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A program for the study of many-body correlations: matrix elements of the generators of U(n)

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Abstract. A procedure has been outlined for generating configuration space basis states of many-particle systems in which the maximal occupancy of any single-particle orbital is arbitrary. An efficient computer program has been developed for determining the matrix elements of the generators of the unitary group U(n) over configuration space basis states. Computer times for generating these matrix elements have been presented for specific examples.

1. Introduction

The study of electron correlation in atoms and molecules has in recent years made increasing use of computer programs based on unitary and permutation group methods (Paldus 1974, 1975, 1976, Shavitt 1978, Brooks and Schaefer 1979, Downward and Robb 1977, Sarma and Rettrup 1977). Efficient algorithms have been developed for generating the Gelfand–Zetlin basis sets (Gelfand and Zetlin 1950) spanning the irreducible representations (ireps), $[2^{N/2-S}1^{2S}0^{n-N/2-S}]$, of the unitary group U(n) over the configuration space of the electrons. In the light of these successes with many-electron systems, it is worth examining whether we could develop equally efficient algorithms in dealing with other many-fermion systems. The algebraic structure of the unitary group underlying these studies was investigated by a number of workers (Biedenharn 1963, Baird and Biedenharn 1963, Ciftan and Biedenharn 1969, Moshinsky 1968). General computational procedures based on these studies have however not received much attention. Such a program could be used to test the efficiency of the algebra in handling large-scale studies of many-body correlations.

In this paper we present generalisations of some of the algorithms used in recent years for the study of many-electron systems. We assume that the system under consideration is described by a basis set of Nth rank tensors in the configuration space. Each of the single-particle orbitals defining the tensor space is assumed to have a maximal occupancy index f. This essentially means that no orbital can be more than f-fold occupied in the set of Nth rank tensors. This restriction implies that the irreducible components of U(n) into which the tensor space decomposes are described by Young shapes (Kaplan 1975, Hamermesh 1962) with no more than f columns. The index f may be conveniently designated the 'spin' of the particle. If we have an N-particle system each component of which has f 'spin' states, we are interested in

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generating the basis states spanning the irreducible representations $[f^{p_1}, (f-1)^{p_2}, \ldots, 1^{p_f}, 0^{p_{f+1}}]$ of U(n) where

$$\sum_{i=0}^{f} p_{i+1} = n, \qquad \sum_{i=0}^{f} (f-i)p_{i+1} = N$$

and

$$p_1, p_2, \ldots, p_f, p_{f+1} > 0.$$

Given a procedure for determining these basis states, the matrix elements of the generators, $\{E_{ij} | i, j = 1, \ldots, n\}$, of U($n$) can be obtained using a well-known algebraic expression (Baird and Biedenharn 1963).

The present work has been carried out in three main stages. Firstly, we have replaced the Gelfand representation of the basis states (Gelfand and Zetlin 1950) by generalised Paldus arrays (Paldus 1974). This leads to economy in storage and retrieval if f is small. Secondly, a procedure was developed for generating Paldus arrays corresponding to a specific component of the tensor space. Finally, the Baird–Biedenharn (1963) expression for the matrix elements of the generators of U(n) was adapted to suit the use of Paldus arrays in place of the Gelfand tableaux.

In § 2 we describe the procedure used and present the CPU times for some specific examples as illustrations of the efficiency of the program. A brief discussion of the method is presented in § 3.

2. Present method

Consider an N-particle system, each component of which has f possible 'spin' states. Let the configuration space of the system be described by n orthonormal single-particle basis states $\Phi_1, \Phi_2, \ldots, \Phi_n$. This basis set spans the carrier space V_n of U(n). A primitive tensor basis set spanning $V_n \otimes^N$ then defines a reducible configuration space for the N-particle system. An element of this set may be designated by the occupancy index of the set, $(N_1, N_2, \ldots, N_n)$, where $N_i \leq f$ for all $i = 1, \ldots, n$ and $\Sigma_{i=1}^{n} N_i = N$. In view of the occupancy restriction, we are interested only in the ireps $[f^{p_1}(f-1)^{p_2} \ldots 1^{p_1} 0^{p_{f+1}}]$ obtained in the reduction of $V_n \otimes^N$. A more compact notation for this irep is $[p_1^n, p_2^n, \ldots, p_f^n, p_{f+1}^n]$ indicating the frequency of occurrence of row lengths $f, f-1, \ldots, 0$ respectively in the corresponding Young shape. Since U(n) admits the canonical subgroup chain $\mathrm{U}(n) \supset \ldots \supset \mathrm{U}(1)$, we find that the subgroup U(i)($1 \leq i \leq n$) can be similarly characterised by $[p_1^i p_2^i \ldots p_f^i p_{f+1}^i]$, where

$$\sum_{R=0}^{f} p_{R+1}^i = i, \tag{1}$$

$$\sum_{R=0}^{f} (f-R)p_{R+1}^i = N^{(i)}, \qquad N^{(i)} = \sum_{R=1}^{i} N_R \tag{2}$$

and $p_1^i, p_2^i, \ldots, p_{f+1}^i$ are integers ≥ 0. The set of indices $[p_1^i, p_2^i, \ldots, p_{f+1}^i]$ $(i = 1, \ldots, n)$ provides a one-to-one correspondence with the rows of a Gelfand

tableau, so that

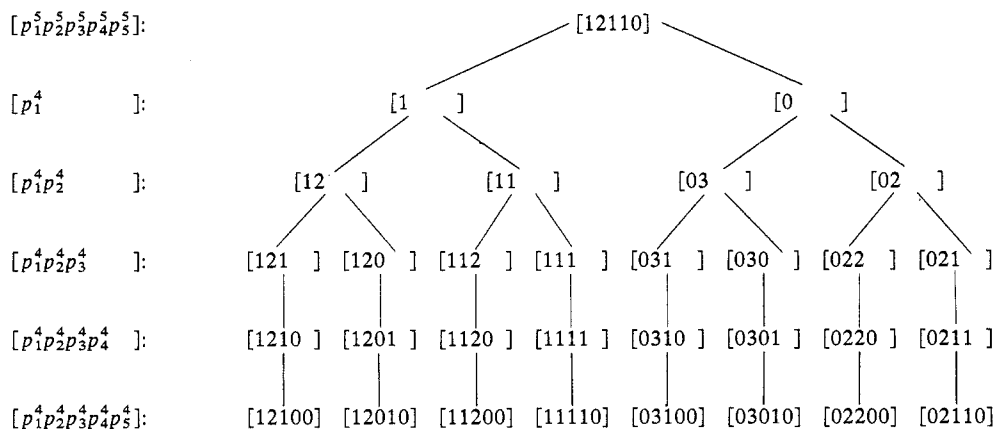
$$\begin{array}{ccccc} & & & & \\ & & & & \\ m_{1n} & m_{2n} & \cdots & m_{nn} & \\ m_{1n-1} & m_{2n-1} & & m_{n-1n-1} & \\ & \cdots & & & \\ & \cdots & & & \\ & m_{12} & m_{22} & & \\ & & m_{11} & & \end{array} \equiv \begin{bmatrix} p_1^n & p_2^n & \cdots & p_{f+1}^n \\ p_1^{n-1} & p_2^{n-1} & \cdots & p_{f+1}^{n-1} \\ & & & \\ & & & \\ p_1^2 & p_2^2 & \cdots & p_{f+1}^2 \\ p_1^1 & p_2^1 & \cdots & p_{f+1}^1 \end{bmatrix}. \tag{3}$$

The representation of the right-hand side of equation (3) may be labelled a Paldus array in a manner similar to the one obtained for the irep $[N/2-S, 2S, n-N/2-S]$ of U(n) for describing the configuration space of electrons (Paldus 1974, 1975, 1976). If $f \ll n$, we find that the Paldus array requiring $n(f+1)$ entries is a more compact representation than the corresponding Gelfand tableau with $n(n+1)/2$ entries.

Given a Gelfand tableau having specified entries in the ith row, we can obtain a lexically ordered set of possible $(i-1)$th rows by imposing the betweenness condition on the weights m_{ji} such that $m_{ji} \geqslant m_{ji-1} \geqslant m_{j+1i}$. Though we have not used the complete set of lexically ordered states spanning an irep of U(n), it is interesting to study the corresponding procedure for Paldus arrays. For generating such a basis we first define a set of partial sums for the ith row as

$$M_j^i = \sum_{\alpha=1}^{j} p_\alpha^i \tag{4}$$

where $1 < i < n$. We now generate the possible p_j^{i-1} $(j = 1, 2, \ldots, f+1)$ for the $(i-1)$th row as those which lead to M_j^{i-1} satisfying $M_j^i \geqslant M_j^{i-1} \geqslant M_j^i - 1$ and subject to the condition $M_{f+1}^{i-1} = M_{f+1}^i - 1$. If all $M_{j'}^i$ $(j' > j)$ satisfy $M_{j'}^i = M_j^i$, the last of the above requirements implies that we choose only that p_j^{i-1} which corresponds to $M_j^{i-1} = M_j^i - 1$. This procedure leads to a branching diagram which can be best illustrated using an example. Consider a fifth row, [12110], in a Paldus array corresponding to $f = 4$. We can then generate the possible fourth rows of this array as:



Starting from the nth row specifying the given irep we can successively generate lower rows till we have scanned all of them. Using a suitable indexing system we can

link up different rows to yield distinct lexically ordered Paldus arrays. A computer program has been developed for this part of the procedure.

The dimensionality of an irep of U(n) tends to increase rapidly with increasing values of n. This leads to practical difficulties in using the entire configuration space corresponding to an irep of U(n). A better alternative would be to generate Paldus arrays corresponding to physically interesting allowed values of the occupancy indices $(N_1, N_2, \ldots N_n)$. The problem then is to be able to generate the subset of Paldus arrays corresponding to a definite choice of these occupancy indices. We now outline a scheme for doing this. If a particular $N_i = 0$, we readily find from equations (1) and (2) that the only possible $(i-1)$th row resulting from $[p_1^i p_2^i \ldots p_{f+1}^i]$ is $[p_1^{i-1} p_2^{i-1} \ldots p_{f+1}^{i-1}]$, where $p_j^{i-1} = p_j^i (1 \leqslant j \leqslant f)$ and $p_{f+1}^{i-1} = p_{f+1}^i - 1$. If on the other hand $N_i = 1$, we use the above $(i-1)$th row as an intermediate stage and generate f new $(i-1)$th rows by changing a pair of entries (p_j^i, p_{j+1}^i) $(1 \leqslant j \leqslant f)$ at a time to $(p_j^i - 1, p_{j+1}^i + 1)$, leaving all the others unchanged. In doing this we retain any negative entry which might have been obtained at the $N_i = 0$ stage. In terms of the entries in the ith row, the possible $(i-1)$th rows for $N_i = 1$ are given by $[p_1^i p_2^i \ldots p_f^i - 1 p_{f+1}^i]$, $[p_1^i p_2^i \ldots p_{f-1}^i - 1 p_f^i + 1 p_{f+1}^i - 1]$, $[p_1^i - 1 p_2^i + 1 \ldots p_f^i p_{f+1}^i - 1]$. If $N_i = 1$, we terminate the above procedure and neglect those possibilities for the $(i-1)$th row which have any negative entries. If $N_i > 1$, we use the same techniques as above, but now using each of the f possibilities as intermediate stages. In order to avoid repetitions we use this technique for the pairs (p_j^i, p_{j+1}^i) for $1 \leqslant j \leqslant f-1$ when dealing with the first of the intermediate stages and (p_j^i, p_{j+1}^i) for $1 < j < f-2$ in dealing with the second and so on, and neglect the last one obtained at $N_i = 1$ level. This procedure may be readily continued for any arbitrary N_i, leading finally to all possibilities for the $(i-1)$th row. From among these we neglect those possibilities which contain negative entries and obtain the allowed $(i-1)$th rows. The nature of this construction is such that the conditions set out for equation (4) are automatically fulfilled. This implies that the betweenness conditions for the corresponding Gelfand tableaux are satisfied. The procedure may be used for each of the $(n-1)$ rows following the top row and, using a suitable indexing system, we can generate the possible Paldus arrays corresponding to a given set $(N_1, N_2, \ldots N_n)$. A computer program has been developed for doing this. In column (6) of table 1 we present the CPU times for generating Paldus arrays for all single excitations $(N_1, N_2, \ldots N_i \pm 1, \ldots, N_j \mp 1 \ldots N_n)$ from a reference set $(N_1, N_2, \ldots N_n)$ for an irep of U(9) corresponding to $f = 2, 3, 4, 5, 6$. In view of the extremely short CPU times, we found that it was not necessary to look for any of the simplifications of the type used by Shavitt and others in dealing with electrons (Shavitt 1978, Brooks and Schaefer 1979, Downward and Robb 1977).

As an illustration of the procedure consider the case $N_6 = 2$ corresponding to the sixth row, [22011], of a Paldus array for $f = 4$. We can visualise the process leading to possible fifth rows as

$$
[22011] \xrightarrow{N_6=0} [22010] \xrightarrow{N_6=1} \begin{cases} [22001] \xrightarrow{N_6=2} \begin{cases} [22\text{-}111] \\ [21101] \\ [13001] \end{cases} \\ [22\text{-}120] \xrightarrow{N_6=2} \begin{cases} [21020] \\ [13\text{-}120] \end{cases} \\ [21110] \xrightarrow{N_6=2} [12110] \\ [13010] \xrightarrow{N_6=2} x. \end{cases}
$$

Neglecting the first and the fifth of the final states, we obtain four allowed fifth rows satisfying $N_6 = 2$.

Paldus representation for the basis states of the ireps of U(n) obtained as above may now be used to determine the matrix elements of the generators $E_{ij}(1 \leq i, j \leq n)$. General expressions for these matrix elements over a Gelfand basis set were obtained by Moshinsky using the lowering operator technique (reference to original work in Moshinsky (1968)) and by Baird and Biedenharn (1963) using the hook content of Weyl tableaux. More recently a graphical realisation of these matrix elements was suggested by Sarma and Sahasrabudhe (1979) using permutation group algebra. In all cases, however, the final results were obtained in terms of the weights m_{ij} in the Gelfand tableaux. It is useful to recall the general result obtained in terms of m_{ij} before working out the modifications necessary in using Paldus arrays. For $E_{ij}(i<j)$ we have (Baird and Biedenharn 1963)

$$\langle [m'] | E_{ij} | [m] \rangle = \begin{bmatrix} j \\ s_i : j-1 \end{bmatrix} \prod_{r=1}^{j-i-1} \begin{bmatrix} s_r : j-r \\ s_{r+1} : j-r-1 \end{bmatrix} \times \begin{bmatrix} s_i : i \\ i-1 \end{bmatrix} \tag{5}$$

where $[m']$ differs from $[m]$ in just $j-i$ entries, having locations $s_1, s_2, \ldots s_1$ in the rows $j-1, j-2, \ldots i$ respectively, with the difference being given by $m'_{s_r j-r} = m_{s_r j-r} + 1$. The factors on the right side of equation (5) are given by

$$\begin{bmatrix} j \\ s_1 : j-1 \end{bmatrix} = \left\{ \prod_{\alpha=1}^{j} [\pm(m_{\alpha j} - m_{s_1 j-1} + s_1 - \alpha)] \Big/ \prod_{\substack{\alpha=1 \\ (\alpha \neq s_1)}}^{j-1}{}' [\pm(m_{\alpha_{j-1}} - m_{s_1 j-1} + s_1 - \alpha)] \right\}^{1/2} \tag{6}$$

$$\begin{aligned} \begin{bmatrix} s_r : j-r \\ s_{r+1} : j-r-1 \end{bmatrix} &= \left\{ \left(\prod_{\substack{\alpha=1 \\ (\alpha \neq s_r)}}^{j-r}{}' [\pm(m_{\alpha_{j-r}} - m_{s_{r+1} j-r-1} + s_{r+1} - \alpha)] \Big/ \right. \right. \\ &\quad \left. \prod_{\substack{\alpha=1 \\ (\alpha \neq s_{r+1})}}^{j-r-1}{}' [\pm(m_{\alpha_{j-r-1}} - m_{s_{r+1} j-r-1} + s_{r+1} - \alpha)] \right) \\ &\quad \times \left(\prod_{\substack{\alpha=1 \\ (\alpha \neq s_{r+1})}}^{j-r-1}{}' [\pm(m_{\alpha j-r-1} - m_{s_r j-r} + s_r - \alpha - 1)] \Big/ \right. \\ &\quad \left. \left. \prod_{\substack{\alpha=1 \\ (\alpha \neq s_r)}}^{j-r}{}' [\pm(m_{\alpha j-r} - m_{s_r j-r} + s_r - \alpha - 1)] \right) \right\}^{1/2} Y(s_r - s_{r+1}), \end{aligned} \tag{7}$$

$$\begin{bmatrix} s_i : i \\ i-1 \end{bmatrix} = \left\{ \prod_{\alpha=1}^{i-1} [\pm(m_{\alpha i-1} - m_{s_i i} - \alpha - 1)] \Big/ \prod_{\substack{\alpha=1 \\ (\alpha \neq s_i)}}^{i}{}' [\pm(m_{\alpha i} - m_{s_i i} - \alpha - 1)] \right\}^{1/2} \tag{8}$$

subject to

$$\begin{bmatrix} s_1 : 1 \\ 0 \end{bmatrix} = 1. \tag{9}$$

In all the equations (6)–(8), the +(−) sign is to be used if α is less than (greater than) the reference indices s_1, s_{r+1}, s_r, or s_i involved in the product. In equation (7)

$$Y(s_r - s_{r+1}) = \begin{cases} +1 & \text{if } s_r \leqslant s_{r+1} \\ -1 & \text{if } s_r > s_{r+1}. \end{cases} \tag{10}$$

A restatement of the results of equations (6)–(8) in terms of Paldus arrays now follows if we note that

(i) each row of such an array contains information on the frequency of occurrence (or non-occurrence) of all the possible weights, $0 < m_{ij} < f$, of the Gelfand tableaux consistent with a given irep of U(n). Read from left to right, the column index in the row of a Paldus array uniquely locates a corresponding weight in the Gelfand tableaux.

(ii) A particular weight within an identical set can be located by defining an integer parameter α where α ranges over $M^i_{r-1} \leqslant \alpha \leqslant M^i_r$, with the partial sums as defined in equation (4). These identifications permit us to restate the results of equations (6)–(8) in terms of Paldus arrays as

$$\begin{bmatrix} j \\ s:j-1 \end{bmatrix} = \Bigg\{ \prod_{R=1}^{f+1} \prod_{\alpha = M^j_{R-1}+1}^{M^j_R} [\pm(R - s - M^{j-1}_{s-1} + \alpha)] \Big/ \prod_{R=1}^{f+1} \prod'_{\substack{\alpha = M^{j-1}_{R-1}+1 \\ (\alpha \neq M^{j-1}_{R-1}+1 \text{ if } R = s:j-1)}}^{M^{j-1}_R} [\pm(R - s - M^{j-1}_{s-1} + \alpha)] \Bigg\}^{1/2} \tag{11}$$

$$\begin{aligned} \begin{bmatrix} s':j-r \\ s'':j-r-1 \end{bmatrix} = \Bigg\{ \Bigg(\prod_{R=1}^{f+1} \prod'_{\substack{\alpha = M^{j-r}_{R-1}+1 \\ (\alpha \neq M^{j-r}_{R-1}+1 \text{ if } R = s':j-r)}}^{M^{j-r}_R} [\pm(R - s'' - M^{j-r-1}_{s''-1} + \alpha)] \Big/ \\ \prod_{R=1}^{f+1} \prod'_{\substack{\alpha = M^{j-r-1}_{R-1}+1 \\ (\alpha \neq M^{j-r-1}_{R-1}+1 \text{ if } R = s'':j-r-1)}}^{M^{j-r-1}_R} [\pm(R - s'' - M^{j-r-1}_{s''-1} + \alpha)] \Bigg) \\ \times \Bigg(\prod_{R=1}^{f+1} \prod_{\substack{\alpha = M^{j-r-1}_{R-1}+1 \\ (\alpha \neq M^{j-r}_{R-1}+1 \text{ if } R = s'':j-r-1)}}^{M^{j-r-1}_R} [\pm(R - s' - M^{j-r}_{s'-1} + \alpha - 1)] \Big/ \\ \prod_{R=1}^{f+1} \prod'_{\substack{\alpha = M^{j-r}_{R-1}+1 \\ \alpha \neq M^{j-r}_{R-1}+1 \text{ if } R = s':j-r}}^{M^{j-r}_R} [\pm(R - s' - M^{j-r}_{s'-1} + \alpha - 1)] \Bigg) \Bigg\}^{1/2} \\ \times Y(M^{j-r-1}_{s''-1} - M^{j-r}_{s'-1}), \end{aligned} \tag{12}$$

$$\begin{bmatrix} s''':i \\ i-1 \end{bmatrix} = \Bigg\{ \prod_{R=1}^{f+1} \prod_{\alpha = M^{i-1}_{R-1}+1}^{M^{i-1}_R} [\pm(R - s''' - M^i_{s'''-1} + \alpha - 1)] \Big/ \prod_{R=1}^{f+1} \prod'_{\substack{\alpha = M^i_{R-1}+1 \\ (\alpha \neq M_{R-1}+1 \text{ if } R = s''':i)}}^{M_R} [\pm(R - s''' - M^i_{s'''-1} + \alpha - 1)] \Bigg\}^{1/2}. \tag{13}$$

In the above expression the row indications for k, s, s', s'', and s''' are given by the superscripts on the corresponding partial sum. Further, on the right of equation (12) we have

$$Y(M^{j-r-1}_{s''-1} - M^{j-r}_{s'-1}) = \begin{cases} +1 & \text{if } M^{j-r-1}_{s''-1} \leqslant M^{j-r}_{s'-1} \\ -1 & \text{if } M^{j-r-1}_{s''-1} > M^{j-r}_{s'-1}. \end{cases} \tag{14}$$

The $-(+)$ sign is to be used on the right of equations (11)–(13) when $R < s (R \geqslant s)$. The condition given in equation (9) still holds.

A computer program has been developed for determining the matrix elements of equation (5) using the factors obtained in equations (11)–(14). This part of the program has been combined with the one described earlier for generating the basis states. Some test calculations have been performed to determine the efficiency of the procedure. The results are summarised in column (7) of table 1.

Table 1. Timings for generating basis states and evaluating the matrix elements of the generators of U(n) for all single excitations: $(N_1 N_2 \ldots N_i \ldots N_j \ldots N_n) \rightarrow (N_1 N_2 \ldots N_i + 1 \ldots N_j - 1 \ldots N_n)$, $(i, j = 1, 2, \ldots n)$.

Maximal single particle orbital occupancy index (f)	Reference occupancy $(N_1 N_2 \ldots N_n)$	Dimensionality of configuration space	The irep of U(n) $[p_1^n p_2^n \ldots p_{f+1}^n]$	Number of basis states generated	Time for generating basis states (CPU-sec)†	Time for evaluation of matrix elements (CPU-sec)†
2	(111111111)	73	[414]	1050	1·0	57·2
3	(222221100)	57	[2223]	1218	1·4	79·4
4	(332111100)	57	[11133]	1016	1·5	69·8
5	(443211000)	49	[111114]	1400	2·1	119·0
6	(554331000)	49	[1111113]	1240	2·7	119·0

† IBM 370/165.

3. Discussion

The procedure oulined in § 2 is in three main parts. Firstly, the Gelfand representation was replaced by Paldus arrays leading to considerable compactness in notation when $f \ll n$. Secondly, a simple procedure was developed for generating the Paldus arrays corresponding to given $(N_1, N_2, \ldots, N_n) \in V_n \otimes^N$. The program using this procedure was found to perform efficiently for all cases studied. Finally, the Baird–Biedenharn (1963) expression expressed in terms of the Gelfand basis set was modified to suit Paldus arrays. The program for using this expression was also carried out successfully. As the illustrative examples demonstrate, this part of the program is equally efficient considering the fact that the configuration space used was strongly interacting. It can of course be made more efficient by simplifying equations (11)–(13) for specific values of f, as was done by Paldus (1974, 1975, 1976) and Shavitt (1978). Since we wished to retain the program in its most general form, no attempt was made to incorporate any of these simplifications.

In conclusion it is to be noted that most of the physically interesting operators of U(n) are polynomials of E_{ij}. Obvious illustrations are the pair interactions, Casimir invariants of U(n) and its physical chain of subgroups such as O(n), etc (Moshinsky 1968). Programming procedures for handling such operators are in progress at present.

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References

Baird G F and Biedenharn L C 1963 *J. Math. Phys.* **4** 1449
Biedenharn L C 1963 *J. Math. Phys.* **4** 436
Brooks B R and Schaefer H F 1979 *J. Chem. Phys.*
Ciftan M and Biedenharn L C 1969 *J. Math. Phys.* **10** 221
Downward M J and Robb M A 1977 *Theor. Chim. Acta* **46** 129
Gelfand I M and Zetlin M L 1950 *Dokl. Akad. Nauk SSSR* **71** 825
Hamermesh M 1962 *Group Theory and Its Applications to Physical Problems* (Reading, Mass.: Addison-Wesley)
Kaplan I G 1975 *Symmetry of Many-Electron Systems* (New York: Academic)
Moshinsky M 1968 *Group Theory and the Many-Body Problem* (London: Gordon and Breach)
Paldus J 1974 *J. Chem. Phys.* **61** 5321
—— 1975 *Int. J. Quant. Chem.* **S9** 165
—— 1976 *Phys. Rev.* A **14** 1620
Sarma C R and Rettrup S 1977 *Theor. Chim. Acta* **46** 63 73
Sarma C R and Sahasrabudhe G G 1979 *J. Math. Phys.*
Shavitt I 1978 *Int. J. Quant. Chem.* S **12** 5