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Modification of the Liu–Davidson Method for Obtaining One or Simultaneously Several Eigensolutions of a Large Real-Symmetric Matrix

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A new and efficient iteration method for obtaining simultaneously several eigensolutions, and even for obtaining only one solution, of a large real-symmetric matrix is presented by modifying the simultaneous expansion method by Davidson and Liu. The method is basically the Ritz iteration method to correct trial vector(s) simultaneously using correction vectors. However, the number of the correction vectors determined in each iteration need not be the same as the number of the desired solutions; it is advantageous for the former number to be smaller than the latter when many eigensolutions are sought. In addition, trial vectors which need not be obtained exactly nor be corrected are included so as to bound the desired solutions which are to be obtained exactly from above and/or below (when interior solutions are sought). The correction vector space may be kept constant throughout the iterations. When the correction vector space has room enough to include the trial vectors of the previous iterations, the old trial vectors can serve as expansion vectors. The performance of the algorithm is tested for five matrices and is compared with the original Liu–Davidson algorithm. The results demonstrate that the present algorithm attains efficient use of memory space and reduction of iteration cycles, arithmetic operations and *I/O* processings.

I. INTRODUCTION

The relaxation method, which had been originally developed by Southwell [1] for solving coupled linear equations within the framework of the iteration (successive approximation) method, was applied to the eigenvalue problem by Cooper [2]. Large-scale matrix eigenproblems are familiar to quantum chemists in configuration interaction calculations of electronic wavefunctions of atoms and molecules. Several quantum chemists [3–5] have adopted the relaxation method for the diagonalization of large Hamiltonian matrices. The original relaxation method, i.e., the coordinate relaxation method, improves one element in the trial vector at a time based on the linear (first-order) minimization of the Rayleigh quotient (expectation value of the Hamiltonian, in quantum mechanics) or the linear vanishing of the residual. Within the coordinate relaxation algorithm, Shavitt *et al.* [6] corrected the trial vector based on the quadratic (exact) minimization of the Rayleigh quotient. Their method, which

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is called the method of optimal (coordinate) relaxations (MOR), is the most widely used algorithm for the non-degenerate lowest eigenproblem in quantum chemistry.

A modification of the coordinate relaxation method has been presented: the simultaneous improvement of several elements in the trial vector [7, 8]. This group-coordinate relaxation method is a natural extension of the two-by-two Ritz iteration algorithm [2], and can also be effective in resolving convergence difficulties for nearly degenerate eigensolutions.

Algorithms to generate only one correction vector to improve all elements in the trial vector at a time have also been presented. The gradient method by Hestenes and Karush [9] is based on the two-by-two Ritz iteration algorithm, but gives much poorer convergence than the above-mentioned relaxation methods. In order to remedy the gradient method, generation of a series of correction vectors (expansion vectors) is necessary. The Lanczos method [10], which originally is a modification of the power method based on the Krylov sequence, can be regarded as an extension of the gradient method. The Lanczos method has some weak points but is widely used, especially by nuclear physicists.

Another algorithm for generating only one correction vector to improve all elements in the trial vector has been used, in which the correction vector has individual coordinate relaxations. In quantum chemistry we can regard the variational perturbation method [3, 11] as its origin. This algorithm may be better than the gradient method, but undoubtedly gives slower convergence than the relaxation methods which continuously update a trial vector as soon as one or several elements are corrected. In order to improve this algorithm and the Lanczos method, Davidson [12] proposed the use of this type of correction vectors as expansion vectors in a Lanczos-like algorithm. Davidson's method overcomes the convergence difficulties for nearly degenerate eigensolutions by solving a small eigenvalue problem within the expansion space, and is widely used by quantum chemists as well as the MOR [6].

Some schemes [6] for obtaining higher eigensolutions have been proposed within the above-mentioned methods. In the methods adopting Ritz iteration, the orthogonality-constraint procedure [6, 9] of the trial vector to lower eigenvectors is effective; in the other methods, the root-shifting procedure [6] to mimic the deflation is effective. Against these procedures, the variance minimization version [13] of MOR and the root-homing version [14] of Davidson's method make possible the direct determination of higher eigensolutions without knowledge of the exact lower ones.

Recently new methods for obtaining several eigensolutions, not based on the sequential iteration algorithms which require knowledge of the exact lower solutions in advance, but based on a simultaneous iteration algorithm for all the trial solutions to be corrected, have been developed in order to improve computational efficiency [8, 15–20]. Clint and Jennings [15] combined the power method with a Ritz-like diagonalization algorithm. Cheung and Bishop [8] corrected several trial vectors simultaneously within the group-coordinate relaxation method. Raffenetti [16] and Liu [17]. (See also Ref. [18]) have proposed simultaneous versions of MOR and of

Davidson's method, respectively. Golebiewski [19] combined the power method with a new orthogonalization procedure, but his method is basically equivalent to the single-premultiplication version of the Jennings method [15]. Iwata [20] proposed the simultaneous gradient method without explicit orthogonalization among trial and correction vectors and even previously obtained eigenvectors.

The Ritz iteration algorithm becomes more powerful as the correction vector space is increased. The simultaneous group-coordinate relaxation method [8] keeps the number of correction vectors fixed in each group; on the other hand, the Liu–Davidson method [12, 17, 18] increases the number of correction vectors by the number of desired solutions in each iteration cycle. The latter method has the disadvantage of increased memory requirements. In the present work, modification of the Liu–Davidson method is proposed for obtaining one or simultaneously several eigensolutions combined with the simultaneous group-coordinate relaxation method. The essence of the modification is that the number of the correction vectors determined in each iteration need not be the same as the number of the desired solutions and that additional trial vectors are used in order to prevent variational collapse of higher eigensolutions. The advantage of the proposed method is clearly shown for five test matrices.

II. Modification of the Liu–Davidson Method

1. *Scheme*

The method proposed in the present work is basically the Ritz iteration method to correct trial vector(s) simultaneously using correction vectors and keeps the number of correction vectors fixed throughout the iteration cycles. Correction vectors for trial vectors are individually evaluated in each iteration cycle according to the Liu–Davidson method [12, 17, 18], but unimportant constituents of the correction vectors obtained in the previous iteration cycle are neglected in the next cycle. This point is different from the Liu–Davidson expansion method in which the correction-vector space used in an iteration cycle is basically always (within the limits of the main-memory space admitted) included in the successive iteration cycles. The purpose of including constituents of old correction vectors in the Ritz iteration does lie in the optimal extra- or inter-polation. A criterion for important constituents of the correction vectors is their contribution to corrections for the trial vectors; that is, the trial vectors improved in the previous iteration cycles include important constituents of the correction vectors. The present algorithm does not keep old correction vectors but keeps old trial vectors in the successive iteration cycles.

When only the lowest eigensolution is desired, it is preferred to choose the number of trial vectors to be greater than 1, because trial vectors for the higher (second, third, and so on) eigensolutions are important to exclude constituents of the higher solutions from a trial vector for the lowest one and to bound the lowest solution from above. Here, the higher solutions need not be obtained exactly and correction vectors are all for the lowest solution. This discussion is valid not only for the cases in which

some lowest solutions are desired but also for one or several interior solutions. In the latter case, trial vectors for lower solutions than those desired are always necessary to bound the solutions from below and to avoid variational collapse to the lower solutions.

2. *Procedure*

The equation to be solved is $\mathbf{XC} = \mathbf{CE}$. $\mathbf{X}$ is a large real-symmetric matrix (dimension $N \times N$) having real eigenvalues E_k and eigenvectors $\mathbf{C}_k$ ($k = 1 \sim n_{\text{solv}}$; $n_{\text{solv}} = n_{\text{exact}} + n_{\text{approx}}$). The number of approximate eigensolutions, which need not be obtained exactly, is n_{approx}, and the number of desired exact solutions is n_{exact}.

A. *Initialization*

1. Form initial trial vectors $\mathbf{C}_k^{(0)}$ and the Rayleigh quotients $E_k^{(0)}$ ($k = 1 \sim n_{\text{solv}}$).

2. Form $\mathbf{D}^{(0)} = \mathbf{XC}^{(0)}$, where $\mathbf{D}^{(0)}$ and $\mathbf{C}^{(0)}$ are of $N \times n_{\text{solv}}$ dimension.

3. Form the initial residual vectors $\mathbf{q}_k^{(0)} = \mathbf{D}_k^{(0)} - E_k^{(0)}\mathbf{C}_k^{(0)}$, ($k = 1 \sim n_{\text{exact}}$).

4. Form the initial correction vectors $\mathbf{b}_k^{(0)} = (\mathbf{X}^{\text{diag}} - E_k^{(0)}\mathbf{I})^{-1} \cdot \mathbf{q}_k^{(0)}$, ($k = 1 \sim n_{\text{exact}}$), where the diagonal matrix $\mathbf{X}^{\text{diag}}$ has the diagonal elements of $\mathbf{X}$. (If the maximum number of correction vectors, n_{corr}, is greater than n_{exact}, scatter $\mathbf{b}_k^{(0)}$ ($k = 1 \sim n_{\text{exact}}$) over $\mathbf{b}^{(0)}$ ($N \times n_{\text{corr}}$ dimension) or add $n_{\text{corr}} - n_{\text{exact}}$ coordinate vectors.)

B. *Iteration* ($i = 0, 1, \ldots$)

5. Form the orthonormalized correction vectors $\mathbf{C}_{\text{corr}}^{(i)}$ from $\mathbf{b}^{(i)}$ by Schmidt orthogonalization; then, ${}^t(\mathbf{C}^{(i)}, \mathbf{C}_{\text{corr}}^{(i)}) \cdot (\mathbf{C}^{(i)}, \mathbf{C}_{\text{corr}}^{(i)}) = \mathbf{I}$.

6. Form $\mathbf{D}_{\text{corr}}^{(i)} = \mathbf{XC}_{\text{corr}}^{(i)}$.

7. Form $\mathbf{H}^{(i)} = {}^t(\mathbf{C}^{(i)}, \mathbf{C}_{\text{corr}}^{(i)}) \cdot (\mathbf{D}^{(i)}, \mathbf{D}_{\text{corr}}^{(i)})$, and solve the reduced eigenvalue problem (Ritz iteration) of $n_{\text{solv}} + n_{\text{corr}}$ dimension: $\mathbf{H}^{(i)}\mathbf{T}^{(i,i+1)} = \mathbf{E}^{(i+1)}\mathbf{T}^{(i,i+1)}$. In this step the root-homing pattern search [14] is incorporated.

8. Form $\mathbf{C}^{(i+1)} = (\mathbf{C}^{(i)}, \mathbf{C}_{\text{corr}}^{(i)}) \cdot \mathbf{T}^{(i,i+1)}$ and $\mathbf{D}^{(i+1)} = (\mathbf{D}^{(i)}, \mathbf{D}_{\text{corr}}^{(i)}) \cdot \mathbf{T}^{(i,i+1)}$.

9. Form $\mathbf{q}_k^{(i+1)} = \mathbf{D}_k^{(i+1)} - E_k^{(i+1)}\mathbf{C}_k^{(i+1)}$, and check convergence by $|\mathbf{q}_k^{(i+1)}|^2$, ($k = 1 \sim n_{\text{exact}}$).

10. Form $\mathbf{b}_k^{(i+1)} = (\mathbf{X}^{\text{diag}} - E_k^{(i+1)}\mathbf{I})^{-1} \cdot \mathbf{q}_k^{(i+1)}$ for unconverged $\mathbf{C}_k^{(i+1)}$. If $n_{\text{corr}} > n_{\text{exact}} - n_{\text{conv}}$ (n_{conv} is the number of converged solutions), fill $\mathbf{b}^{(i+1)}$ with $\mathbf{C}^{(i)}$ and, if necessary, $\mathbf{C}_{\text{corr}}^{(i)}$ for unconverged solutions.

11. Return to step 5 with $i = i + 1$.

3. *Some Comments*

It is preferred that the large real-symmetric matrix $\mathbf{X}$ to be diagonalized should be rearranged with the low-lying diagonal elements $\mathbf{X}^{\text{diag}}$ near the beginning when the

matrix $\mathbf{X}$ is diagonally dominant, because it is easy to construct initial trial vectors for lowest eigensolutions by solving the small eigenvalue problem for the submatrix $\mathbf{X}^{(0)}$ of N_{guess} dimension (step 1). The off-diagonal elements of $\mathbf{X}$ need not be used in any specific sequence; then, only nonzero elements (semimatrix) can be stored in auxiliary memory. (A specific sequence might be required in a certain type of array processors.)

The $\mathbf{X}$ matrix multiplication steps (2 and 6) are time-determining, even if limited to nonzero multiplication, and are bound by the *I/O* processing. In Davidson's method and its modifications multiplication and accumulation per one off-diagonal element are performed only twice per iteration cycle. The present algorithm, in which the multiplication and accumulation are performed simultaneously in proportion to n_{solv} or n_{corr} per only one read-processing of large-matrix elements, is capable of avoiding being I/O bound; this is very important in using recent and near-future array processors.

In order to avoid round-off errors, explicit orthogonalization is required even among trial vectors $\mathbf{C}^{(i)}$ in step 5, and the procedure $\mathbf{D}^{(i)} = \mathbf{X}\mathbf{C}^{(i)}$ (step 6′) is required before step 7. In the program EMOR1 [21], the explicit orthogonalization and step 6′ are performed every iteration cycle and every fifth cycle, respectively. Because the Schmidt orthogonalization procedure is completely array processing-adapted, its computational time is negligible compared with the $\mathbf{X}$ matrix multiplication.

The computer program (named EMOR1) coded in FORTRAN 77 by the present author is available in the Computer Centre of the University of Tokyo [21]. The small eigenvalue problems in steps 1 and 7 are solved with a Householder-bisection-*QR*-inverse-iteration routine modified from the original version [22] by the present author so as to adapt it for array processing. In the present version of EMOR1 on the HITAC M-280H computer with an integrated array processor (IAP) of the Computer Centre the maximum values for parameters are as follows: $N_{\text{guess}} \leqslant 750$; $(N, n_{\text{solv}} + n_{\text{corr}}) \leqslant (13000, 26)$, $(20000, 17)$, or $(30000, 10)$. The extension to non-symmetric matrix eigenproblems and generalized eigenproblems ($\mathbf{X}\mathbf{C}_k = E_k\mathbf{Y}\mathbf{C}_k$) is under consideration.

III. Test Problems

1. *Results*

The program EMOR1 was applied to five test matrices. The structure of the matrices, which are the original Nesbet [4] (matrix $\mathbf{X}_1$) and modified Nesbet matrices ($\mathbf{X}_2 \sim \mathbf{X}_5$), is summarized in Table I. Eigenvalues for the matrices are summarized in Table II.

In Tables III, IV and V, test results for many sets of parameters in the matrices $\mathbf{X}_1$, $\mathbf{X}_2$ and $\mathbf{X}_3$ are shown, respectively. Throughout these examples N_{guess} is equal to

TABLE I

The Structure of Test Matrices[a]

Matrix X	Dimension N	Matrix elements X_{ii}	Matrix elements $X_{ij}(=X_{ji})$	No. of non-zero elements	Diagonal dominance (%)	Density (%)
$\mathbf{X}_1$	300	$2i-1$	1	45150	100	100
$\mathbf{X}_2$	300	$1.0+0.1\times(2i-1)$	1	45150	96.0	100
$\mathbf{X}_3$	300	$1.00+0.01\times(2i-1)$	1	45150	68.8	100
$\mathbf{X}_4$	1000	$2i-1$	$1, \lvert i-j\rvert < 50$	48775	100	9.75
$\mathbf{X}_5$	1000	$1.0+0.1\times(2i-1)$	$0, \lvert i-j\rvert \geqslant 50$	48775	98.8	9.75

[a] Diagonal dominance = fraction of the cases which satisfy that $|X_{ij}| < |X_{ii} - X_{jj}|$; density = ratio of non-zero elements.

n_{solv} and n_{approx} is zero. The maximum value of $|\mathbf{q}_k^{(0)}|^2$ is rather large. We solved the problems from such poor initial guesses because eigenvalue problems for matrices of $\approx$300 dimension can be easily solved by standard direct-diagonalization algorithms. For the matrix $\mathbf{X}_1$ the condition that $n_{\text{corr}} = n_{\text{exact}}$ is quite enough except when $n_{\text{exact}} = 1$. The condition that $n_{\text{corr}} = n_{\text{exact}}/2$ is sufficient when $n_{\text{exact}} \gtrsim 8$. On the other hand, the condition that $n_{\text{corr}} = n_{\text{exact}}$ is not sufficient when $n_{\text{exact}} \lesssim 6$ for $\mathbf{X}_2$ and even when $n_{\text{exact}} = 10$ for $\mathbf{X}_3$. For $\mathbf{X}_3$ the parameter n_{corr} should be chosen to be at least $4 \cdot n_{\text{exact}}$ ($n_{\text{exact}} \leqslant 3$) and about 12 ($n_{\text{exact}} \geqslant 4$); that is, the number of effective correction vectors does not depend on n_{exact} when n_{exact} becomes large.

TABLE II

Lowest Eigenvalues of Test Matrices

n	$\mathbf{X}_1$	$\mathbf{X}_2$	$\mathbf{X}_3$	$\mathbf{X}_4$	$\mathbf{X}_5$
1	0.2355346	0.1296170	0.01303906	0.2791881	−4.456670
2	2.262109	0.3336875	0.03346562	2.316219	−2.594780
3	4.278451	0.5362786	0.05373813	4.339914	0.07319100
4	6.290699	0.7382596	0.07394690	6.358201	0.2732267
5	8.300687	0.9398978	0.09411976	8.373496	0.4739468
6	10.30922	1.141313	0.1142692	10.38687	0.6756589
7	12.31674	1.342569	0.1344020	12.39891	0.8781389
8	14.32349	1.543706	0.1545223	14.40997	1.081195
9	16.32966	1.744750	0.1746327	16.42027	1.284691
10	18.33535	1.945719	0.1947352	18.42997	1.488534

TABLE III

Test Results[a] for Matrix $\mathbf{X}_1$

n_{solv}	n_{corr}	N_{guess}	$\mathbf{q}^2_{guess}$	$n_{it}(-6)$	$n_{it}(-10)$
1	1	1	$0.299\ 10^{+3}$	>20	
	2			6	9
	3			5	7
2	2	2	$0.508\ 10^{+3}$	4	6
	3			3	4
4	2	4	$0.917\ 10^{+3}$	8	9
	4			3	5
6	3	6	$0.132\ 10^{+4}$	5	8
	6			2	3
8	4	8	$0.173\ 10^{+4}$	5	6
	8			2	3
10	5	10	$0.213\ 10^{+4}$	4	5
	10			2	2
15	5	15	$0.311\ 10^{+4}$	5	6
	10			3	5
20	5	20	$0.407\ 10^{+4}$	5	6
	10			4	5

Note: $\mathbf{q}^2_{guess}$, maximum value of $|\mathbf{q}_k^{(0)}|^2$ for initial trial vectors; $n_{it}(-x)$, number of iterations required for converging $\mathbf{q}_k^2$ to less than 10^{-x}.

[a] $n_{solv} = n_{exact}$; namely, $n_{approx} = 0$.

TABLE IV

Test Results[a] for Matrix $\mathbf{X}_2$

n_{solv}	n_{corr}	N_{guess}	$\mathbf{q}^2_{guess}$	$n_{it}(-6)$	$n_{it}(-10)$
1	1	1	$0.299\ 10^{+3}$	>20	
	2			10	16
	3			7	12
	4			6	9
2	2	2	$0.594\ 10^{+3}$	>20	
	4			5	11
	6			4	6
4	4	4	$0.118\ 10^{+4}$	7	11
	6			3	5
	8			3	3
6	6	6	$0.175\ 10^{+4}$	4	8
	9			2	3
8	8	8	$0.232\ 10^{+4}$	3	5
	12			2	2
10	10	10	$0.289\ 10^{+4}$	2	4
	15			2	3

[a] $n_{solv} = n_{exact}$; $n_{approx} = 0$.

TABLE V

Test Results[a] for Matrix $\mathbf{X}_3$

n_{solv}	n_{corr}	N_{guess}	$\mathbf{q}^2_{guess}$	$n_{it}(-6)$	$n_{it}(-10)$
1	2	1	$0.299\ 10^{+3}$	13	>20
	3			11	>20
	4			9	17
2	4	2	$0.595\ 10^{+3}$	9	>20
	6			6	>20
	8			5	9
4	6	4	$0.119\ 10^{+4}$	>20	
	8			3	9
	12			3	4
6	6	6	$0.176\ 10^{+4}$	>20	
	9			3	6
	12			3	5
8	8	8	$0.233\ 10^{+4}$	>20	
	12			3	4
	16			2	3
10	10	10	$0.289\ 10^{+4}$	9	15
	15			2	4

[a] $n_{solv} = n_{exact}$; $n_{approx} = 0$.

Results of eigenvalue problems for the matrices $\mathbf{X}_4$ and $\mathbf{X}_5$ are shown in Tables VI and VII, respectively. Throughout these examples, $n_{approx} = 0$ and the parameter n_{exact} is fixed at 10; the parameters N_{guess} and n_{corr} are varied. For the matrix $\mathbf{X}_4$ when $N_{guess} = 10$, the conditions $n_{corr} = 20$ and 30 give the same result. The reason is that near linear dependence among correction vectors is encountered when $n_{corr} \gtrsim 20$. The condition $(N_{guess}, n_{corr}) = (50, 20)$ or $(100, 10)$ is sufficient. When $N_{guess} = 200$, the problem is nearly solved at the initial stage. For the matrix $\mathbf{X}_5$, the lowest two eigenvalues are unusual (Table II). The parameter N_{guess} should be chosen to be at least ≈ 100 and in practice ≈ 300.

Results of interior-eigenvalue problems for the matrix $\mathbf{X}_4$ are shown in Table VIII, where the initial trial vectors are unit vectors. The parameter n_{solv} corresponds to the number of solutions from the lowest (root 1) to the highest to be obtained either exactly or approximately. Added trial vectors to bound desired solution(s) from above improve convergence slightly; on the other hand, trial vectors to bound interior solution(s) from below work very well though the corresponding solutions are not converged at all, and convergence behaviors change little by comparison with the lowest-eigenvalue problems.

2. *Discussion*

The choice of the parameters N_{guess} and n_{corr} is quite important for efficiently solving eigenproblems. The larger N_{guess}, the better is convergence; on the other

TABLE VI

Test Results[a] for Matrix $\mathbf{X}_4$

n_{solv}	n_{corr}	N_{guess}	$\mathbf{q}^2_{guess}$	$n_{it}(-6)$	$n_{it}(-10)$
10	10	10	$0.327\ 10^{+3}$	13	16
	20			6	8
	30			6	8
10	10	50	$0.457\ 10^{+1}$	8	10
	20			6	8
10	10	100	$0.481\ 10^{-1}$	5	8
10	10	200	$0.188\ 10^{-7}$	1	2

[a] $n_{solv} = n_{exact}$; $n_{approx} = 0$.

TABLE VII

Test Results[a] for Matrix $\mathbf{X}_5$

n_{solv}	n_{corr}	N_{guess}	$\mathbf{q}^2_{guess}$	$n_{it}(-6)$	$n_{it}(-10)$
10	10	100	$0.369\ 10^{+2}$	>20	
	20			17	>20
	30			13	17
10	10	200	$0.801\ 10^{0}$	17	>20
	20			10	16
10	10	300	$0.154\ 10^{-2}$	6	12
	20			4	8
10	10	400	$0.153\ 10^{-5}$	2	4

[a] $n_{solv} = n_{exact}$; $n_{approx} = 0$.

TABLE VIII

Test Results[a] for Matrix $\mathbf{X}_4$

n_{exact}(Root No.)	n_{solv}	n_{corr}	$n_{it}(-6)$	$n_{it}(-10)$
1(1)	1	1	>20	
		3	9	12
		5	8	11
	3	3	8	11
		5	7	10
5(1 ~ 5)	5	5	15	>20
		7	9	13
		10	8	11
10(1 ~ 10)	10	10	13	18
		15	7	11
		20	7	9
1(5)	5	3	8	12
		5	7	9
	7	3	8	10
5(6 ~ 10)	10	5	16	>20
		7	9	12
		10	8	12
	13	7	7	11

[a] $N_{guess} = 0$; namely, the initial vectors are unit vectors.

hand, convergence is not improved when n_{corr} is too large. An optimum value for the parameter n_{corr} is strongly dependent on the problem (the structure of the matrix). The value $\mathbf{q}^2_{guess}$ is a criterion in determining an optimum n_{corr}. When n_{exact} is greater than ≈ 10, we may choose n_{corr} to be nearly constant (less than n_{exact}). This feature results in a similar approach to the group-coordinate relaxation method [7, 8].

In Table IX convergence behavior of the present algorithm is compared with the original Liu–Davidson algorithm in the same problem by imposing the same convergence criterion as in Ref. [17]. The present algorithm needs only four correction vectors in order to solve the problem with the same number of iterations as taken in the Liu–Davidson algorithm [17]; it is not necessary at all to expand n_{corr} up to 16.

The additional trial vectors to bound desired solutions from above are not so important; in any case, two or three vectors may be sufficient to improve convergence. For the interior-eigenvalue problem, all the initial trial vectors to bound the desired solutions from below are necessary, but correction vectors for the additional trial vectors are not necessary at all. The number of iterations is almost the same as for the lowest-eigenvalue problems. The present algorithm for directly determining higher eigensolutions seems superior to the method proposed by Butscher and Kammer [14] because theirs requires more iteration steps and correction vectors.

If the number n_{exact} of eigensolutions to be sought is too large to store all the vectors of $n_{exact} + n_{corr}$ in the main-memory, partitioning, such as $n_{exact} = n_{exact\,1} + n_{exact\,2} + \cdots$, is required and the problem is solved for $n_{exact\,1}$, $n_{exact\,2}$, and so on, sequentially from the lower solutions. Converged eigenvectors are saved in auxiliary memory. They are read out and used only at Schmidt orthogonalization step (step 5).

The present algorithm has advantages to use memory space efficiently and to reduce iteration steps, arithmetic operations and I/O processings.

TABLE IX

The Comparison with the Liu–Davidson Algorithm for the Same Problem[a] [17]

	$n_{solv}(=n_{exact})$	n_{corr}	N_{guess}	n_{it}
This work	4	$3 \to \to \to \to \to 3$	5	6
		$4 \to 4 \to 4 \to 4$		4
		$5 \to 5 \to 5$		3
		$6 \to 6 \to 6$		3
		$7 \to 7$		2
Ref. [17]	4	$4 \to 8 \to 12 \to 16$	5	4

[a] $X_{ij} = X_{ji} = 1, \quad 1 \leqslant i < j \leqslant 250$

$$X_{ii} = \begin{cases} 1 + 0.1(i-1), & 1 \leqslant i \leqslant 5 \\ 2i - 1, & 6 \leqslant i \leqslant 250. \end{cases}$$

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REFERENCES

1. A. PELLEW AND R. V. SOUTHWELL, *Proc. Roy. Soc. London A* **175** (1940), 262.
2. J. L. B. COOPER, *Quart. Appl. Math.* **6** (1948), 179.
3. S. F. BOYS, *Proc. Roy. Soc. London Ser. A* **201** (1950), 125.
4. R. K. NESBET, *J. Chem. Phys.* **43** 1965, 311.
5. I. SHAVITT, *J. Comput. Phys.* **6** (1970), 124.
6. I. SHAVITT, C. F. BENDER, A. PIPANO, AND R. P. HOSTENY, *J. Comput. Phys.* **11** (1973), 90.
7. Z. FALK, *Z. Angew. Math. Mech.* **53** (1973), 73.
8. L. M. CHEUNG AND D. M. BISHOP, *Comput. Phys. Commun.* **13** (1977), 247.
9. M. R. HESTENES AND W. KARUSH, *J. Res. Nat. Bur. Stand.* **47** (1951), 45.
10. C. LANCZOS, *J. Res. Nat. Bur. Stand.* **45** (1950), 255.
11. A. DALGARNO AND A. L. STEWART, *Proc. Phys. Soc.* **77** (1961), 467.
12. E. R. DAVIDSON, *J. Comput. Phys.* **17** (1975), 87.
13. M. G. FELER, *J. Comput. Phys.* **14** (1974), 341.
14. W. BUTSCHER AND W. E. KAMMER, *J. Comput. Phys.* **20** (1976), 313.
15. M. CLINT AND A. JENNINGS, *Comput. J.* **13** (1970), 76.
16. R. C. RAFFENETTI, *J. Comput. Phys.* **32** (1979), 403.
17. B. LIU, The simultaneous expansion method, *in* "Report on the Workshop: Numerical Algorithms in Chemistry: Algebraic Methods" (C. Moler and I. Shavitt, Eds.), p. 49, Lawrence Berkeley Lab., Univ. of California, 1978.
18. E. R. DAVIDSON, *J. Phys. A* **13** (1980), L179.
19. A. GOLEBIEWSKI, *Int. J. Quantum Chem.* **XV** (1979), 693.
20. S. IWATA, private communication.
21. N. KOSUGI, Program EMOR1, Program Library, The Computer Centre, The Univ. of Tokyo, 1982.
22. Y. BEPPU AND I. NINOMIYA, *Comput. Phys. Commun.* **23** (1981), 123; *Comput. Chem.* **6** (1982), 87.