/2}(\alpha\cdot\alpha)^{(n-l)/2}\mathscr{Y}_{lm}(\alpha). \tag{11}$$

Thirdly, one can decompose any U(3) basis state in coherent states using

$$|[N]nlm\rangle = (2\pi A_{nl})^{-1}(2^N/N!)^{1/2}\times\int_0^{2\pi}d\chi\int_{-1}^{1}d\cos\theta\int_0^{2\pi}d\phi\times\exp(-in\chi)Y^l_m(\theta,\phi)|[N]\alpha_\mu(\chi,\theta,\phi)\rangle, \tag{12}$$

with

$$\alpha_\mu(\chi,\theta,\phi)=\frac{1}{\sqrt{2}}e^{i\chi}\begin{pmatrix}-(1/\sqrt{2})\sin\theta\,e^{-i\phi}\\ \cos\theta\\ (1/\sqrt{2})\sin\theta\,e^{i\phi}\end{pmatrix}. \tag{13}$$

An important point to note is that one can replace the three-dimensional integral in Eq. (12) by a summation in an *exact* fashion due to the fact that the states in the representation $[N]$ of U(4) are polynomials in the boson operators of (finite) order N. In particular the decompositon (12) of a general U(3) basis state remains exact if we replace the integration over ϕ by a $(2N+1)$-point, the one over χ by an $(N+1)$-point equidistant summation, and the integral over $\cos\theta$ by an $(N+1)$-point Gaussian summation. We replace symbolically: $\int\to\sum\!\!\!\!\!\!\int$. Using Eqs. (9)–(13), one obtains the result

$$\langle[N]nlm|\hat{U}|[N]n'l'm\rangle = 2^{N/2}A_{nl}A^{-1}_{n'l'}\exp(i\beta N)\times\sum_0^{2\pi}\!\!\!\!\!\!\int d\chi\sum_{-1}^{1}\!\!\!\!\!\!\int d\cos\theta\sum_0^{2\pi}\!\!\!\!\!\!\int d\phi\exp(-in'\chi)\times Y^{l'}_{m'}(\theta,\phi)(1-\alpha'\cdot\tilde{\alpha}'^*)^{(N-n)/2}(\alpha'\cdot\alpha')^{(n-l)/2}\mathscr{Y}_{lm}(\alpha'). \tag{14}$$

If one considers a general boson-number-conserving, rotationally invariant Hamiltonian,[6] its eigenstates can be expressed in the U(3) basis as

$$|[N]vlm\rangle=\sum_n a^v_n(l)|[N]nlm\rangle, \tag{15}$$

where the $a^v_n(l)$ are the expansion coefficients.

To obtain matrix elements of $\hat{U}$ between the eigenstates without the necessity of determining all matrix elements (7) (which is particularly convenient if the number of states in the representation $[N]$ is large and if one is interested in only a few matrix elements in the basis of eigenstates), one replaces in Eq. (14)

$$A_{nl}(1-\alpha'\cdot\tilde{\alpha}'^*)^{(N-n)/2}(\alpha'\cdot\alpha')^{(n-l)/2}$$

by

$$\sum_n a^v_n(l)A_{nl}(1-\alpha'\cdot\tilde{\alpha}'^*)^{(N-n)/2}(\alpha'\cdot\alpha')^{(n-l)/2}, \tag{16}$$

and

$$A^{-1}_{n'l'}\exp(-in'\chi)$$

by

$$\sum_{n'}a^{v'}_{n'}(l')A^{-1}_{n'l'}\exp(-in'\chi). \tag{17}$$

In particular, this last replacement will be efficient regarding computational time.

IV. DISCUSSION

There are two main reasons why the above described procedure is attractive. First, this method is numerically efficient. Because of the unique property (9) of coherent states one only needs to decompose the ket of a matrix element (7). In any other basis one would need to calculate *all* the matrix elements of $\hat{U}$ and use transformation brackets to return to the U(3) basis [for both the bra and the ket in Eq. (7)], which is inconvenient for large N {this advantage of the coherent state basis is partly compensated for by the fact that the decomposition (12) in order to be exact involves a number of coherent states that is larger than the dimension of the representation $[N]$}. In addition, one is usually interested in only few matrix elements of $\hat{U}(\epsilon_j)$ (particularly for large N) and these are easily provided by Eq. (14). Instead of transformation brackets only simple numerical procedures and functions are involved. Secondly, if one considers a typical Hamiltonian possessing a dynamical symmetry [corresponding to the group chains (3a) or (3b)] the ground state has special properties and can be decomposed rather easily. For example, in the U(3) limit one obtains

$$|[N],\mathrm{gs}\rangle=(1/\sqrt{N!})(s^\dagger)^N|0\rangle, \tag{18}$$

and in the O(4) limit

$$|[N],\mathrm{gs}\rangle=\mathscr{N}\int_{-1}^{1}d\cos\theta\int_0^{2\pi}d\phi\times[(1/\sqrt{2})s^\dagger+(1/\sqrt{2})\tilde{\alpha}(\chi=0,\theta,\phi)\cdot p^\dagger]^N|0\rangle. \tag{19}$$

Therefore, the evolution of the ground state of such a system under an operator (6) can be calculated rather simply. Also certain symmetries in the problem can easily be implemented, for instance, in the case of cylindrical symmetry one can omit the ϕ integration in (14).

We have written a computer code based upon this algorithm. It is available on request.

Extensions of these techniques to U(6) are straightforward, although the resulting expressions are more involved. The U(6) formula corresponding to Eq. (4) is given in Ref. 7, where also the generalizations of the spherical harmonics appropriate for the U(6) problem are treated. An equation analogous to (14) would involve a five-dimensional integral and contain more complicated functions. Simplifications in the spirit of the points mentioned above could be applied.

Let us finally emphasize that the special realization of the U(4) group, and in particular the O(3) structure assumed here, is by no means essential. An appropriate coherent state basis can also be found for other chains of subgroups.

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