Extension of an iterative method to obtain low-lying eigenstates of unbounded Hermitian operators

Extension of an iterative method to obtain low-lying eigenstates of unbounded Hermitian operators

K G Kreuzer†, H G Miller†, R M Dreizler† and W A Berger‡

† Institut für Theoretische Physik, Universität Frankfurt am Main, Robert-Mayer-Strasse 8-10, 6000 Frankfurt/Main 1, West Germany
‡ Institut für Theoretische Physik, Universität Giessen, West Germany

Abstract. An iterative method which determines the low-lying eigenvalues of a Hermitian operator defined in a finite-dimensional vector space is extended to a specific type of unbounded Hermitian operator defined in a Hilbert space. As an illustrative numerical example the extended algorithm has been applied to the quantum mechanical harmonic oscillator problem.

1. Introduction

In the last few years iterative algorithms have been used extensively to obtain acceptable approximations for the low-lying eigenstates of a quantum mechanical system (see the list of references given by Stewart (1974) or Berger (1979)). These algorithms are usually formulated for Hermitian operators defined in a finite-dimensional vector space and can also be extended to compact Hermitian operators defined in a Hilbert space (Vorobyev 1965). However, in most cases of interest the Hamiltonian of a quantum mechanical system is a Hermitian operator possessing a spectrum with a lower bound only. Hence in order to make use of such algorithms a projection of the Hamiltonian onto a finite-dimensional subspace of the entire Hilbert space is required.

To avoid this projection and the subsequent errors inherent in the eigenstates obtained in this manner we have extended the simple 2×2 algorithm described previously by us (Berger *et al* 1977) to include also unbounded Hermitian operators. In this case iterations can be performed with the full (that is the unprojected) Hamiltonian provided that this operator possesses a special kind of continuity and that an appropriate trial vector is available.

In this paper we reformulate the algorithm and prove its convergence properties. Furthermore we make some remarks about error estimates and the occurrence of pseudoconvergence. An application to a well-known Hamiltonian illustrates the numerical behaviour of the present algorithm.

2. The extended 2×2 algorithm

2.1. Statement of the algorithm

Let $\mathcal{H}$ be a separable Hilbert space and $\hat{H}$ a Hermitian operator having a discrete spectrum with a lower bound only. Let $\mathcal{D}$ be the domain of $\hat{H}$ and E and $|E\pi\rangle$ its

eigenvalues and eigenvectors respectively. The index π labels a possible degeneracy of the eigenvalues. Furthermore let $|T\rangle \in \mathcal{D}$ be a vector normalised to unity, the so-called trial vector. The expansion of the trial vector in terms of the eigenvectors is given by

$$|T\rangle = \sum_{E\pi} t_{E\pi} |E\pi\rangle \tag{2.1}$$

or equivalently as

$$|T\rangle = \sum_{E} t_E |E\rangle \tag{2.2}$$

where all eigenvectors and expansion coefficients corresponding to the same eigenvalue E are collected in the normalised vectors $|E\rangle$ and in the coefficients t_E, that is

$$|E\rangle = \frac{1}{t_E} \sum_{\pi} t_{E\pi} |E\pi\rangle \tag{2.3}$$

with

$$t_E = \left(\sum_{\pi} |t_{E\pi}|^2 \right)^{1/2}. \tag{2.4}$$

The algorithm is now defined by the following steps:

(i) From the given trial vector construct the orthonormal vectors

$$\begin{aligned} |\Phi_1\rangle &:= |T\rangle \\ |\Phi_2\rangle &:= \frac{\hat{H}|T\rangle - |T\rangle\langle T|\hat{H}|T\rangle}{\|\hat{H}|T\rangle - |T\rangle\langle T|\hat{H}|T\rangle\|}. \end{aligned} \tag{2.5}$$

Linear independence of $|T\rangle$ and $\hat{H}|T\rangle$ is guaranteed if the trial vector is not an eigenvector of $\hat{H}$.

(ii) Diagonalise $\hat{H}$ in the subspace $\mathcal{H}_\Phi$ spanned by $|\Phi_1\rangle$ and $|\Phi_2\rangle$ in order to obtain the orthonormal vectors

$$|e_i\rangle = \left(1 + \left(\frac{e_i - v_1}{w} \right)^2 \right)^{-1/2} \left(|\Phi_1\rangle + \frac{e_i - v_1}{w} |\Phi_2\rangle \right) \tag{2.6}$$

where

$$v_i = \langle \Phi_i | \hat{H} | \Phi_i \rangle, \qquad w = \langle \Phi_1 | \hat{H} | \Phi_2 \rangle, \qquad i = 1, 2.$$

Their expectation values are

$$e_i = \tfrac{1}{2}(v_1 + v_2) + (-1)^i (w^2 + \tfrac{1}{4}(v_1 - v_2)^2)^{1/2}, \tag{2.7}$$

and

$$e_1 < v_1, \qquad e_2 > v_2. \tag{2.8}$$

Here the diagonal matrix elements v_1 and v_2 are real since $\hat{H}$ is a Hermitian operator. The off-diagonal matrix element w is also real since its square is nothing more than the variance of $\hat{H}$ with respect to the trial vector, that is

$$w^2 = \langle T|\hat{H}^2|T\rangle - \langle T|\hat{H}|T\rangle^2. \tag{2.9}$$

(iii) Choose the vector $|e_1\rangle$ as a new trial vector and restart at step (i).

The algorithm defines the sequences $(w(I))$, $(e_1(I))$ and $(|e_1(I)\rangle)$ whose convergence properties are given by

$$\lim_{I \to \infty} e_1(I) = E_T \tag{2.10}$$

$$\lim_{I \to \infty} w(I) = 0 \tag{2.11}$$

$$\lim_{I \to \infty} |e_1(I)\rangle = |E_T\rangle. \tag{2.12}$$

Here E_T is the lowest eigenvalue that corresponds to the eigenvector $|E_T\rangle$ contained in the expansion (2.2) of the trial vector.

To prove the statements (2.10), (2.11) and (2.12) we cannot proceed as in the original case of a bounded Hermitian operator since there we used essentially the fact that the sequence $(v_2(I))$ is bounded. In the present case of an unbounded Hermitian operator this is not guaranteed, except in the trivial case where the trial vector contains only a finite number of eigenvectors. The proof of the convergence properties of the extended 2×2 algorithm requires that the trial vector $|T\rangle$ and the operator $\hat{H}$ must be assumed to satisfy additional restrictions. These are that $\hat{H}$ is positive and τ-continuous in $\mathscr{L}$ and $|T\rangle$ is contained in $\mathscr{F}$. Here $\mathscr{L}$ is defined to be the space of all finite linear combinations of eigenvectors of $\hat{H}$. τ-continuity of $\hat{H}$ is continuity with respect to the topology which is defined by the additional scalar products in $\mathscr{L}$

$$\langle \phi | \psi \rangle_k := \langle \phi | \hat{H}^k | \psi \rangle, \qquad k = 0, 1, 2, 3, \ldots \tag{2.13}$$

and $\mathscr{F}$ is defined to be the completion of $\mathscr{L}$ with respect to this topology, that is

$$\mathscr{F} := \mathscr{L} \cup \{\text{limits of all } \tau\text{-Cauchy sequences of } \mathscr{L}\} \tag{2.14}$$

or equivalently

$$\mathscr{F} := \mathscr{L} \cup \left\{ |\phi\rangle \in \mathscr{H} : \sum_{E_\pi} |\langle E_\pi | \phi \rangle|^2 E^k < \infty \; \forall \; k = 0, 1, 2, 3, \ldots \right\}. \tag{2.15}$$

Requiring $\hat{H}$ to be positive ensures that $\langle \; | \; \rangle_k$ has indeed the properties of a scalar product while τ-continuity of $\hat{H}$ in $\mathscr{L}$ guarantees that $\hat{H}$ possesses a unique (τ-continuous) extension onto $\mathscr{F}$. Hence $\mathscr{F}$ is included in the domain of $\hat{H}$ and for every $|T\rangle \in \mathscr{F}$ the vectors $\hat{H}^k | T\rangle$ are defined for all $k = 1, 2, 3, \ldots$. This guarantees that an arbitrary number of iterations can actually be performed. Note that τ-continuity of $\hat{H}$ does not imply the usual continuity and hence does not contradict the unboundedness of $\hat{H}$. This stems from the fact that the set of Cauchy sequences in $\mathscr{L}$ is larger than the set of τ-Cauchy sequences in $\mathscr{L}^\dagger$.

2.2. Proof of convergence

The proof given below can be briefly outlined as follows. The sequences $(e_1(I))$ and $(\langle E_T | e_1(I) \rangle)$ can be shown to be convergent with limits x and y. If $(|e_1(I)\rangle)$ is τ-Cauchy then the iterative structure of the algorithm requires that the limit is an eigenvector of $\hat{H}$. Therefore it is guaranteed that zero is an accumulation point of $(w^2(I))$. This finally implies that $x = E_T$ and $y = 1$ and hence that $(|e_1(I)\rangle)$ and $(w(I))$ converge to $|E_T\rangle$ and zero. We now give the proof in detail.

† For further details and references see Böhm (1978).

2.2.1. Proof that $(e_1(I))$ *and* $(\langle E_T|e_1(I)\rangle)$ *converge.* From relation (2.8) and step (iii) of the algorithm we obtain

$$E_T < e_1(I) < e_1(I-1) < \langle T|\hat{H}|T\rangle. \tag{2.16}$$

Hence $(e_1(I))$ is bounded and monotonically decreasing and therefore must converge to some x with $E_T \leqslant x \leqslant \langle T|\hat{H}|T\rangle$. From equations (2.5) and (2.6) and step (iii) of the algorithm we obtain

$$\frac{\langle E|e_1(I)\rangle}{\langle E|e_1(I-1)\rangle} = \frac{1 + (e_1(I-1) - e_1(I))(e_1(I-1) - E)/w^2(I-1)}{[1 + (e_1(I-1) - e_1(I))(e_1(I-1) - e_1(I))/w^2(I-1)]^{1/2}}. \tag{2.17}$$

For $E = E_T$ relation (2.16) guarantees that the right-hand side of equation (2.17) is greater than 1. This together with the fact that $\langle E_T|T\rangle$ is real and positive and that $|E_T\rangle$ and $|e_1(I)\rangle$ are normalised to unity implies that $(\langle E_T|e_1(I)\rangle)$ is real, positive, mononotically increasing and bounded by the values $\langle E_T|T\rangle$ and 1. Consequently $(\langle E_T|e_1(I)\rangle)$ converges to some y with $\langle E_T|T\rangle < y < 1$.

2.2.2. Proof that if $(|e_1(I)\rangle)$ *is* τ-*Cauchy then its limit is contained in* $\mathcal{F}$, *normalised to unity, and an eigenvector of* $\hat{H}$. Let $|\tilde{T}\rangle$ be the limit vector of $(|e_1(I)\rangle)$. The first two statements follow from the fact that $\mathcal{F}$ is complete with respect to the τ-topology and that all vectors $|e_1(I)\rangle$ are normalised to unity. Since $\hat{H}$ is τ-continuous the convergence of $(|e_1(I)\rangle)$ implies the convergence of $(\hat{H}^k|e_1(I)\rangle)$ for each $k = 1, 2, 3 \ldots$. Since expectation value and variance are continuous functionals, $(v_{1/2}(I))$, $(w(I))$ and $(e_1(I))$ are also convergent with limits $\tilde{v}_{1/2}$, $\tilde{w}$, $\tilde{e}_1$ which are related by (see equation (2.7))

$$\tilde{e}_1 = \tfrac{1}{2}(\tilde{v}_2 + \tilde{v}_1) - (\tilde{w}^2 + \tfrac{1}{4}(\tilde{v}_2 - \tilde{v}_1)^2)^{1/2}. \tag{2.18}$$

From the algorithm we have $v_1(I) = e_1(I-1)$ and therefore $\tilde{v}_1 = \tilde{e}_1$. This implies that $\tilde{w} = 0$ which means that $|\tilde{T}\rangle$ is an eigenvector of $\hat{H}$.

2.2.3. Proof that zero is an accumulation point of $(w^2(I))$. Suppose zero is not an accumulation point. From step 1 of the proof, we obtain

$$\frac{e_1(I-1) - e_1(I)}{w^2(I-1)} \xrightarrow[I\to\infty]{} 0 \tag{2.19}$$

and inserting this into equation (2.17)

$$\frac{E^k\langle E|e_1(I)\rangle}{E^k\langle E|e_1(I-1)\rangle} \xrightarrow[I\to\infty]{} 1. \tag{2.20}$$

From relation (2.20) and from the fact that for arbitrary large but fixed value of k the sequence $(E^k\langle E|e_1(I)\rangle)$ is real and bounded we conclude that $(\langle E|\hat{H}^k|e_1(I)\rangle)$ converges for all $|E\rangle$. This implies that $(|e_i(I)\rangle)$ is τ-Cauchy and, according to step 2 of the proof, its limit is an eigenvector of $\hat{H}$. Hence $(w^2(I))$ converges to zero, since the variance is a continuous functional. But this contradicts the assumption that zero is not an accumulation point of $(w^2(I))$. Hence zero must be an accumulation point.

2.2.4. Proof that $x = E_T$, $y = 1$, $|E_T\rangle = \lim_{I\to\infty}|e_1(I)\rangle$ *and* $0 = \lim_{I\to\infty}w(I)$. Step 3 of the proof guarantees the existence of a partial sequence $(w^2(I_j))$ which converges to zero.

Since $w^2(I_j)$ is the variance of $\hat{H}$ with respect to $|e_1(I_j - 1)\rangle$,

$$0 = \lim_{j \to \infty} w^2(I_j)$$

$$= \lim_{j \to \infty} \sum_E \langle E|e_1(I_j - 1)\rangle^2 (E - e_1(I_j - 1))^2 \tag{2.21}$$

and

$$1 = \sum_E \langle E|e_1(I_j - 1)\rangle^2 \tag{2.22}$$

since $|e_1(I_j - 1)\rangle$ is normalised. According to step 1 of the proof we have

$$x = \lim_{j \to \infty} e_1(I_j - 1), \qquad y = \lim_{j \to \infty} \langle E_T|e_1(I_j - 1). \tag{2.23}$$

From these equations we infer that $x = E_T$ and $y = 1$, since all other values of x and y would contradict equation (2.21) or equation (2.22). The value $y = 1$ implies that

$$\| |e_1(I)\rangle - |E_T\rangle\|^2 = 2(1 - \langle E_T|e_1(I)\rangle^2) \xrightarrow[I \to \infty]{} 2(1 - y^2) = 0, \tag{2.24}$$

hence $|E_T\rangle = \lim_{I \to \infty} |e_1(I)\rangle$ and $0 = \lim_{I \to \infty} w(I)$.

2.3. Error estimates and the numerical problem of pseudoconvergence

The convergence properties of the algorithm imply that E_T can be determined with an arbitrary degree of accuracy. In practice, however, one can perform only a finite number of iterations. The eigenvalue E_T is then approximated by the expectation value $e_1(I_{max})$. Besides this upper bound for E_T a lower bound may also be obtained. According to Kato (1949) the interval

$$[\langle \hat{H}\rangle_\phi - (\langle \hat{H}^2\rangle_\phi - \langle \hat{H}\rangle_\phi^2)^{1/2}, \langle \hat{H}\rangle_\phi + (\langle \hat{H}^2\rangle_\phi - \langle \hat{H}\rangle_\phi^2)^{1/2}]$$

includes at least one eigenvalue of $\hat{H}$ for any $|\phi\rangle \in \mathcal{D}$. In the present algorithm this yields the relation

$$v_1(I) - w(I) \le E \le v_1(I) + w(I) \tag{2.25}$$

where E is one of the eigenvalues that corresponds to the eigenvectors $|E\rangle$ contained in the expansion (2.2). In the region where the sequences $(e_1(I))$ and $(w(I))$ have already reached their limits E_T and zero within some small interval the inequality (2.25) demonstrates that $v_1(I) - w(I)$ is a lower bound for E_T. If after I_{max} iterations the sequence $(e_1(I))$ has almost converged the eigenvalue E_T is then contained in the small interval $(v_1(I_{max}) - w(I_{max}), e_1(I_{max}))$.

In the 2×2 algorithm as in most iterative algorithms the numerical problem of pseudoconvergence may occur. In this case the expectation value $e_1(I)$ approaches an eigenvalue $E_{pseudo} > E_T$ and remains constant for a number of iterations. Furthermore the variance of the vectors $|e_1(I)\rangle$ and their overlap with the eigenvector $|E_{pseudo}\rangle$ exhibit simultaneously a local minimum and maximum respectively. At this iteration step the vector $|e_1(I)\rangle$ represents an approximation to the eigenvector $|E_{pseudo}\rangle$. In the case of pseudoconvergence the eigenvalue E_{pseudo} itself can be specified within a small interval which is given by relation (2.25). As can be seen from previous calculations with the 2×2 algorithm (Berger *et al* 1977) pseudoconvergence occurs whenever the trial vector

$|T\rangle$ has the property that one or more of its components in the eigenvectors $|E\rangle$ are large compared to the rest. The fact that the variance of the vectors $|e_1(I)\rangle$ does not decrease monotonically with increasing number of iterations merely provides a means to identify pseudoconvergence in practical calculations. Instead of trying to obtain the final convergence in the conventional manner, that is by performing more iterations or to begin with another trial vector, the 2×2 algorithm may be modified in a manner suggested in one of our previous publications (Miller and Berger 1979). In this case pseudoconvergence is more easily identified and as soon as it occurs it may be eliminated.

3. Application to a well-known problem

In order to demonstrate the numerical behaviour of the 2×2 algorithm when it is applied directly to the full Hamiltonian of a quantum mechanical system, we have considered a well-known one-particle system, the harmonic oscillator in one dimension. In coordinate representation the eigenvalue problem of the Hamiltonian reads

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+x^2\right)\langle x|E\rangle = E\langle x|E\rangle \tag{3.1}$$

and has the well-known solution

$$E_n = \left(\frac{\hbar^2}{2m}\right)^{1/2}(2n+1), \qquad n = 0, 1, 2, 3, \ldots \tag{3.2}$$

$$\langle x|E_n\rangle = \left(\frac{1}{\pi}\left(\frac{\hbar^2}{2m}\right)^{-1/2}\right)^{1/4}(2^n n!)^{-1/2}H_n(\xi)\exp\left[-\left(\frac{\hbar^2}{2m}\right)^{-1/2}\frac{x^2}{2}\right] \tag{3.3}$$

where $\xi = (\hbar^2/2m)^{-1/4}x$ and $H_n(\xi)$ are the Hermite polynomials.

For this Hamiltonian the space $\mathscr{F}$ consists of the states which are represented by the infinitely differentiable functions $\langle x|T\rangle$ which together with their derivatives tend to zero for $|x| \to \infty$ more rapidly than any power of $1/|x|$, and in this space the Hamiltonian is τ-continuous (Böhm 1978). Thus we choose the trial state to be a wave packet of the form

$$\langle x|T\rangle = \alpha \exp(-\beta\gamma x^2/2) =: a(x). \tag{3.4}$$

Here α is a normalisation constant, $\gamma = (\hbar^2/2m)^{-1/2}$ and the real parameter β determines the width of the wave packet. For $\beta = 1$ the trial state is just the exact groundstate of the Hamiltonian and for $\beta \neq 1$ this parameter can be interpreted as a measure of the difference between the trial state and the exact groundstate. In the case $\beta \neq 1$ one can easily show that $\langle E_0|T\rangle$ does not vanish. Therefore, starting with this trial state, application of the 2×2 algorithm should yield the groundstate of the system and its groundstate energy. The choice of our trial state is most appropriate since it is closely related to the asymptotic form of the exact eigenstates, especially to the exact groundstate. Furthermore it has the property that for $\langle x|\hat{H}^I|T\rangle$ and $\langle x|e_1(I)\rangle$ recursion relations in terms of functions $a(x), x^2 a(x), \ldots, x^{2I}a(x)$ may be given. The existence of such recursion relations simplifies the numerical calculation considerably.

The convergence rate of the sequences $(e_1(I))$, $(w(I))$ and $(\langle E_T|e_1(I)\rangle)$ for different values of β is given in figure 1. Here it can be seen that the convergence rate improves
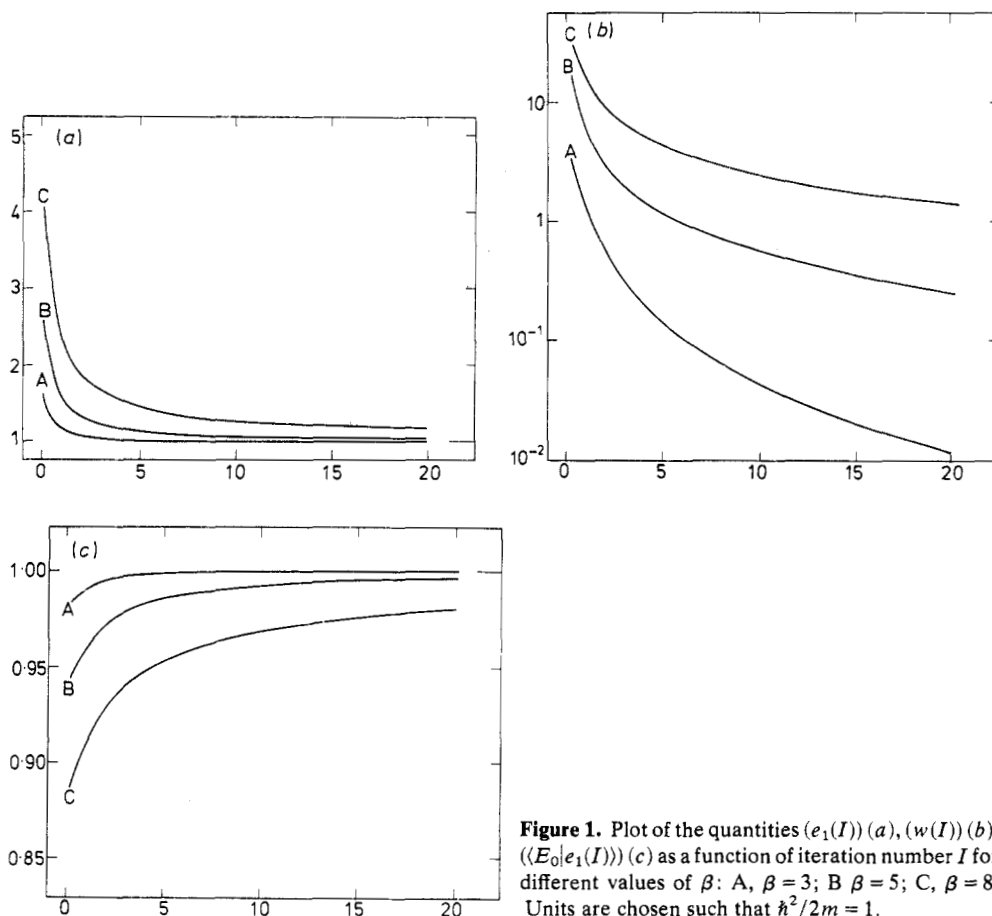
Figure 1. Plot of the quantities $(e_1(I))$ (a), $(w(I))$ (b), $(\langle E_0|e_1(I)\rangle)$ (c) as a function of iteration number I for different values of β: A, $\beta = 3$; B $\beta = 5$; C, $\beta = 8$. Units are chosen such that $\hbar^2/2m = 1$.

as β approaches 1. This, of course, corresponds to the fact that the closer the parameter β is to 1, the larger the overlap of the trial state with the exact groundstate.

If we choose a trial state of the form

$$\langle x|T\rangle = \alpha(1 + 1000x + x^2 + \ldots + x^9 + 1000x^{10}) \exp(-\gamma x^2/2) \qquad (3.5)$$

where the parameters α and γ have the same meaning as in equation (3.4), the trial state contains a non-vanishing component of the groundstate $|E_0\rangle$ and also a large component of the first excited state $|E_1\rangle$ and pseudoconvergence may be expected to occur. Indeed, as can be seen in figure 2, the expectation values remain constant in the interval $3 \leqslant I \leqslant 8$ and the local extrema for the variance and the overlap occur at $I = 5$ and $I = 6$. From relation (2.25) the eigenvalue E_{pseudo} lies in the interval $[2\cdot63, 3\cdot36]$. This, of course, corresponds to $E_1 = 3$, the energy of the first excited state.

4. Summary and discussion

The present investigation demonstrates that the 2×2 algorithm can be reformulated and its convergence properties can be proved even in a Hilbert space for Hermitian
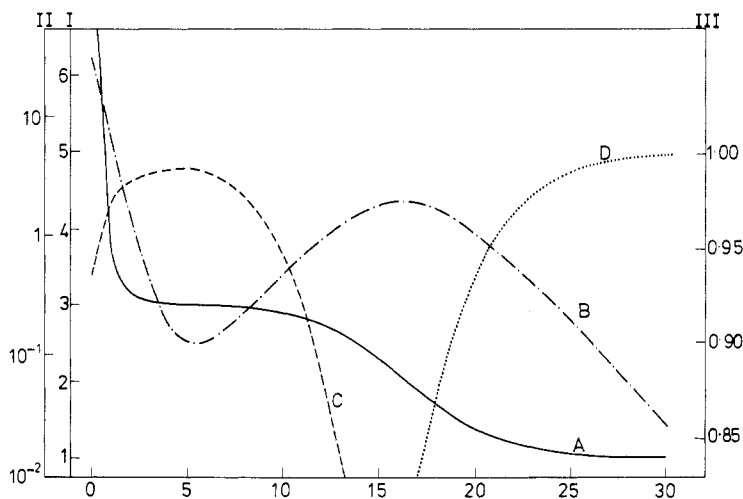
Figure 2. Plot of the quantities $(e_1(I))$ (curve A, scale *I*), $(w(I))$ curve B, scale *II*) $(\langle E_1|e_1(I)\rangle)$ (curve C, scale *III*), $(\langle E_0|e_1(I)\rangle)$ (curve D, scale *III*) in the case where pseudoconvergence occurs.

operators which are bounded only from below, provided the trial vector and the operator satisfy additional restrictions.

The advantage for quantum mechanical applications is that the actual groundstate and corresponding groundstate energy of a given Hamiltonian can be determined, provided that the trial state has a non-vanishing overlap with the groundstate. Furthermore the magnitude of this overlap determines to a large extent the convergence rate. This may at most be retarded by the occurrence of pseudoconvergence.

In practice the application of the 2×2 algorithm for a given Hamiltonian requires that there is an appropriate trial state available, that is a state belonging to the space $\mathcal{F}$. This space, however, is generally not easy to specify unless, of course, the eigenvalue problem of the Hamiltonian has already been solved. Iterating with the full (unprojected) Hamiltonian in either its coordinate or momentum representation restricts at present the applicability of the algorithm to quantum mechanical systems which can be described by a small number of coordinates.

References

Berger W A 1979 *PhD Dissertation* University of Frankfurt
Berger W A, Miller H G, Kreuzer K G and Dreizler R M 1977 *J. Phys. A: Math. Gen.* **10** 1089
Böhm A 1978 *The Rigged Hilbert Space and Quantum Mechanics* (Berlin: Springer) p 41
Kato T 1949 *J. Phys. Soc. Jap.* **4** 434
Miller H G and Berger W A 1979 *J. Phys. A: Math. Gen.* **12** 1693
Stewart G W 1974 *Proc. IFIP Congress, Stockholm* 1974 p 666
Vorobyev Y V 1965 *Methods of Moments in Applied Mathematics* (New York: Gordon and Breach) p 153