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A Thorough Analysis and Exposition of the Four-Index Transformation

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The nature of two-electron integral transformations as a major stumbling block to configuration interaction calculations is discussed. An N^5 general procedure utilizing positional algorithms for all members of specially ordered lists of partial summations is presented. Theoretical analysis detailing sequencing and calculational algorithms is included, augmented by results of FORTRAN programmed versions of the method. Two program versions differing in the manner of dividing the partially summed integrals into blocks give practical orders $N^{5.5\pm0.2}$ and $N^{6.23\pm0.05}$, the former approaching theoretical order.

INTRODUCTION

With the advent of large and extremely fast computers, the development of programs utilizing self-consistent field (SCF) methods, and the increasing availability of these programs, more researchers are using calculations to support and illuminate the observed behavior of molecules. The successes and shortcomings of SCF methods have been well documented[1] and viable alternatives have been mentioned. For those who wish to proceed beyond the limitations of SCF calculations, configuration interaction (CI) is now an economically and programmatically feasible route.

Of primary importance to the CI calculation are the integral transformations

$$\mathrm{B} = \mathrm{C}^{\dagger}\mathrm{bC} \tag{1}$$

$$\mathrm{R}_{ijkl} = \mathrm{C}_i{}^{\dagger}\mathrm{C}_j{}^{\dagger}\mathrm{rC}_k\mathrm{C}_l \tag{2}$$

from atomic to molecular bases. In Eqs. (1) and (2) C is the molecular orbital coefficient matrix, the r are the two-electron integrals over the atomic basis and b the one-electron integrals. The one-electron transformation Eq. (1) presents

[1] See for example, H. F. Schaefer III, "The Electronic Structure of Atoms and Molecules—A Survey of Rigorous Quantum Mechanical Results," Addison-Wesley (1972).

little problem as even grossly inefficient routines can handle the work with speed. The same statement does not hold for Eq. (2), however. Because of the enormous number of terms involved in the transformation expressed in Eq. (2) even for a moderate number (N) of atomic basis functions, considerable attention must be paid to the efficiency of the algorithms employed. A number of efficient algorithms [1–3] have been proposed, all of which have a work dependence of N^5. The recent proposal of Bender [1] appears to be maximally efficient, but suffers from the requirement of random access to the intermediate partial sums with its attendant demands for large fast memory storage. Tang and Edmiston [2] have proposed a method similar in some respects to the analysis presented here. The present work addresses itself to a highly detailed exposition of sequencing and of calculational algorithms effecting the transformation expressed in Eq. (2) without utilizing specific savings due to highly symmetrical situations. In addition, the algorithms discussed have been programmed and comparisons between the functioning programs and the theoretical analysis are presented.

METHOD

The two electron transformation (Eq. (2)) utilizes the symmetric permutations of integral indices

$$\begin{aligned} \langle ab \mid cd \rangle &= \langle ab \mid dc \rangle \\ &= \langle ba \mid dc \rangle \\ &= \langle ba \mid cd \rangle \\ &= \langle cd \mid ab \rangle \\ &= \langle cd \mid ba \rangle \\ &= \langle dc \mid ba \rangle \\ &= \langle dc \mid ab \rangle \end{aligned} \tag{3}$$

As a result of these equalities the input and transformed bases need only contain

$$\frac{W^4}{8} + \frac{W^3}{4} + \frac{3W^2}{8} + \frac{W}{4} \tag{4}$$

entries (where W is the length of the basis). Such a set may be defined by $\langle ab \mid cd \rangle$,

$$\begin{aligned} 1 &\leqslant [ab] \leqslant (W^2 + W)/2 \\ [ab] &\leqslant [cd] \leqslant (W^2 + W)/2 \end{aligned} \tag{5}$$

where $[ab] \equiv$ pair position of the pair ab in a list of unique pairs of a and b

$$\begin{aligned} 1 &\leqslant a \leqslant W \\ a &\leqslant b \leqslant W \end{aligned} \tag{6}$$

in which there are $(W^2 + W)/2$ unique pairs. The position, I, of any integral with known indices $\langle ij \mid kl \rangle$ in a canonically ordered list may then be determined by the equations[2]

$$\begin{aligned} P(ij) &= (i - 1)[W + 1 - i/2] + j - i + 1 \\ P(kl) &= (k - 1)[W + 1 - k/2] + l - k + 1 \end{aligned} \tag{7}$$

$$I = (P(ij) - 1)[W(W + 1)/2 + 1 - P(ij)/2] + P(kl) - P(ij) + 1 \tag{8}$$

As a result of the retention of only unique integrals in each respective list, the transformation, expressed as

$$\begin{aligned} \langle \alpha\beta \mid \gamma\delta \rangle &= \sum_p \sum_q \sum_r \sum_s C_{p\alpha} C_{q\beta} C_{r\gamma} C_{s\delta} \langle pq \mid rs \rangle \\ &= \sum_p C_{p\alpha} \sum_q C_{q\beta} \sum_r C_{r\gamma} \sum_s C_{s\delta} \langle pq \mid rs \rangle, \end{aligned} \tag{9}$$

which may then be written as the partial summations

$$\langle pq \mid r\delta \rangle = \sum_s C_{s\delta} \langle pq \mid rs \rangle \tag{10}$$

$$\langle pq \mid \gamma\delta \rangle = \sum_r C_{r\gamma} \langle pq \mid r\delta \rangle \tag{11}$$

$$\langle p\beta \mid \gamma\delta \rangle = \sum_q C_{q\beta} \langle pq \mid \gamma\delta \rangle \tag{12}$$

$$\langle \alpha\beta \mid \gamma\delta \rangle = \sum_p C_{p\alpha} \langle p\beta \mid \gamma\delta \rangle, \tag{13}$$

may not be carried out as the straightforward summations of Eqs. (10–13) without

[2] See Appendix A for a derivation of these expressions. The more usual lower triangle indexing has the somewhat simpler formulae

$$p(ij) = \frac{i(i-1)}{2} + j, \quad I = \frac{p(ij)[p(ij) - 1]}{2} + p(kl)$$

some manipulation of the input list to each partial summation. It is proposed that such manipulation be carried out in the formation of the sets from Eq. (10) and Eq. (12) in order that Eq. (11) and Eq. (13) apply exactly as written. The resulting list of $\langle pq \mid r\delta \rangle$ from Eq. (10) would then be sequenced as

$$1 \leqslant r \leqslant N \text{ for every } pq\delta,\ 1 \leqslant [pq] \leqslant (N^2 + N)/2 \text{ for every } \delta,\ 1 \leqslant \delta \leqslant M, \quad (14)$$

where N is the length of the expansion basis and M that of the transformed basis, resulting in $M(N^3 + N^2)/2$ items created. The second partial summation, Eq. (11), then becomes a trivial exercise of N multiplications and additions to form each member of a list, $\langle \delta\gamma \mid pq \rangle$,

$$1 \leqslant [pq] \leqslant (N^2 + N)/2 \text{ for every } \delta\gamma,\ 1 \leqslant [\delta\gamma] \leqslant (M^2 + M)/2, \quad (15)$$

consisting of $(N^2 + N)(M^2 + M)/4$ entries. Minor manipulations of the indices of this set in concert with application of Eq. (12) yields a list $\langle \delta\gamma \mid \beta p \rangle$

$$1 \leqslant p \leqslant N \text{ for every } \delta\gamma\beta,\ \delta \leqslant \beta \leqslant M \text{ for every } \delta\gamma,\ 1 \leqslant [\delta\gamma] \leqslant (M^2 + M)/2, \quad (16)$$

of $N(2M^3 + 3M^2 + M)/6$ unique terms required for Eq. (13). Consequently, Eq. (13) may be utilized to form the completely transformed set, $\langle \delta\gamma \mid \beta\alpha \rangle$

$$[\delta\gamma] \leqslant [\beta\alpha] \leqslant (M^2 + M)/2 \text{ for every } \delta\gamma,\ 1 \leqslant [\delta\gamma] \leqslant (M^2 + M)/2. \quad (17)$$

The total number of operations in the transformation (an operation being defined as a multiplication and addition) is then

$$\sum_{i=1}^{4} Z_i \cdot N \quad (18a)$$

where $Z_i \equiv$ number of terms produced in partial summation i.

$$\sum_{i=1}^{4} Z_i N = \frac{N^4 M}{2} + \frac{N^3 M^2}{4} + \frac{N^2 M^3}{3} + \frac{N M^4}{8} + \frac{3N^3 M}{4} + \frac{3N^2 M^2}{4} + \frac{N M^3}{4} + \frac{5N^2 M}{12} + \frac{3N M^2}{8} + \frac{NM}{4}, \quad (18b)$$

which in the worst possible case ($N = M$) leads to

$$\frac{29}{24} N^5 + \frac{7}{4} N^4 + \frac{19}{24} N^3 + \frac{N^2}{4} \quad (18c)$$

operations, yielding what should be an N^5 procedure. Table I demonstrates the magnitude of the problem for N and M values up to 50.

TABLE I

Number of Operations Required for Various N and M Values

M/N	10	20	30	40	50
10	139150	1255800	5344950	15601600	36420750
20		4153100	14547150	38606200	85420250
30			30801600	74073800	154323500
40				128264400	251955500
50					388641250

CALCULATIONS

Because of the large number of integrals created and used during the course of the transformation and the general inadequacy of computer fast storage to handle this number of items, the transformed and incoming integral sets will probably be divided into blocks. The result of these arbitrary divisions is a sizable increase in the amount of work the computer must perform (and thus the time involved).

A program utilizing the basic algorithms given in Eqs. (10–17) has been written entirely in FORTRAN and tested using two types of fixed block dimensions. In the first version a list as described in Eq. (14) is created such that each block of the transformed list contains at least all possible p, q, and r values for a given δ. Since there are $(N^2 + N)/2$ pairs pq and N r's for every pq, the blocksize must be at least $(N^3 + N^2)/2$. Since only the unique integrals are kept in the atomic basis list, the creation of the list of the first partial sum requires that each of the unique atomic basis integrals $\langle tu \mid vw \rangle$ be treated as two permutations such that in Eq. (10)

(a) $p = t, q = u, r = v, s = w$

$$1 \leqslant [pq] \leqslant [rs]$$

(b) $p = v, q = w, r = t, s = u$

$$[pq] > [rs] \geqslant 1.$$

Case (a) treats each integral $\langle tu \mid vw \rangle$ as $\langle tu \mid vw \rangle$ and as $\langle tu \mid wv \rangle$ (except when $w = v$) while case (b) treats the integral as $\langle vw \mid tu \rangle$ and as $\langle vw \mid ut \rangle$ (except when $u = t$) with the case $[pq] = [rs]$ being treated only in (a). For each block of the partially transformed list the peripheral unit (either tape or disk) containing the atomic basis set must be read through completely. After completion of a partially

transformed block, that block may be stored on a peripheral unit and the next block calculated. After completion of the list, application of Eq. (11) to each block of the new list results in the list described by Eq. (15), which is stored in blocks. Again, because only unique entries are retained, resultant partial sums must be treated as $\langle \delta\gamma \mid pq \rangle$ and $\langle \delta\gamma \mid qp \rangle$ to create the set described by Eq. (16). The completely transformed list is then a straightforward result of Eq. (13).

The second version, which requires more computation, involves a fixed block size in the output list of the first partial summation with the only restriction being that the r index (see Eq. (14)) be completed at the end of a block, i.e., if

$$N \equiv \text{length of input basis}$$
$$A \equiv \text{size of block,}$$

the effective block size will be the largest multiple of N which is still less than or equal to A. The first entry in a partially transformed list block (as described in Eq. (14)) will then have indices $\langle p_b q_b \mid 1\delta_b \rangle$ and the last entry will have indices $\langle p_l q_l \mid N\delta_l \rangle$. (Set $D = [p_b q_b]$). There are then two cases which yield all necessary atomic basis integrals for the partial summation of Eq. (10). Again, the integral indices t, u, v and w must be permuted[3] such that in Eq. (10)

(I) (i) $p = t, q = u, r = v, s = w$

$$[pq] < D, \qquad 1 \leqslant [pq] \leqslant [rs] \leqslant (N^2 + N)/2 \equiv [NN]$$

(ii) $p = v, q = w, r = t, s = u$

$$1 \leqslant [rs] < [pq] \leqslant [NN], \qquad [rs] < D$$

(II) (i) $p = t, q = u, r = v, s = w$

$$D \leqslant [pq] \leqslant [rs]$$

(ii) $p = v, q = w, r = t, s = u$

$$[pq] > [rs] \geqslant D$$

Case (I) is used for all integrals in the atomic basis list which precede the integral with indices $\langle p_b q_b \mid p_b q_b \rangle$. Case (II) then applies to the integral with the aforementioned indices and all that follow it in the list. In all cases with the obvious exception of $r = s$ the r and s indices must be permuted i.e., the integrals $\langle pq \mid rs \rangle$ and $\langle pq \mid sr \rangle$ are required for the partial summation.

In the formation of the list $\langle pq \mid r\delta \rangle$ in version 1 the atomic integral list must

[3] See Appendix B.

be read through completely for each block of the partially summed list. There exist possible savings in version 2, however in that if a block is so structured that $[p_b q_b] \leqslant [p_l q_l]$, $\delta_b = \delta_l$, then no $[pq] < D$ would occur in the current block of the output list of $\langle pq \mid r\delta \rangle$ and the operations in case (I).(i) above need not be performed. Further, all atomic integrals necessary for the partial summation in Eq. (10) would occur before and up to the integral with indices $\langle p_l q_l \mid NN \rangle$. However if there exists any pq pair within the partially summed list block such that $[pq] > [p_l q_l]$ (thus implying $\delta_b \neq \delta_l$) then these savings are not possible and all operations above must be performed on the entire list of atomic integrals.

While a brief flow chart of each partial summation is presented in Appendix C, some details of the method seem in order.

First partial summation (FRST). The set described in Eq. (14) is formed. Initially the effective block size and first and last integral indices of each block in both the incoming and producted lists are computed. Then, in a loop over the number of blocks of items to be created, the atomic basis integral list is read through to the appropriate place; the position of the $\langle pq \mid r\delta \rangle$ to which a $\langle pq \mid rs \rangle$ contributes is calculated and the contributions $C(s, \delta) \cdot \langle pq \mid rs \rangle$ and $C(r, \delta) \cdot \langle pq \mid sr \rangle$ are added to the appropriate places. It is here that version 1 and version 2 differ. For an arbitrarily cut list of $\langle pq \mid r\delta \rangle$, more than one value of δ may exist within a block i.e., the range of p, q, and r values specified by Eq. (14) may have ended for one value of δ but not for another. For this reason the position calculated for the partial sum must be checked to see if a given atomic basis integral need contribute to more than one value of δ in a block. Where all possible p, q, and r values for a given δ exist within a block, such a check is unnecessary.

Second partial summation (SCND). Equation (11) is applied to the list formed above to create the list described by Eq. (15).

Third partial summation (THRD). (1) Determines the indices of the first and last partial sum of each block of the list from Eq. (15) and the list to be created. (2) Does the actual transformation treating each $\langle \delta\gamma \mid pq \rangle$ as $\langle \delta\gamma \mid pq \rangle$ and $\langle \delta\gamma \mid qp \rangle$.

Fourth partial summation (FRTH). Equation (13) is applied to the list formed in the third partial summation.

Discussion

Version 1, through the utilization of one large block structured such that all p, q, and r values for a given δ exist within the block, compared with version 2,

exhibits a marked time savings in subroutines FRST and THRD.[4] As demonstrated in Table II, savings in FRST (for moderate N) range from 42–52 %. THRD time savings are respectable for large M/N ratios but drop off rapidly (as do the savings in FRST) as the number of items created in THRD (FRST) diminish with decreasing $M(N)$. Total time savings are expected in going from version 2 to version 1 from a comparison of the practical order of the transformations with respect to N. A plot of log N vs log t (t being the process time) for versions 1 and 2 gave least squares slopes

Version 1	5.5 ± 0.2
Version 2	6.23 ± 0.05

implying order 5.5 for version 1 and 6.2 for version 2. The departure from ideality arises from two factors: 1. Counting through the integral lists index by index. 2. I0 operations. Thus version 2, which must of necessity do more work in FRST and THRD in view of its smaller block size and the arbitrary indexing within a block, exhibits, as would be expected, a much larger order (with respect to N) for the transformation.

Table III shows a comparison among

(1) Calculated percent work

(2) Percent time for version 1

(3) Percent time for version 2

for a series of M and N values. The calculated percent work is

$$\left(Z_i \Big/ \sum_{i=1}^{4} Z_i\right) \times 100,$$

Z_i defined in Eq. (18).

Invariably, version 2 values for FRST exceed the calculated percent time while version 1 values are too low for FRST and too high for SCND. The result of handling the transformed list in two entirely different manners in FRST and THRD is very noticeable. The change from four different series of operations to two (plus the loss of the position check) accounts for the reduction of percent time spent. The reasons for the increase in percent time spent on SCND in version 1 are the same as above.

[4] In the following test section the version 1 maximum block size of the lists from the first and third partial summations was set equal to 8125 [$= (25^3 + 25^2)/2$] while the block size for the lists from the second and fourth partial summations was set at 2000. Version 2 had a set maximum block size of 2000. The incoming atomic basis integral list was divided into blocks of 1000 integrals each.

TABLE II

Percent Time Savings of Version 1 over Version 2 by Subroutine

N	M		FRST	% Saving	SCND	% Saving	THRD	% Saving	FRTH	% Saving	Total	% Saving
20	20	1	18460[a]	51.04	14791	3.25	20079	40.81	2907	−2.04	56237	37.35
		2	37703		15288		33921		2849		89761	
20	18	1	15822	52.06	12001	−.46	12217	37.62	1890	−3.62	41930	36.81
		2	33003		11946		19586		1824		66359	
20	16	1	15248	48.33	10101	2.24	7432	27.16	1242	−7.44	34023	33.55
		2	29512		10332		10203		1156		51203	
20	14	1	12606	52.55	7409	2.05	3912	33.14	713	−1.86	24640	39.43
		2	26567		7564		5851		700		40682	
20	12	1	11474	48.12	6121	−2.32	2555	10.35	439	−13.14	20589	34.30
		2	22117		5982		2850		388		31337	
20	10	1	9413	48.19	3539	−4.06	1155	9.62	209	−7.73	14316	37.86
		2	18167		3401		1278		194		23040	
16	16	1	4581	46.64	4881	4.31	3323	43.63	943	2.68	13728	33.20
		2	8585		5101		5895		969		20550	
16	14	1	3805	47.80	3763	0.58	2138	36.86	611	−5.89	10317	31.39
		2	7289		3785		3386		577		15037	
16	12	1	3278	47.97	2883	−.56	1279	27.78	330	−6.11	7770	30.93
		2	6300		2867		1771		311		11249	
16	10	1	2964	42.47	1848	−12.41	759	19.85	179	−9.82	5750	27.27
		2	5152		1644		947		163		7906	
12	12	1	1043	27.72	900	2.49	757	10.84	269	−7.17	2969	14.34
		2	1443		923		849		251		3466	
12	10	1	856	25.89	680	2.44	453	2.79	130	−6.56	2119	13.16
		2	1155		697		466		122		2440	
10	10	1	437	10.08	371	−9.44	351	−20.21	110	−8.91	1269	−4.19
		2	486		339		292		101		1218	

TABLE III

Comparison of Actual Percent Time and Calculated Percent Work by Subroutine

	$N = 12$ $M = 12$			$N = 12$ $M = 10$			$N = 16$ $M = 16$		
	1[a]	2[b]	3[c]	1	2	3	1	2	3
FRST	35.13	41.63	39.84	40.40	47.34	47.25	33.37	41.77	40.22
SCND	30.31	26.63	21.58	32.09	28.52	21.66	35.56	24.82	21.37
THRD	25.50	24.50	27.66	21.38	19.10	23.32	24.21	28.69	27.65
FRTH	9.06	7.24	10.92	6.13	5.04	7.77	6.86	4.72	10.76
	$N = 16$ $M = 14$			$N = 16$ $M = 12$			$N = 16$ $M = 10$		
FRST	36.88	48.47	45.78	42.19	56.00	52.01	51.55	65.17	58.91
SCND	36.47	25.17	21.46	37.10	25.50	21.13	32.14	20.79	20.25
THRD	20.72	22.52	24.40	16.46	15.74	20.72	13.20	11.98	16.68
FRTH	5.92	3.84	8.36	4.25	2.76	6.14	3.11	2.06	4.16
	$N = 20$ $M = 20$			$N = 20$ $M = 18$			$N = 20$ $M = 16$		
FRST	32.83	42.00	40.45	37.73	49.73	44.89	44.82	57.64	49.78
SCND	26.30	17.03	21.24	28.62	18.00	21.32	29.69	20.18	21.16
THRD	35.70	37.80	27.64	29.14	29.52	25.05	21.84	19.93	22.16
FRTH	5.17	3.17	10.67	4.51	2.75	8.74	3.65	2.26	6.90
	$N = 20$ $M = 14$			$N = 20$ $M = 12$			$N = 20$ $M = 10$		
FRST	51.16	65.30	55.10	55.73	70.58	60.82	65.75	78.85	66.89
SCND	30.07	18.59	20.67	29.73	19.09	19.77	24.72	14.76	18.39
THRD	15.88	14.38	19.02	12.41	9.09	15.69	8.07	5.55	12.26
FRTH	2.89	1.72	5.21	2.13	1.24	3.72	1.46	0.84	2.45

[a] Version 1.
[b] Version 2.
[c] Calculated.

These methods were compared with a working transformation program (4) to establish the validity of the calculational algorithms and to obtain some comparative times. For $N = M = 12$ version 2 required 1.00 minutes execution; the working routine required 1.86 minutes. All transformed integrals agreed to 10^{-9}, the effective word length limit.

CONCLUSION

An entirely general N^5 procedure for the two-electron integral transformation has been presented. Also included are the formulae for atomic integral index manipulation which are needed for a general partial summation approach to

Eq. (2). Actual time tests have demonstrated the order of the work with respect to the basis length N. Symmetry savings have been ignored in a deliberate attempt to examine the efficiency of straight-forward procedures which will be necessary when asymmetrical molecular problems are undertaken. The method requires a canonically ordered atomic integral list. A simple reordering of integrals is required if they were not generated in this order. The programs written to accomplish the transformations need only moderate core storage; massive storage on large machines is unnecessary. The effectiveness of block sizes structured to the problem has been demonstrated, wherein theoretical and calculated orders of the transformation approach one another.

APPENDIX A: Determination of the Position of a Member with Known Indices of a List in Each of the Partial Summations

The sequencing of the list of all integrals $\langle pq \mid rs \rangle$ is best viewed as a tabular array. First arrange all unique pairs as shown below.

Position	Pair	Position	Pair		Position	Pair
1	11	$N+1$	22	$\cdots$	$\frac{N^2+N}{2}$	NN
2	12	$N+2$	23			
3	13	$\vdots$	$\vdots$			
$\vdots$	$\vdots$	$2N-1$	$2N$			
N	$1N$					

For each p there are $(N-p+1)$ q's; the total number of pq pairs is then

$$\sum_{m=0}^{N-1} (N-m) = \frac{N^2+N}{2} \tag{A.1}$$

since

$$\sum_{\epsilon=0}^{N-1} \epsilon = \frac{N(N-1)}{2}.$$

The number of pq pairs through $(p-1)N$ is

$$\sum_{q=1}^{p-1} (N-q+1) = N(p-1) - \frac{(p-1)p}{2} + p - 1$$

$$= (p-1)\left[N+1-\frac{p}{2}\right]. \tag{A.2}$$

The number of pq pairs since the last change in p is $q - p + 1$. The pair position of pq is thus

$$P(pq) = (p - 1)\left[N + 1 - \frac{p}{2}\right] + q - p + 1 \tag{A.3}$$

The position of the pair may now be used as a designator of that pair and a similar array used to display all combinations of the pairs.

For each pq pair there exist all rs pairs such that the pair position of the rs pair is greater than or equal to $P(pq)$. Every pq pair has then

$$\frac{N^2 + N}{2} - P(pq) + 1$$

rs's. The total number of items is then

$$\sum_{i=1}^{(N^2+N)/2}\left[\frac{N^2 + N}{2} - i + 1\right] = \left(\frac{N^2 + N}{2}\right)\left(\frac{N^2 + N}{2} + 1\right)\Big/2. \tag{A.4}$$

In order to determine the position of a given integral we need to know the pair position of each pair $P(pq)$ and $P(rs)$. Then, noting the manner in which the pairs combine, the final position determination is completely analogous to the determination of the pair position and is

$$\text{Position} = (P(pq) - 1)\left[\frac{N(N + 1)}{2} + 1 - \frac{P(pq)}{2}\right] + P(rs) - P(pq) + 1. \tag{A.5}$$

Similar arguments for the partial sums lead to the following expressions for the position of a given integral in each list.

$\langle \delta r \mid pq \rangle$, $1 \leqslant r \leqslant N$ for every $pq\delta$, $1 \leqslant [pq] \leqslant (N^2 + N)/2$ for every δ, $1 \leqslant \delta \leqslant M$

$$\text{Position} = (\delta - 1) \cdot \frac{N(N + 1)}{2} \cdot N + N \cdot \left[\frac{(p - 1)(2N - p)}{2} + q - 1\right] + r. \tag{A.6}$$

$\langle \delta\gamma \mid pq \rangle$, $1 \leqslant [pq] \leqslant (N^2 + N)/2$ for $\delta\gamma$, $1 \leqslant [\delta\gamma] \leqslant (M^2 + M)/2$

$$\text{Position} = (\delta - 1)\left[M + 1 - \frac{\delta}{2}\right] \cdot \frac{N(N + 1)}{2} + \left[(\gamma - \delta) \cdot \frac{N(N + 1)}{2}\right] + \left\{(p - 1)\left[n + 1 - \frac{p}{2}\right]\right\} + q - p + 1. \tag{A.7}$$

$$\langle \delta\gamma \mid \beta p\rangle,\ 1 \leqslant p \leqslant N \text{ for every } \delta\gamma\beta,\ \delta \leqslant \beta \leqslant M \text{ for every } \delta\gamma,$$
$$1 \leqslant [\delta\gamma] \leqslant (M^2 + M)/2$$

$$\text{Position} = \left\{\left[(\delta - 1)(M^2 + M - M(\delta - 1) + 1) + \frac{\delta(\delta - 1)(2\delta - 7)}{6}\right] N\right\}$$
$$+ (\gamma - \delta)(M - \delta + 1)\, N + (\beta - \delta)\, N + p. \tag{A.8}$$

APPENDIX B: Atomic Basis Integral List Manipulations Necessary to to Accomplish the First Partial Summation

A list of $\langle pq \mid r\delta\rangle$, sequenced as

$$1 \leqslant r \leqslant N \text{ for every } pq\delta,\ 1 \leqslant [pq] \leqslant (N^2 + N)/2 \text{ for every } \delta,\ 1 \leqslant \delta \leqslant M, \tag{B.1}$$

is to be formed from a list $\langle tu \mid vw\rangle$, sequenced as

$$[tu] \leqslant [vw] \leqslant (N^2 + N)/2 \text{ for every } tu,\ 1 \leqslant [tu] \leqslant (N^2 + N)/2 \tag{B.2}$$

by means of the equation

$$\langle pq \mid r\delta\rangle = \sum_s C_{s\delta} \cdot \langle pq \mid rs\rangle. \tag{B.3}$$

If the output list (B.1) is cut into blocks with the only restriction being a complete range over r, the first and last entries in a block will have the indices $\langle p_b q_b \mid 1\delta_b\rangle$ and $\langle p_l q_l \mid N\delta_l\rangle$ respectively. The integral immediately preceding the integral with indices $\langle p_b q_b \mid p_b q_b\rangle$ in the list (B.2) will have the indices $\langle ab \mid NN\rangle$ (except of course if $p_b = q_b = 1$), where

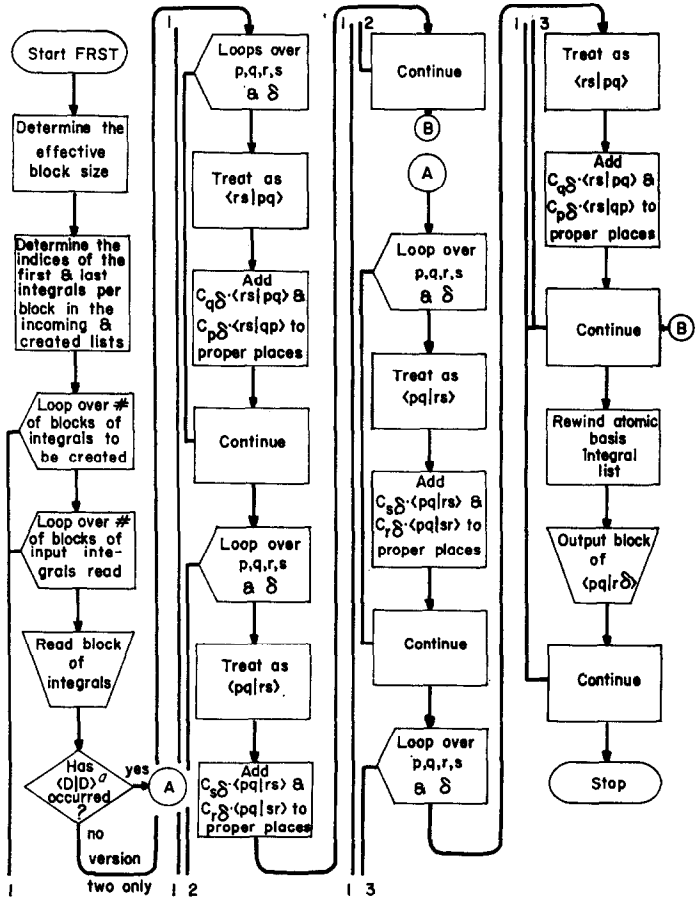
$$a = p_b - 1 \quad \text{if} \quad p_b = q_b$$
$$a = p_b \quad \text{otherwise}$$
$$b = N \quad \text{if} \quad p_b = q_b$$
$$b = q_b - 1 \quad \text{otherwise,}$$

or more simply, $[ab] = [p_b q_b] - 1$. For all pq in the block of the list defined by (B.1) lying between [1 1] and $[p_b q_b] - 1$, all integrals necessary for the summation (B.3) occur in the input list (B.2) before $\langle p_b q_b \mid p_b q_b\rangle$. Difficulties arise because of the restriction of the indices of the list (B.2) in that for all $[vw] > 1$ the permutation of indices (as given in Eq. (3)) is necessary for the completion of (B.3). The integral list (B.2) is initially treated as follows:

$$p = t, \qquad q = u, \qquad r = v, \qquad s = w$$

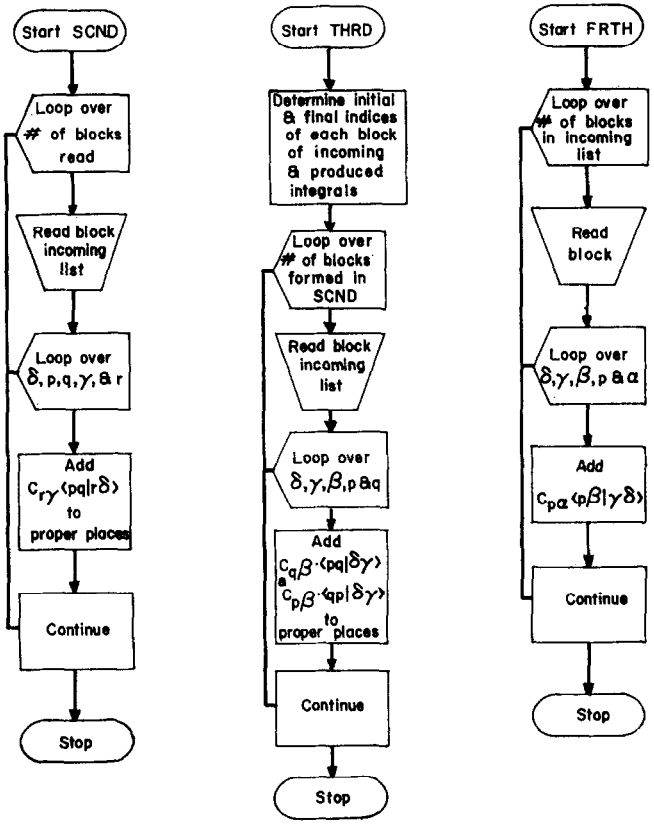
(with the appropriate interchange of r and s for all $r \neq s$). Finishing (B.3) then requires the permutation $p = v$, $q = w$, $r = t$, $s = u$ (again with interchange of r and s when $r \neq s$). At this point the partial summation for all entries in (B.1) with $[pq] < [p_b q_b]$ is completed. In addition, the range of the pq pair during the permutation has allowed required contributions to (B.1) to be added for all $\langle pq \mid rs \rangle$ such that $[p_b q_b] \leqslant [pq] \leqslant [NN]$ with $[1\ 1] \leqslant [rs] < [p_b q_b]$. The summations are completed through similar treatment of the list for all pq and rs pairs with pair positions greater than or equal to $[p_b q_b]$.

APPENDIX C: FLOW CHART OF THE FOUR PARTIAL SUMMATIONS



[a] $\langle D \mid D \rangle \equiv \langle p_b q_b \mid p_b q_b \rangle$. See text.

APPENDIX C (*continued*)



REFERENCES

1. C. F. BENDER, *J. Comp. Phys.* **9** (1972), 547.
2. K. C. TANG AND C. EDMISTON, *J. Chem. Phys.*, **52** (1970), 997.
3. R. K. NESBET, *Rev. Mod. Phys.*, **35** (1963), 552.
4. J. L. WHITTEN, private communication.