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Orthogonal subspaces in an iterative method for the diagonalisation of Hermitian operators

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Abstract. An iterative method for calculating low-lying eigenvalues of a Hermitian operator is extended and modified so as to provide an efficient algorithm that yields the whole spectrum.

1. Introduction

In recent years, the Lanczos algorithm (Lanczos 1950) for the diagonalisation of quantum mechanical operators has been widely utilised (Sebe and Nachamkin 1969, Cole *et al* 1973, 1974a, b, c, 1975a, b, c, d, Toepfer 1975, Whitehead 1972). Recently, a most interesting iterative method has been presented by Berger and co-workers (Berger *et al* 1977, Miller and Berger 1979) which may, under certain circumstances, be considered as an alternative to the Lanczos procedure. This new algorithm, which for the sake of brevity shall be referred to as the BMKD one, has the great advantage of drastically reducing the computer storage space and is both simple and elegant (Berger *et al* 1977).

As presented originally (Berger *et al* 1977) the method is ideally suited for obtaining the lowest-lying eigenvalue (and eigenvector). Having nicely surmounted the so-called pseudoconvergence problem (Miller and Berger 1979), the first excited state can also be easily obtained. However, were one faced with the necessity of finding the complete spectrum of a given Hermitian operator of not exceedingly large dimensions (say, 40×40), the set of 'parallel iterations' (Miller and Berger 1979) to be performed may give rise to numerical complications. At the very least, steps would have to be adopted that may defile the extreme simplicity and beauty of the algorithm.

Since among the existent diagonalisation schemes, the BMKD is in many circumstances the simplest available one, we feel that the problem mentioned in the previous paragraph deserves some consideration. The purpose of the present work is to present a modified version of the method that renders it more manageable in those cases in which the complete spectrum is sought. We have in mind, of course, medium-size matrices ($\sim 100 \times 100$) only.

We shall briefly review, for the sake of completeness, the BMKD scheme in § 2, and present our amended version of the algorithm in § 3. Section 4 is devoted to some small numerical examples and some conclusions are drawn in § 5.

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2. The BMKD scheme

This is an algorithm (Berger *et al* 1977) that, supported by the variational principles of Padé–Rayleigh–Ritz (Bessis 1976), allows one to evaluate the eigenvectors (and eigenvalues) of a given Hermitian operator $\hat{A}$ defined everywhere in a finite dimensional vector space V_n of dimension n. It yields the eigenvalues (and corresponding eigenvectors) one at a time, starting with the calculation of the lowest one (and in increasing order), via an iterative process which can be succinctly described as follows. A given initial vector (normalised) $|k\rangle \in V_n$ is chosen. When $\hat{A}$ operates on $|k\rangle$ one obtains

$$\hat{A}|k\rangle = e_k|k\rangle + v_k|kp\rangle \tag{2.1}$$

with (Berger *et al* 1977)

$$\begin{aligned} &\langle k\,|\,kp\rangle = 0 \\ &\langle kp\,|\,kp\rangle = 1 \\ &e_k = \langle k|\hat{A}|k\rangle \\ &v_k = (\langle k|\hat{A}^2|k\rangle - e_k^2)^{1/2}. \end{aligned} \tag{2.2}$$

The states $|k\rangle$ and $|kp\rangle$ define a 2×2 subspace of V_n in which $\hat{A}$ is to be diagonalised, the corresponding matrix being

$$M = \begin{bmatrix} e_k & v_k \\ v_k & \alpha_k \end{bmatrix} \tag{2.3}$$

with

$$\alpha_k = \langle kp|\hat{A}|kp\rangle. \tag{2.4}$$

The eigenvector $|k+1\rangle$ of M corresponding to its lowest eigenvalue now takes the place of $|k\rangle$ in equation (2.1), thus generating, in the same fashion, a new 2×2 matrix to be diagonalised, and so on. Let K denote the set $\{|\lambda\rangle\}$ of eigenvectors of $\hat{A}$ whose overlap with the initial vector $|k\rangle$ is different from zero. Berger *et al* (1977) have shown that the iterative process described above converges to that member of K whose corresponding eigenvalue is the lowest.

The BMKD algorithm neatly avoids some numerical and computational problems that may arise when dealing with the original Lanczos approach (Lanczos 1950). As the BMKD iterations involve only 2×2 matrices, in a given iteration step only two vectors are needed and, moreover, just *one* new vector ($|kp\rangle$) orthogonal to the iterating one ($|k\rangle$ in equation (2.1)) is to be built. On the other hand, in employing Lanczos' method, one must enforce the orthogonality of its new basis vector with respect to *all* those previously generated. This may entail the task of reorthogonalising, in step number m, say, the mth basis vector with respect to the preceding $m-1$ ones, which obviously demands both a larger storage space and additional computing time than in the BMKD case.

As stated by the authors (Berger *et al* 1977), their method may in principle be utilised to obtain additional eigenvalues (and eigenvectors) of $\hat{A}$, other than the lowest one ($|\lambda = 1\rangle$). The idea is to project out of the original start vector $|k\rangle$ the vector $|\lambda = 1\rangle$ already found, and repeat the procedure with the new initial vector thus constructed, which may ultimately yield $|\lambda = 2\rangle$, etc.

Two types of difficulties may arise in applying this beautiful scheme. On the one hand, the component of the desired eigenvector in the original (arbitrarily chosen) start vector may be small (although non-vanishing) compared with the components of one or more of the neighbouring eigenvectors. In other words, the selection of the initial vector has not been appropriate. As a consequence, the method may converge to the wrong eigenvalue. This pseudoconvergence can be avoided by using the 'parallel iterations' scheme (PIS) of Miller and Berger (1979). A different (although not unrelated) problem may also present itself, no matter how good the choice of the start vector, because of the unavoidable loss of precision inherent to data processing in a computer. As a consequence, in evaluating some 'excited' eigenvalue (i.e. not the lowest one) the iterating vector may acquire a non-vanishing overlap with a previously evaluated one. The iterative process will then converge to this last vector. Even a very small spurious overlap will have this effect, an annoying numerical feature which may well make it impossible, in many circumstances, to obtain high-lying eigenvalues with the BMKD method. It is our purpose to implement a simple device that circumvents this difficulty (see §3).

It should be explicitly pointed out that the PIS of Miller and Berger (1979) has been implemented by them in order to obtain the lowest two eigenvalues. The authors suggest the possibility of extending their approach by inclusion of additional sets of parallel iterations, in order to evaluate more than two eigenvectors. In doing this, however, still another difficulty appears (again, not unrelated to the previous ones), i.e. numerical instabilities which may even prevent the process from converging and will be illustrated below. This last problem can also be surmounted by recourse to the algorithm to be presented in the following section.

3. A modified BMKD algorithm

The purpose of the present section is to present a modified version of the BMKD algorithm in order to overcome some difficulties, mentioned in the previous section, that arise in applying the original formulation of the method.

We consider again the Hermitian operator $\hat{A}$ defined in V_n and denote by $\{|\lambda\rangle\}$ the set of its eigenvectors.

$$\hat{A}|\lambda\rangle = E_\lambda|\lambda\rangle \qquad \lambda = 1, \ldots, n \tag{3.1}$$

where we assume

$$E_1 \leqslant E_2 \leqslant E_3 \leqslant \ldots \leqslant E_n. \tag{3.2}$$

Let B_n be an arbitrary basis in V_n and A_n the corresponding matrix of $\hat{A}$ in that basis

$$\|\hat{A}\|_{B_n} = A_n. \tag{3.3}$$

As usual, we need a starting vector $|k_1\rangle$ and, for convenience, we assume

$$\langle\lambda|k_1\rangle \neq 0 \qquad \lambda = 1, 2, \ldots, n. \tag{3.4}$$

We shall now regard the BMKD algorithm as a set of operations that define an 'operator' $\hat{\mu}_{\hat{A}}$, such that $\hat{\mu}_{\hat{A}}$ acts on a given vector $|k_1\rangle \in V_n$ yielding that eigenvector of $\hat{A}$, selected among those having non-zero overlap with $|k_1\rangle$, whose eigenvalue is the

lowest. Thus

$$\hat{\mu}_{\hat{A}}|k_1\rangle = |\lambda = 1\rangle \tag{3.5}$$

$$\hat{A}|\lambda = 1\rangle = E_1|\lambda = 1\rangle. \tag{3.6}$$

We point out that the set of 'parallel iterations' proposed by Miller and Berger (1979) are included in the definition of $\hat{\mu}_{\hat{A}}$.

3.1. Orthogonal subspaces

Consider now the subspace S_{n-1} (of dimension $n-1$) of V_n orthogonal to $|\lambda = 1\rangle$

$$S_{n-1} = \{|x\rangle / |x\rangle \in V_n \wedge \langle x|\lambda = 1\rangle = 0\} \tag{3.7}$$

and B_{n-1} a given orthonormal basis of S_{n-1}

$$B_{n-1} = \{|f_i\rangle; i = 1, \ldots, n-1\}. \tag{3.8}$$

Since $\langle \lambda = 1|f_i\rangle = 0$ for all i, the set $D_{n,1}$

$$D_{n,1} = \{|f_1\rangle, |f_2\rangle, \ldots, |f_{n-1}\rangle, |\lambda = 1\rangle\} \tag{3.9}$$

is a basis of V_n. Now, denote the matrix representing the change of basis $B_n \to D_{n,1}$ as H_n; then

$$|x\rangle_{B_n} = H_n|x\rangle_{D_{n,1}} \tag{3.10}$$

where $|x\rangle_Q$ denotes the vector $|x\rangle$ developed according to the basis Q.

The matrix of $\hat{A}$ in the basis $D_{n,1}$ is

$$\|\hat{A}\|_{D_{n,1}} = H_n^{-1}\|\hat{A}\|_{B_n}H_n = H_n^{-1}A_nH_n. \tag{3.11}$$

We introduce now the operator $\hat{A}_1$ as the restriction of $\hat{A}$ to the subspace S_{n-1}, and the $(n-1)\times(n-1)$ matrix A_{n-1} defined as

$$\|\hat{A}_1\|_{B_{n-1}} = A_{n-1}. \tag{3.12}$$

It should be clear now (we shall show it formally below) that the matrix of $\hat{A}$ in the basis $D_{n,1}$ adopts the form

$$\|\hat{A}\|_{D_{n,1}} = \begin{bmatrix} & & 0 \\ & A_{n-1} & \vdots \\ & & 0 \\ 0 & \ldots 0 & E_1 \end{bmatrix} \tag{3.13}$$

where E_1 denotes the lowest eigenvalue of $\hat{A}$.

In a way, we have 'diagonalised' $\hat{A}$ with respect to its lowest eigenvector. Although $\|\hat{A}\|_{D_{n,1}}$ possesses identical information to that of $\|\hat{A}\|_{B_n}$, the structure (3.13) makes it clear that its $n-1$ remaining eigenvectors may be computed by diagonalisation of A_{n-1} (a $(n-1)\times(n-1)$ procedure).

The BMKD algorithm is now to be applied to the operator $\hat{A}_1$, whose matrix is given by (3.12). The start vector should now be chosen within the subspace S_{n-1}, which leads one to consider the initial vector

$$|k_2\rangle = |k_1\rangle - \langle \lambda = 1|k_1\rangle|\lambda = 1\rangle \tag{3.14}$$

which obviously satisfies $\langle k_2|\lambda = 1\rangle = 0$, i.e. $|k_2\rangle \in S_{n-1}$.

This new application of the BMKD formalism

$$\hat{\mu}_{\hat{A}_1}|k_2\rangle = |\lambda = 2\rangle_{B_{n-1}} \tag{3.15}$$

yields the second eigenvector of $\hat{A}$, expressed in the basis B_{n-1} of S_{n-1}. In order to obtain the expression of $|\lambda = 2\rangle$ in the original basis B_n it suffices to add to $|\lambda = 2\rangle_{B_{n-1}}$ a null nth component. This gives us the corresponding coordinates in $D_{n,1}$, which, using (3.10), finally leads to

$$|\lambda = 2\rangle_{B_n} = H_n|\lambda = 2\rangle_{D_{n,1}}. \tag{3.16}$$

Knowing both $|\lambda = 1\rangle$ and $|\lambda = 2\rangle$, a new reduction of V_n is feasible, that defines S_{n-2} according to

$$S_{n-2} = \{|y\rangle / |y\rangle \in S_{n-1} \wedge \langle y|\lambda = 2\rangle = 0\}. \tag{3.17}$$

A new operator $\hat{A}_2$ (the restriction of $\hat{A}_1$ to the subspace S_{n-1}) should now be introduced and the procedure (3.8)–(3.13) can be repeated, yielding $|\lambda = 3\rangle$,

$$\hat{\mu}_{\hat{A}_2}|k_3\rangle = |\lambda = 3\rangle_{B_{n-2}}. \tag{3.18}$$

In a similar fashion, higher-lying eigenvalues may be found, until the whole spectrum of $\hat{A}$ is exhausted. Now, one wishes to express the eigenvectors $|\lambda = j+1\rangle$ thus obtained in the original basis B_n rather than in the reduced one B_{n-j}. This entails a product of matrices of the form

$$|\lambda = j+1\rangle_{B_n} = h_{n,0}h_{n,1} \ldots h_{n,j-1}|\lambda = j+1\rangle'_{B_{n-j}} \tag{3.19}$$

where

$$|\lambda = j+1\rangle'_{B_{n-j}} \equiv (|\lambda = j+1\rangle_{B_{n-j}}, 0, \ldots, 0) \tag{3.20}$$

is a vector with the last j components equal to zero, and

$$h_{n,k} = \begin{bmatrix} & & 0 \\ & H_{n-k} & \vdots \\ 0 & \ldots & 0 \end{bmatrix} \tag{3.21}$$

is an $n \times n$ matrix which is built by completing with zeros in the appropriate places the $(n-k) \times (n-k)$ matrix H_{n-k}.

Notice now that, in order to obtain $|\lambda = j\rangle_{B_n}$, one needs the product

$$P_j \equiv h_{n,0}h_{n,1} \ldots h_{n,j-2} \tag{3.22}$$

with the property

$$P_j = P_{j-1}h_{n,j-2}. \tag{3.23}$$

So that the procedure of expressing a given vector $|\lambda = j+1\rangle$ in the original basis B_n *requires the storage of only two matrices*, i.e. P_j and $h_{n,j-1}$.

Obviously, as we deal with higher and higher eigenvalues, both the number of iterations implied in $\hat{\mu}_{\hat{A}}$ (until convergence is reached) and the CPU computer time required in each iteration drastically decreases, since the dimensions of the matrices involved diminish steadily. In particular, in the case of the last two eigenvalues, no iterations are needed, since only a 2×2 matrix remains.

One should point out that, within the present framework, the second of the problems mentioned in § 2 with reference to the BMKD scheme *cannot arise* (at least as

posed there) because of the orthogonality of the corresponding subspaces involved (see, however, § 3.3).

3.2. Construction of H_n

Let B_n be the initial basis in V_n:

$$B_n = \{|v_i\rangle\}_{i=1,\ldots,n}. \tag{3.24}$$

The expansion of $|\lambda = 1\rangle$ in such a basis will be

$$|\lambda = 1\rangle = \sum_{i=1}^{n} \beta_i |v_i\rangle \tag{3.25}$$

where the coefficients β_i are determined by the action of $\hat{\mu}_{\hat{A}}$ upon the starting vector. As an example, the basis B'_{n-1} introduced in the previous subsection is

$$B'_{n-1}: \{|v_1\rangle - \beta_1/\beta_k |v_k\rangle; \ldots; |v_{k-1}\rangle - \beta_{k-1}/\beta_k |v_k\rangle; |v_{k+1}\rangle - \beta_{k+1}/\beta_k |v_k\rangle; \ldots; |v_n\rangle - \beta_n/\beta_k |v_k\rangle\}. \tag{3.26}$$

We choose $k = n$ for convenience. In such a case

$$B'_{n-1}: \{|g_i\rangle\}_{i=1,\ldots,n-1}. \tag{3.27}$$

with

$$|g_i\rangle = |v_i\rangle - \beta_i/\beta_n |v_n\rangle \qquad i = 1, \ldots, n-1. \tag{3.28}$$

Obviously, the $|g_i\rangle$ are linearly independent and generate S_{n-1}. The Gram–Schmidt orthonormalisation process allows one to obtain an orthonormal basis of S_{n-1}, constructed from B'_{n-1} and which we call B_{n-1}.

$$B_{n-1}: \{|f_i\rangle, i = 1, \ldots, n-1\} \tag{3.29}$$

where

$$|f_i\rangle = \sum_{j=1}^{i} \alpha_{ji} |g_j\rangle \qquad i = 1, \ldots, n-1. \tag{3.30}$$

The Gram–Schmidt algorithm determines the coefficients α_{ji}. The bases B'_{n-1} and B_{n-1}, extended to the space V_n, are given by

$$D'_{n,1}: \{|g_1\rangle, |g_2\rangle, \ldots, |g_{n-1}\rangle, |\lambda = 1\rangle\} \tag{3.31}$$

and

$$D_{n,1}: \{|f_1\rangle, |f_2\rangle, \ldots, |f_{n-1}\rangle, |\lambda = 1\rangle\} \tag{3.32}$$

respectively. Now we introduce the matrix

$$H'_1 = \begin{bmatrix} \alpha_{11} & \alpha_{12} & \ldots & \alpha_{1,n-1} & 0 \\ 0 & \alpha_{22} & \ldots & \alpha_{2,n-2} & 0 \\ \vdots & & & \vdots & \\ 0 & 0 & \ldots & \alpha_{n-1,n-1} & 0 \\ 0 & 0 & \ldots & 0 & 1 \end{bmatrix} \tag{3.33}$$

such that

$$|x\rangle_{D'_{n,1}} = H'_1 |x\rangle_{D_{n,1}} \tag{3.34}$$

and the matrix H_2'

$$H_2' = \begin{bmatrix} 1 & 0 & \dots & 0 & \beta_1 \\ 0 & 1 & \dots & 0 & \beta_2 \\ \vdots & & & & \vdots \\ \gamma_1 & \gamma_2 & \dots & \gamma_{n-1} & \beta_n \end{bmatrix} \tag{3.35}$$

where

$$\gamma_k = -\beta_k/\beta_n \tag{3.36}$$

with the property

$$|x\rangle_{B_n} = H_2' |x\rangle_{D_{n,1}'}. \tag{3.37}$$

The passage from the basis $D_{n,1}$ to the B_n is finally accomplished by the matrix H_n given by

$$H_n = H_2' H_1' \tag{3.38}$$

since

$$|x\rangle_{B_n} = H_n |x\rangle_{D_{n,1}}. \tag{3.39}$$

Of course, similar procedures yield the matrices H_{n-1}, H_{n-2} etc.

3.3. Practical considerations

In applying the formalism discussed in the present work an unpleasant feature may arise, that stems from the difficulty in numerically achieving the form (3.13) for $\|\hat{A}\|_{D_{n,1}}$ (the form (3.38) for H_n). That is, A_n is not 'exactly' diagonalised with respect to $|\lambda = 1\rangle$. This effect is due to one of the following reasons.

(i) $|\lambda = 1\rangle$ is not the 'exact' eigenvector of A_n (by 'exact' one should understand infinite precision).

(ii) Error accumulation in computing H_n.

As a consequence S_{n-1} is not a subspace strictly orthogonal to $|\lambda = 1\rangle$, and contains a small projection of $|\lambda = 1\rangle$, with a spurious eigenvalue $\varepsilon = 0$.

This does not constitute any problem as long as one deals with the negative region of the spectrum of $\hat{A}$, because $\hat{\mu}_{\hat{A}}$ always converges to the lowest available eigenvalue (Berger *et al* 1977). On the other hand, if one is working with the positive region, the procedure will converge to ε.

This is not the pseudoconvergence problem discussed in Miller and Berger (1979) although it could be regarded as its counterpart within the present scheme, and can be circumvented with their PIS treatment. In our case, of course, there can be no convergence to a previously found eigenvector, since they do not exist in the space one is working with. The point is however that the problem we are discussing in this subsection (*a*) can only appear if one deals with positive eigenvalues and (*b*) can be surmounted by recourse to a much simpler device than the parallel iterations scheme: Assume that an upper bound γ to the absolute value of the eigenvalues of $\hat{A}$ is known. A trivial upper bound of this sort, for a given matrix, is the sum of the absolute values of its diagonal elements. One simply considers the operator $\hat{A} - \gamma\hat{I}$, $\hat{I}$ denoting the identity operator, which possesses an entirely negative spectrum (the eigenvectors, of course, do not change).

4. Numerical examples

As a practical application we discuss here the complete diagonalisation of the 41×41 energy matrix that arises in the modified Lipkin model of Abecasis *et al* (1969) for 40 particles and coupling constant equal to 0.015.

This matrix possesses both negative and positive eigenvalues and the relevant results are illustrated in figure 1.

Let ν_j denote the number of BMKD iterations required to obtain the jth eigenvector, and n_j the dimension of the subspace in which one works to obtain it. We plot ν_j/ν_1 against n_j. (In particular, if $j = 2$, only a 2×2 matrix remains, so no iteration is needed.)

Figure 1(a) shows that the pseudoconvergence discussed in § 3.3 arises for $j < 18$. Recourse is then made to the parallel iterative procedure (Miller and Berger 1979), and the relative number of iterations increases. In figure 1(b) we plot the same quantities. Pseudoconvergence has here been circumvented with the prescription (§ 3.3), so that ν_j decreases monotonically.

We shall now consider a very simple example that clearly illustrates the numerical difficulties that one may face in trying to implement the PIS of Miller and Berger (1979) in order to obtain *more* than two eigenvalues (see the last paragraph of § 2). Let us diagonalise the 5×5 matrix that arises in the model of Abecasis *et al* (1969) for four

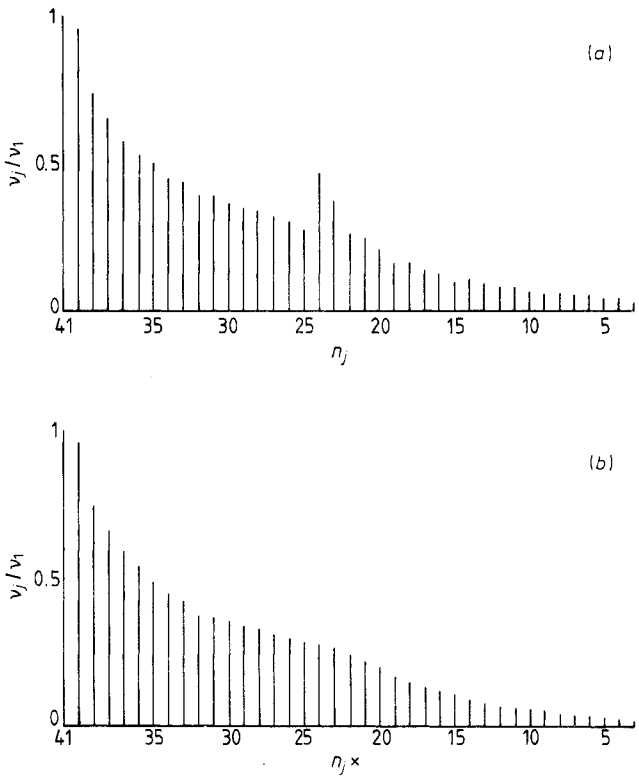

Figure 1. Relative number of iterations ν_j/ν_1 needed to obtain the jth eigenvector plotted against the dimension of the corresponding linear space n_j. The calculation reported corresponds to a 41×41 matrix; (a) straightforward procedure, (b) pseudoconvergence is avoided.

particles and coupling constant equal to 0.1. Our version of the BMKD method and the PIS yield, of course, the first two eigenvalues without difficulties. Things are different, however, in the case of higher eigenvalues, as shown in table 1. Let us denote by E the 'exact' eigenvalue and consider the quantity $\sigma_i^2 = (E_i - E)^2/E^2$, where i is an integer number that counts the successive iterations one must perform in applying any of these two schemes. Table 1 displays the behaviour of σ_i^2, both for our version of the BMKD method and for the PIS of Miller and Berger (1979). Notice that in the case of the last two eigenvalues, the method of the present work yields the final result after the first iteration†. On the other hand, the numerical instabilities that arise with the PIS may even prevent convergence, as illustrated in the case of the highest eigenvalue. In any case, our approach converges much sooner.

Table 1. Relative deviation $\sigma_i^2 = (E - E_i)^2/E^2$, with respect to the exact eigenvalue E, of the approximate one E_i obtained, using the iterative diagonalisation schemes discussed in the text, after performing the ith iteration. A 5×5 matrix is considered. In the case of the last two eigenvalues the method of the present work (PW) yields the correct answer after just one iteration, so that the corresponding σ^2 are not shown. The BMKD approach fails to converge for the last eigenvalue.

Iteration number \ Eigenvalue	3		4	5
	σ^2_{BMKD}	σ^2_{PW}	σ^2_{BMKD}	σ^2_{BMKD}
3	0.8733	0.667×10^{-7}	0.0546	0.4557
4	0.2048	0.0	0.0079	0.2623
7	0.0001	0.0	0.0001×10^{-8}	0.8392
8	0.0001	0.0	0.0985	1.2717
11	0.0170	0.0	0.2865	0.6292
12	0.0001×10^{-3}	0.0	0.2680	0.5046
15	2.3228	0.0	1.4088	0.6307
16	2.3224	0.0	0.0001×10^{-3}	0.1772
19	0.0001×10^{-2}	0.0	1.4094	0.8845
20	2.3229	0.0	1.4094	0.1850
23	0.0001×10^{-9}	0.0	0.2854	0.6108
24	0.0001×10^{-2}	0.0	0.2992	0.6153
27	0.0901	0.0	0.0002	0.1773
28	0.1980	0.0	0.2964	0.5648
31	0.0001×10^{-3}	0.0	0.0021	0.1772
32	0.0001×10^{-9}	0.0	0.0001×10^{-8}	0.6233
35	0.0001×10^{-14}	0.0	0.4060	0.6373
36	0.0001×10^{-16}	0.0	0.0001×10^{-2}	0.1772
39	0.0	0.0	0.2394	0.7291
40	0.0	0.0	0.0046	0.6684
43	0.0	0.0	0.4548	0.1981

These and many other numerical examples that we have studied exhibit an additional advantage of our procedure. After each successive reduction to a smaller subspace, the corresponding reduced matrices A_{n-j} tend to adopt forms increasingly closer to the diagonal one. This allows for a more rapid convergence in the action of the operator $\hat{\mu}_A$ than could otherwise be expected.

† See § 3.1.

5. Conclusions

A quite convenient method for the evaluation of the low-lying eigenvalues of a Hermitian operator (Berger *et al* 1977) has been modified in the present work so as to provide a rapid and economical algorithm that enables one to compute the whole spectrum.

Notice that, although our scheme has been devised with the BMKD algorithm in mind, it ought to work for any other procedure with the restriction that the corresponding operator $\hat{\mu}_{\hat{A}}$ should yield the eigenvalues individually and in an ordered sequence.

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