PHYSICAL REVIEW B VOLUME 27, NUMBER 1 1 JANUARY 1983

Unitary group approach to the theory of nuclear magnetic resonance of higher-spin nuclei

R. D. Kent
Department of Applied Mathematics, University of Western Ontario, London, Ontario N6A 5B9, Canada

M. Schlesinger
Department of Physics, University of Windsor, Windsor, Ontario N9B 3P4, Canada

(Received 9 July 1982)

The unitary group approach to the treatment of nuclear-magnetic-resonance spectra of A_n systems with nuclei of higher than $\frac{1}{2}$ spin is presented. The treatment of one- and two-body operator matrix elements in this context is discussed and some actual examples are worked out. The development is made with NMR in mind but it is otherwise completely general.

I. INTRODUCTION

In a recent paper Siddall[1] has discussed the use of so-called many-spin basis sets in evaluating matrix elements of the NMR Hamiltonian. In that paper the matrix elements of the nuclear-spin unit irreducible tensor were obtained using various basis systems and the computational efficiency of each method was discussed. It was concluded that by adapting the pure nuclear-spin configurations to permutational symmetry maximum efficiency was obtained.

Siddall's paper treats the case of two particles in each pure configuration and the coupling of two pure configurations to a resultant mixed configuration. The symmetry-adapted basis states are defined in terms of the total spin of each pure configuration and the total resultant spin of the mixed configuration. It is not fully evident from that treatment, however, that either the construction of basis states or the evaluation of matrix elements of the coupling tensor operators is simplified when one considers an arbitrary number of particles in a pure configuration or a mixed configuration comprised of pure configurations of differing spins.

In this paper we outline the use of the unitary group approach (UGA) to symmetry-adapted basis states of pure σ^N configurations where for an N-particle system σ is the single-particle spin. The mathematical formalism for this procedure has existed[2] in the literature for some time, but only recently has it been actively investigated in the context of atomic, molecular, and nuclear applications.[3]

This paper is divided into the following parts. In Sec. II we present the general theory for treating pure configuration cases, σ^N. Section III is a reformulation of the two-particle spin-1 case of Siddall and is presented for comparison purposes. We present in Sec. IV the example of the completely symmetric basis states of four spin-$\frac{3}{2}$ particles. Finally, in Sec. V we discuss various programming aspects of the unitary group approach.

II. GENERAL THEORY

In a pure configuration of N particles with single-particle spins σ the permutational symmetry-adapted basis states will be labeled $|\sigma^{[\lambda]},(\alpha)_I M\rangle$ where $[\lambda]$ designates the various partitions or irreducible representations of the symmetric group $S(N)$. The arrangements of numbers in the tableau boxes (α), formed by taking all possible numerical combinations satisfying lexicality conditions (α_i increase down the columns and are nondecreasing across the rows) designate the uniquely labeled basis vectors, or constitute what are called Weyl-Young tableaux. Each entry α_i $(i=1,2,\ldots,N)$ is defined in terms of the single-particle spin and its z projection; $\alpha_i=\sigma+1-m_i$ $(\alpha_i=1,2,\ldots,2\sigma+1)$, and M is the sum, $M=\sum_{i=1}^{N} m_i$. Within each M family there will be a number of tableaux Q_M which we can label $(\alpha)_I$ $(I=1,2,\ldots,Q_M)$.

For a complete description of the unitary group approach to σ^N configurations we refer the reader to Refs. 4–6. For spin-$\frac{1}{2}$ configurations, in particular, we refer the reader to Refs. 7–9 and references contained therein.

Each irreducible representation of $S(N)$, labeled by a given tableau shape, has a unique, highest total spin-basis vector. It is formed by filling in the tableau boxes with the smallest allowed numerical entries α_i. The remaining basis vectors are generated from the highest tableau using the unitary group generators $E(\alpha_i,\alpha_j')$ which destroy the α_j' labeled particle and create the α_i labeled particle.

We define the nuclear-spin unit irreducible tensor operator

$$I^k_q = \sum_{i,j} (-1)^{\sigma - m'_j} \begin{pmatrix} \sigma & k & \sigma \\ -m_i & q & m'_j \end{pmatrix} E(\alpha_i, \alpha'_j) \, . \tag{2.1}$$

The matrix elements of I^k_q are particularly easy to calculate in the tableau basis. There are two types of nonzero matrix elements. First, there are diagonal matrix elements where the bra and ket states are the same. In this case the operator $E(\alpha_i,\alpha_i)$ simply counts the number of α_i entries in the tableau. Second, off-diagonal matrix elements are found from only one term of the sum (2.1) since the bra and ket tableaux may differ by one box only in order that the matrix element be nonzero. These two points greatly simplify the computational procedure. In addition it should be pointed out that nonzero matrix elements exist only between tableaux of the same $[\lambda]$ and not between those belonging to different irreducible representations of $S(N)$.

The NMR coupling Hamiltonian is defined as

$$H_{\mathrm{NMR}} = - \sum_{k=1}^{2\sigma} T^k I^k \cdot I^k \, . \tag{2.2}$$

T^k are unit tensor operator coupling constants. The scalar product of unit tensor operators is written

$$I^k \cdot I^k = \sum_q \sum_{i \le j} \sum_{t \le r} (-1)^q (-1)^{\sigma - m'_j} \begin{pmatrix} \sigma & k & \sigma \\ -m_i & q & m'_j \end{pmatrix} \times (-1)^{\sigma - m'_t} \begin{pmatrix} \sigma & k & \sigma \\ -m_r & -q & m'_t \end{pmatrix} [E(\alpha_i,\alpha'_j)E(\alpha_r,\alpha'_t) + E(\alpha_r,\alpha'_t)E(\alpha_i,\alpha'_j)] \, . \tag{2.3}$$

This form of coupling operator necessitates the evaluation of the two-particle generator product $E(\alpha_i,\alpha'_j)E(\alpha_r,\alpha'_t)$. Once again, however, this procedure is simplified by the fact that for off-diagonal matrix elements, at most two-boxes may differ between bra and ket tableaux and for diagonal matrix elements the manner in which the sum (2.3) is performed is prescribed by the tableau entries α_i themselves. In this respect one of the major computational advantages of the tableau scheme is in the automatic bookkeeping arrangement afforded by the labeling.

The actual evaluation of multistep $(\alpha_i > \alpha'_j + 1)$ matrix elements is performed iteratively using the commutation relations

$$[E(\alpha_i,\alpha'_j), E(\alpha_r,\alpha'_t)] = \delta(\alpha_r,\alpha'_j)E(\alpha_i,\alpha_t) - \delta(\alpha_i,\alpha'_t)E(\alpha_r,\alpha'_j) \, . \tag{2.4}$$

The right-hand side can then be evaluated as a sum of products of one-step matrix elements. These in turn would be evaluated using Harter's "jawbone" formula.[10] In practice this iteration is performed as a matrix multiplication involving sparse banded matrices. Two-body operator matrix elements require the following expression:

$$E(\alpha_i,\alpha'_j)E(\alpha_r,\alpha'_t) = \sum_{(\alpha)} E(\alpha_i,\alpha'_j) \, |(\alpha)\rangle \times \langle(\alpha)| \, E(\alpha_r,\alpha'_t) \, , \tag{2.5}$$

where the sum is over all allowed intermediate tableaux.

Finally, the tableau basis can be transformed into an $R(3)$ adapted basis. The correlation between $\sigma^{[\lambda]}$ and states of definite total spin can be determined by inspection of the Q_M values in each $[\lambda]$ family of tableaux. At a given $M \ge 0$ the difference $\Delta Q = Q_M - Q_{M+1}$ gives the number of states of spin $S = M$. The actual states $|SM\tau\rangle$ [τ is an additional arbitrary label used to distinguish multiple $(\Delta Q > 1)$ total spin states] are linear combinations of tableaux at the M level. The particular coefficients multiplying each tableau are determined either using a combined lowering-projection operator technique (see Refs. 9 and 10) or, alternatively, a raising operator technique (see Ref. 11).

III. TWO-PARTICLE SPIN-1 SYSTEM

In this section we present the detailed description of the basis vectors for a two-particle system, each of spin 1, and the calculation of the matrix elements of the coupling operator (2.3). The tableaux corresponding to the partitions [2] and $[1^2]$ are given in Table I. Only those tableaux are given for which $M \ge 0$ since the full tableau listing is symmetric (in Q_M) about $M=0$. The correlation between the irreducible representations of $\mathrm{SU}(2\sigma+1)^{[\lambda]}$ and those of $R(3)$ is also listed.

There are only six nonzero matrix elements of the generators $E(\alpha_i,\alpha'_j)$ which are required here for our purposes, namely,

$$\begin{aligned}
&\langle 11 \mid E(1,2) \mid 12\rangle = \sqrt{2}\,, \\
&\langle 12 \mid E(1,2) \mid 22\rangle = \sqrt{2}\,, \\
&\langle 12 \mid E(2,3) \mid 13\rangle = 1\,, \\
&\langle 11 \mid E(1,3) \mid 13\rangle = \sqrt{2}\,, \\
&\langle 12 \mid E(1,3) \mid 23\rangle = 1\,, \\
&\langle 13 \mid E(1,3) \mid 33\rangle = \sqrt{2}\,,
\end{aligned} \tag{3.1}$$

where the first three are one-step and the last three are two-step matrix elements. The matrix elements within $[1^2]$ are all 1.

Using the results (3.1) we can immediately proceed to evaluate the matrix elements of the coupling operators $I^1 \cdot I^1$ and $I^2 \cdot I^2$. These values are listed below:

$$\begin{aligned}
&\langle 11 \mid I^1 \cdot I^1 \mid 11\rangle = \frac{1}{6}, \quad \langle 11 \mid I^2 \cdot I^2 \mid 11\rangle = \frac{1}{30}\,, \\
&\langle 13 \mid I^1 \cdot I^1 \mid 13\rangle = -\frac{1}{6}, \quad \langle 13 \mid I^2 \cdot I^2 \mid 13\rangle = \frac{7}{30}\,, \\
&\langle 13 \mid I^1 \cdot I^1 \mid 22\rangle = \frac{\sqrt{2}}{6}, \quad \langle 13 \mid I^2 \cdot I^2 \mid 22\rangle = \frac{-\sqrt{2}}{10}\,, \\
&\langle 22 \mid I^1 \cdot I^1 \mid 22\rangle = 0, \quad \langle 22 \mid I^2 \cdot I^2 \mid 22\rangle = \frac{2}{15}\,, \\
&\left\langle \begin{matrix}1\\2\end{matrix} \middle| I^1 \cdot I^1 \middle| \begin{matrix}1\\2\end{matrix} \right\rangle = -\frac{1}{6}, \quad \left\langle \begin{matrix}1\\2\end{matrix} \middle| I^2 \cdot I^2 \middle| \begin{matrix}1\\2\end{matrix} \right\rangle = -\frac{1}{6}\,.
\end{aligned} \tag{3.2}$$

TABLE I. Tableau states of $\sigma^{[\lambda]}$ for $\sigma = 1$ including correlation with $R(3)$.

$[\lambda]$	M	Tableau states	ΔQ_M	$R(3)$ correlation
[2]	2	11	1	D
	1	12	0	
	0	13 22	1	S
$[1^2]$	1	$\begin{matrix}1\\2\end{matrix}$	1	P
	0	$\begin{matrix}1\\3\end{matrix}$	0	

The results in (3.2) can be compared with those of Siddall (Table II A of Ref. 1) by first noting the transformation from tableau basis to states of total definite spin $|[\lambda],SM\rangle$. We find that

$$\begin{aligned}
&|[2],22\rangle = |11\rangle\,, \\
&|[2],20\rangle = (\tfrac{1}{3})^{1/2}|13\rangle + (\tfrac{2}{3})^{1/2}|22\rangle\,, \\
&|[2],00\rangle = (\tfrac{2}{3})^{1/2}|13\rangle - (\tfrac{1}{3})^{1/2}|22\rangle\,,
\end{aligned} \tag{3.3}$$

$$|[1^2],11\rangle = \left|\begin{matrix}1\\2\end{matrix}\right\rangle\,.$$

Using (3.2) and (3.3) we find

$$\begin{aligned}
&\langle [2]00 \mid I^1 \cdot I^1 \mid [2]00\rangle = -\tfrac{1}{3}, \quad \langle [2]00 \mid I^2 \cdot I^2 \mid [2]00\rangle = \tfrac{1}{3}\,, \\
&\langle [2]2M \mid I^1 \cdot I^1 \mid [2]2M\rangle = \tfrac{1}{6}, \quad \langle [2]2M \mid I^2 \cdot I^2 \mid [2]2M\rangle = \tfrac{1}{30}\,, \\
&\langle [1^2]1M \mid I^1 \cdot I^1 \mid [1^2]1M\rangle = -\tfrac{1}{6}, \quad \langle [1^2]1M \mid I^2 \cdot I^2 \mid [1^2]1M\rangle = -\tfrac{1}{6}\,,
\end{aligned} \tag{3.4}$$

in agreement with Siddall (note that there is a misprint in Siddall's Table III A for $\langle [2]00 \mid I^2 \cdot I^2 \mid [2]00\rangle$).

For a mixed configuration system A_2B_2 where both A and B species are spin-1 particles we can proceed in either of two ways. Using the transformation to states of definite S within each configuration separately we can vector couple these to a resultant total definite spin I, namely

$$\begin{aligned}
|[\lambda_A]S_A,[\lambda_B]S_B,IM\rangle = \sum_{M_A,M_B} &\langle S_A S_B M_A M_B \mid IM\rangle \\
&\times |[\lambda_A]S_A M_A\rangle \\
&\times |[\lambda_B]S_B M_B\rangle\,.
\end{aligned} \tag{3.5}$$

Alternatively, we can express the mixed configuration tableau basis directly using different labels for

TABLE II. Mixed configuration tableau states of $\sigma_A^{[\lambda_A]}\sigma_B^{[\lambda_B]}$ for $\sigma_A=\sigma_B=1$ including correlation with $R(3)$.

$[\lambda_A][\lambda_B]$	M	Tableau states								ΔQ_M	$R(3)$ correlation
[2][2]	4	11 44								1	G
	3	11 45	12 44							1	F
	2	11 46	11 55	12 45	13 44	22 44				3	$3D$
	1	11 56	12 46	12 55	13 45	22 45	23 44			1	P
	0	11 66	12 56	13 46	22 46	13 55	22 55	23 45	33 44	2	$2S$
$[1^2][2]$	3	144 2								1	F
	2	144 3	145 2							1	D
	1	244 3	145 3	146 2	155 2					2	$2P$
	0	245 3	146 3	155 3	156 2					0	
$[1^2][1^2]$	2	14 25								1	P
	1	14 35	14 26							1	P
	0	24 35	14 36	15 26						1	S

the A and B systems (e.g., $\alpha=1,2,3$ for A and $\alpha=4,5,6$ for B). This approach is demonstrated in Table II. We have compared our results with those of Siddall and found full agreement with his Table III B.

IV. SYMMETRIC FOUR-PARTICLE SPIN-$\frac{3}{2}$ SYSTEM

We now consider a more complex system of four particles with single-particle spin $\frac{3}{2}$. To simplify the discussion we shall deal with the completely symmetric partition [4]. The tableaux for this partition are listed in Table III.

For spin-$\frac{3}{2}$ systems there are three coupling terms [see Eq. (2.2)] corresponding to $k=1$, 2, and 3. The matrix elements of the group generators $E(\alpha_i,\alpha_j')$ are shown in Table IV for the tableaux at level $M=3$, 4, 5, and 6 only. Also, note that $\alpha_i=\alpha_j'+q$ for $q=1$, 2, and 3.

The evaluation of the matrix elements of $I^k\cdot I^k$ now proceeds in the following fashion. For the diagonal terms one performs the sum (2.3) using the

TABLE III. Four-particle spin-$\frac{3}{2}$ tableaux for the completely symmetric partition [4].

M	Tableaux					ΔQ_M	$R(3)$ correlation
6	1111					1	I
5	1112						
4	1113	1122				1	G
3	1114	1123	1222			1	F
2	1124	1133	1223	2222		1	D
1	1134	1224	1233	2223			
0	1144	1234	2224	1333	2233	1	S

TABLE IV. One-body operator matrix elements for $E(\alpha_i,\alpha_j')$ for $\alpha_i=\alpha_j'+q$.

	q	
1	2	3
$\langle 1111 \mid E_{1,2} \mid 1112\rangle=2$	$\langle 1111 \mid E_{1,3} \mid 1113\rangle=2$	$\langle 1111 \mid E_{1,4} \mid 1114\rangle=2$
$\langle 1112 \mid E_{1,2} \mid 1122\rangle=\sqrt{6}$	$\langle 1112 \mid E_{1,3} \mid 1123\rangle=\sqrt{3}$	$\langle 1112 \mid E_{1,4} \mid 1124\rangle=\sqrt{3}$
$\langle 1112 \mid E_{2,3} \mid 1113\rangle=1$	$\langle 1112 \mid E_{2,4} \mid 1114\rangle=1$	
$\langle 1122 \mid E_{1,2} \mid 1222\rangle=\sqrt{6}$	$\langle 1122 \mid E_{1,3} \mid 1223\rangle=\sqrt{2}$	$\langle 1122 \mid E_{1,4} \mid 1224\rangle=\sqrt{2}$
$\langle 1122 \mid E_{2,3} \mid 1123\rangle=\sqrt{2}$	$\langle 1122 \mid E_{2,4} \mid 1124\rangle=\sqrt{2}$	
$\langle 1113 \mid E_{1,2} \mid 1123\rangle=\sqrt{3}$	$\langle 1113 \mid E_{1,3} \mid 1133\rangle=\sqrt{6}$	$\langle 1113 \mid E_{1,4} \mid 1134\rangle=\sqrt{3}$
$\langle 1113 \mid E_{3,4} \mid 1114\rangle=1$		
$\langle 1114 \mid E_{1,2} \mid 1124\rangle=\sqrt{3}$	$\langle 1114 \mid E_{1,3} \mid 1134\rangle=\sqrt{3}$	$\langle 1114 \mid E_{1,4} \mid 1144\rangle=\sqrt{6}$
$\langle 1123 \mid E_{1,2} \mid 1223\rangle=2$	$\langle 1234 \mid E_{1,3} \mid 1233\rangle=2$	$\langle 1123 \mid E_{1,4} \mid 1234\rangle=\sqrt{2}$
$\langle 1123 \mid E_{2,3} \mid 1133\rangle=\sqrt{2}$	$\langle 1123 \mid E_{2,4} \mid 1134\rangle=1$	
$\langle 1123 \mid E_{3,4} \mid 1124\rangle=1$		
$\langle 1222 \mid E_{1,2} \mid 2222\rangle=2$	$\langle 1222 \mid E_{1,3} \mid 2223\rangle=1$	$\langle 1222 \mid E_{1,4} \mid 2224\rangle=1$
$\langle 1222 \mid E_{2,3} \mid 1223\rangle=\sqrt{3}$	$\langle 1222 \mid E_{2,4} \mid 1224\rangle=\sqrt{3}$	

tableau labels to determine which two-body operator combinations are different from zero. The resulting set of labels $(\alpha_j'\to\alpha_i,\alpha_t'\to\alpha_r)$ are used to access a look-up table of $3-j$ coefficients which can be calculated and stored *a priori*. For off-diagonal terms only two-boxes may differ in the tableau. One scans the tableaux to determine these labels and then compiles the appropriate factors in a straightforward manner.[12] A list of several of these two-body matrix elements is given in Table V.

As a final step, if the $I^k\cdot I^k$ matrix elements are required in an $R(3)$ adapted basis one uses the transformation coefficients listed in Table VI (for I, G, and F states). We have performed this transformation for the stretched states $[M_L=L_L(\max)]$. The results are as given in Table VII.

TABLE V. Nonzero matrix elements $\langle(\alpha)\mid I^k\cdot I^k\mid(\alpha')\rangle$ for partition [4] of a four-particle spin-$\frac{3}{2}$ system. The matrix element $\langle(1112)\mid I^k\cdot I^k\mid(1112)\rangle$ is identical with the one at level $M=6$.

			k		
M	$\langle(\alpha)\rangle$	$\mid(\alpha')\rangle$	1	2	3
6	1111	1111	$\frac{14}{5}$	$\frac{8}{5}$	$\frac{38}{35}$
4	1113	1113	$\frac{8}{5}$	$\frac{8}{5}$	$\frac{8}{5}$
	1113	1122	$\frac{2\sqrt{2}}{5}$	0	$-\frac{6\sqrt{2}}{35}$
	1122	1122	$\frac{38}{15}$	$\frac{8}{5}$	$\frac{6}{5}$
3	1114	1114	1	$\frac{8}{5}$	$\frac{13}{7}$
	1114	1123	$\frac{\sqrt{3}}{5}$	0	$-\frac{3\sqrt{3}}{35}$
	1123	1123	$\frac{29}{15}$	$\frac{8}{5}$	$\frac{51}{35}$
	1123	1222	$\frac{4}{5}$	0	$-\frac{12}{35}$
	1222	1222	2	$\frac{8}{5}$	$\frac{10}{7}$

TABLE VI. $R(3)$ adapted states: transformation coefficients.

$$|I,6\rangle = |1111\rangle$$

$$\begin{pmatrix} |I,4\rangle \\ |G,4\rangle \end{pmatrix} = \begin{pmatrix} \left(\frac{2}{11}\right)^{1/2} & \left(\frac{9}{11}\right)^{1/2} \\ \left(\frac{9}{11}\right)^{1/2} & -\left(\frac{2}{11}\right)^{1/2} \end{pmatrix} \begin{pmatrix} |1113\rangle \\ |1122\rangle \end{pmatrix}$$

$$\begin{pmatrix} |I,3\rangle \\ |G,3\rangle \\ |F,3\rangle \end{pmatrix} = \begin{pmatrix} -\left(\frac{1}{55}\right)^{1/2} & -3\left(\frac{3}{55}\right)^{1/2} & -3\left(\frac{3}{55}\right)^{1/2} \\ -\frac{3}{2}\left(\frac{3}{22}\right)^{1/2} & -\frac{5}{2\sqrt{22}} & \frac{3}{\sqrt{22}} \\ \frac{3}{2}\left(\frac{3}{10}\right)^{1/2} & \frac{-3}{2\sqrt{10}} & \frac{1}{\sqrt{10}} \end{pmatrix} \begin{pmatrix} |1114\rangle \\ |1123\rangle \\ |1222\rangle \end{pmatrix}$$

$$\vdots \qquad\qquad \vdots$$

V. PROGRAMING CONSIDERATIONS

With regard to programing, the unitary group approach offers several advantages. The tableaux can be stored economically as binary strings. This allows storage of quite large basis sets. The generation of the tableaux basis and evaluation of one- and two-body generator matrix elements can be performed separately by a sequence of program modules and these results assembled by a master routine.[9] This has the effect of providing a series of short, fast programs and allows one to consider highly complex systems.

The approach outlines in this paper differs in principle only slightly from applicatons to SU(2) as outlined previously.[7,8] Thus in most cases only minor modifications of already existing programs need occur. The Harter formula has been programed in high-level language[10] and further work into low-level language programing is proceeding. The purpose behind this is to optimize the programing strategy in terms of both time and memory use.

Finally, the major advantage of the use of unitary group methods lies in the fact that the procedure retains its simplicity regardless of the complexity of the system. In this sense the example of Sec. IV does not do full justice to UGA.

TABLE VII. Matrix elements of the $I^k \cdot I^k$ operator in total spin adapted basis.

Total spin	k = 1	2	3
I	$\frac{42}{15}$	$\frac{8}{5}$	$\frac{8}{5}$
G	$\frac{4}{3}$	$\frac{8}{5}$	$\frac{12}{7}$
F	$\frac{4}{5}$	$\frac{8}{5}$	$\frac{68}{35}$

VI. CONCLUSION

We have presented an alternative approach to nuclear magnetic resonance NMR-type calculations. The method is sufficiently general so that it can handle a variety of other theoretical problems as well as NMR. Further, it can be used to handle both pure- and mixed-configuration systems, though further work is still required.

One important computational obstacle still remains to be overcome. In the treatment of spin-$\frac{1}{2}$ [SU(2)] systems a direct factorization of one-body, multistep, and two-body operators was achieved.[3,8] This was accomplished through a vector coupling scheme. Presently, we do not see how to avoid the iterative approach to such matrix elements based on either (2.4) or (2.5).

[1]T. H. Siddall, J. Phys. Chem. 86, 91 (1982).
[2]M. Moshinsky, *Group Theory and the Many Body Problems* (Gordon and Breach, New York, 1968).
[3]For a thorough list of references including recent introductory reviews of the unitary group approach see M. J. Boyle and J. Paldus, Phys. Rev. A 22, 2316 (1980).
[4]I. M. Gelfand and M. Zetlin, Dok. Akad. Nauk. SSSR 71, 825 (1950).
[5]G. E. Baird and L. C. Biedenharn, J. Math. Phys. 4, 1449 (1963).
[6]J. D. Louck, Am. J. Phys. 38, 3 (1970), and references therein.
[7]J. Paldus, J. Chem. Phys. 61, 5321 (1974); Phys. Rev. A 14, 1620 (1976).
[8]G. W. F. Drake and M. Schlesinger, Phys. Rev. A 15, 1990 (1977).
[9]R. D. Kent and M. Schlesinger, Phys. Rev. A 23, 979 (1981).
[10]J. Drake, G. W. F. Drake, and M. Schlesinger, J. Phys. B 8, 1009 (1975).
[11]M. Schlesinger, R. D. Kent, and G. W. F. Drake, Can. J. Phys. 60, 357 (1982).
[12]R. D. Kent and M. Schlesinger, Comput. Phys. Commun. 23, 301 (1981).