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The Elimination of Lanczos Ghosting Effects by MINRES Filter Diagonalization

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A recently developed filter diagonalization technique (*Ber. Bunsenges. Phys. Chem*. **101**, 400, 1997), based on the optimal approximation of the Green operator in a finite Lanczos subspace, is investigated in relation to its ability to avoid the phenomenom of ghosting which complicates the interpretation of the regular Lanczos spectrum as the order of the subspace is increased. The origin of this potentially useful property of the algorithm is explained with reference to one- and two-dimensional applications.

Key Words: Lanczos; iterative diagonalization; filter diagonalization.

I. INTRODUCTION

The Lanczos algorithm is perhaps the most commonly used technique for iteratively determining the eigenvalues of large sparse real-symmetric or complex-Hermitian matrices [1–3]. In the context of chemical physics, it has found wide application in the determination of vibrational eigenstates for molecules up to high excitation energies [4–11]. However, as is well known, the algorithm is not a "black box," but rather requires some experience and care to correctly identify the true eigenvalues of the Hamiltonian. The problem is that once some eigenvalues of the matrix have converged, the subsequent vectors in the Lanczos subspace tend to take on unwanted components in the direction of the converged eigenvectors, so that the subspace loses strict orthogonality. Ultimately, the algorithm starts to produce "ghost" eigenvalues, i.e., duplicates of true eigenvalues which are stable with respect to the size of the subspace, and also spurious eigenvalues which are unstable with respect to the size of the subspace (for convenience, we refer to this generally as the "ghosting" problem). The origin of this difficulty is the fact that the Lanczos algorithm uses a three-term recursion to build up the orthogonal subspace, which does not guarantee strict orthogonality due to numerical error. There are two ways out of this. The first approach is to enforce strict orthogonality by explicitly orthogonalizing each new vector against all of the previous

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vectors. In this way the ghosting problem is eliminated, but at a very high price since it will be necessary either (a) to store all of the Lanczos vectors in core memory, placing a severe restriction on the size of the subspace which can be handled, or (b) to write them to disk and then read them sequentially back into memory for reorthogonalization at each iteration, in which case the speed of the calculation is severely limited by the read/write operations. A second approach takes advantage of the error analysis of Paige (see, e.g., Ref. [3]), which demonstrates that the eigenvalues which are duplicated in the presence of ghosting are nevertheless accurate. In this latter approach, one simply lives with the ghosting [2] and devises a means of sorting out the true eigenvalues from the spurious ones. Hence, some care and time is required on the part of the user to sort out precisely which are the true eigenvalues.

A characteristic property of the Lanczos algorithm is that it converges eigenvalues in the sparse regions of the spectrum quickly and only slowly resolves the eigenvalues in the dense regions as the order of the subspace is increased. This has motivated alternative approaches to computing vibrational eigenvalues at higher energies, where the spectrum is dense. One such approach is to use a spectral transform in order to make this property of the Lanczos algorithm work in the user's favor. The idea is to use an operator which is a function of H and has eigenvalues of greatest magnitude and separation at the energy of interest, for example, a sharply peaked Gaussian [7, 9] or a Green operator [10]. An alternative approach is that of filter diagonalization (FD), first introduced by Neuhauser [12, 13]. In the FD approach, one calculates a set of filtered states with mean energies spaced evenly through a nominated energy window. These filtered states are then used as a basis in which to represent and diagonalize the Hamiltonian. The method has been used successfully by a number of different groups [13–17].

In our recent work, we have introduced a new FD approach which is based on the Lanczos algorithm [17]. The idea is to generate filtered states within a nominated energy window by approximating the action of the Green operator at different energies spaced through the window. The filtered states are generated within a Lanczos subspace of order k by applying the minimum residual (MINRES) algorithm of Paige and Saunders [18]. The subsequent representation of the Hamiltonian and the overlap matrices in terms of this filtered (non-orthogonal) basis are trivially generated using the tridiagonal matrix $\mathbf{T}_k$, which is the representation of H in the Lanczos basis, and the residual β_{k+1}. Solution of the generalized eigenvalue problem then yields approximations to the true eigenvalues of the Hamiltonian. The main storage cost of the method is just that of the primitive Lanczos algorithm—two real vectors—and the Lanczos subspace need be generated only once in order for *all* eigenvalues to be obtained. In the earlier work [17], it was shown that the MINRES filter diagonalization (MFD) method has two very attractive properties: (a) at high energies, where the Lanczos eigenvalues are not converged, it gives significantly improved estimates of the true eigenvalues and eigenvectors, and (b) at lower energies, where the Lanczos algorithm rapidly converges the eigenstates and starts to produce ghost and duplicate eigenvalues, the MFD algorithm produces only true eigenvalues and eigenvectors. It is the elimination of the ghosting problem which we seek to further investigate in this paper. In Section II, we consider a one-dimensional Morse oscillator problem to illustrate the MFD method and demonstrate its capacity for removing ghost and duplicate eigenvalues. In Section III, we show that the reason for this behavior is a very fortunate coincidence of the properties of the MINRES algorithm in combination with those of singular value decomposition. Finally, in Section IV, we present results of a more challenging application to a special test matrix first introduced by Wyatt [19].

II. THE MFD ALGORITHM

We begin with a brief summary of the MFD algorithm (for further details see Ref. [17]). As described above, the basic idea of filter diagonalization is to compute a set of filtered states in a given energy window and then use these states as a basis for diagonalizing the Hamiltonian to obtain the true eigenvalues in this region of the spectrum. In principle, one might expect to have to carry out a separate filtering calculation for each different energy; however, Wall and Neuhauser [13] showed that this is not necessary if one uses time-to-energy Fourier filtering. In the MFD approach, we use an approximation to the action of the Green operator $G(E) = (H - E)^{-1}$ in order to create filtered states from an initial random vector $\mathbf{r}$. This is achieved by generating a Lanczos subspace from an initial seed vector $\mathbf{v}_1 = \mathbf{r}/|\mathbf{r}|$ and solving the linear system of equations

$$(H - E_j)\,\mathbf{z}\,(E_j) = \mathbf{v}_1 \tag{1}$$

optimally within the given Lanczos subspace of order k. This is achieved by using the MINRES equations of Paige and Saunders [18] to determine the linear combination of Lanczos basis vectors $\mathbf{v}_1, \ldots, \mathbf{v}_k$ which minimizes the residual norm for the linear system.

There are two key observations which make the MFD calculation very convenient and efficient. The first is that the Lanczos subspace obtained from a given seed vector $\mathbf{v}_1$ is independent of the shift energy E_j. When large basis sets are involved, the compute time in a Lanczos calculation is dominated by the matrix-vector multiples required to generate the Lanczos basis vectors. Hence, this fact is very convenient since one need only generate the Lanczos subspace *once* and then solve the MINRES equations for a series of shift energies to obtain the expansion coefficients of the filtered states in terms of the Lanczos basis vectors. Hence, we have the solution

$$\mathbf{z}(E_j) = \sum_{i=1}^{k} y_i^j \mathbf{v}_i = \mathbf{V}_k \mathbf{y}^j, \qquad j = 1, m, \tag{2}$$

where $\mathbf{V}_k$ is a matrix whose columns are the Lanczos basis vectors, $\mathbf{y}^j$ is the representation of $\mathbf{z}(E_j)$ in the Lanczos basis, and m is the number of filtered states to be computed in a given energy window. The second observation is that although it is possible to explicitly construct the filtered states $\{\mathbf{z}(E_j),\ j = 1, m\}$ in the primary basis at a storage cost of $3m + 2$ vectors, this is not necessary if just eigenvalues are sought. We need only the representations $\{\mathbf{y}^j,\ j = 1, m\}$ in the Lanczos subspace. This is because the Hamiltonian and overlap matrices for the $\mathbf{y}^j$ vectors (and indeed any set of vectors in the Lanczos subspace) are simply evaluated by invoking orthonormality of the Lanczos basis vectors and using the tridiagonal representation $\mathbf{T}_k$ of the Hamiltonian in the Lanczos subspace. The solution of the eigenvalue problem proceeds by standard methods. Firstly the non-orthogonal basis $\{\mathbf{y}^j,\ j = 1, m\}$ is contracted to form an orthonormal set $\{\mathbf{u}_i,\ i = 1, n\}$ using singular value decomposition [3, 20]. Then the representation of the Hamiltonian in this orthonormal basis is diagonalized to yield approximations $\mathbf{x}_i$ to the true eigenvectors, still represented in the Lanczos subspace, and their corresponding eigenvalues ε_i. If the Lanczos basis is sufficiently large, the eigenvalues thus obtained will be excellent approximations to the true eigenvalues in the window of interest. One also obtains some eigenvalues outside the window which can be discarded since they will be less well converged [12, 13]. In

principle, the eigenvectors can be constructed in the primary basis by regenerating the Lanczos subspace and accumulating the linear combinations prescribed by the vectors $\mathbf{x}_i$ at a storage cost of $m + 2$ vectors.

In order to illustrate the MINRES filter diagonalization method described above, we begin with a simple problem involving a one-dimensional Morse potential. The Hamiltonian is thus

$$H = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial R^2} + D_e\left[1 - e^{-\alpha(R-R_e)}\right]^2, \tag{3}$$

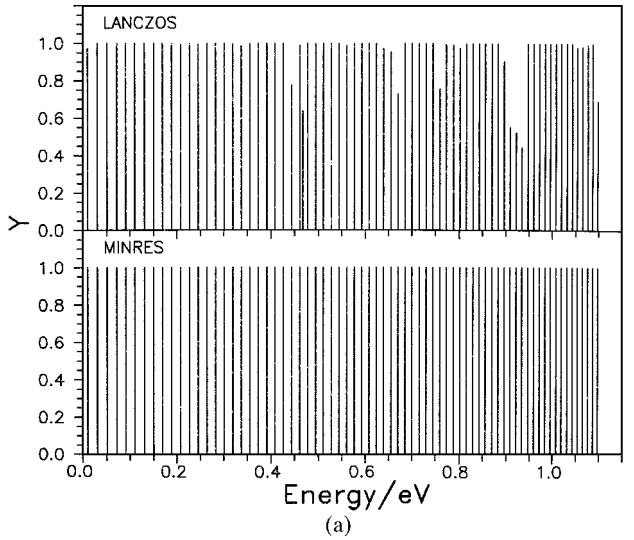
the eigenvalues of which are given analytically given by

$$E_n = \left(n + \frac{1}{2}\right)\hbar\sqrt{\frac{2D_e\alpha^2}{\mu}} - \left(n + \frac{1}{2}\right)^2\frac{\hbar^2\alpha^2}{2\mu}. \tag{4}$$

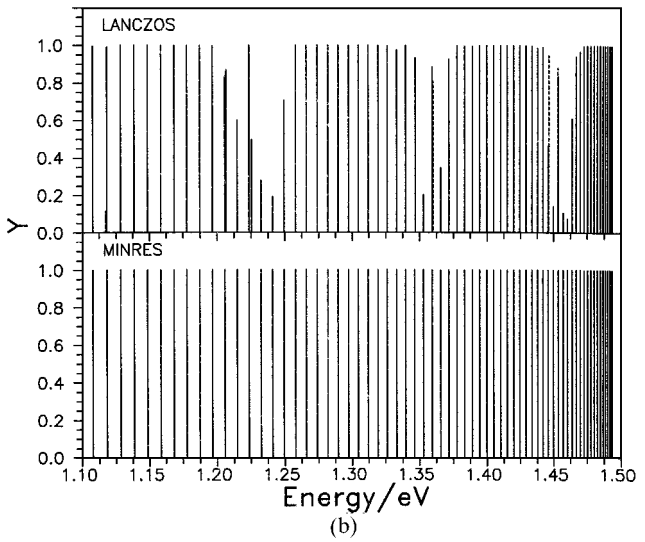
The parameters in Eqs. (3) and (4) were chosen to be

$$\begin{aligned} \mu &= 45.0 \text{ a.m.u.} \\ D_e &= 1.50 \text{ eV} \\ \alpha &= 0.65a_0^{-1} \\ R_e &= 2.00a_0, \end{aligned} \tag{5}$$

for which one obtains 146 bound states. We utilized a primary basis consisting of 812 evenly spaced sinc-function discrete variable representation (DVR) points [21] in the region $0.50 < R < 25.0$ Bohr. A random vector was normalized and used as the initial Lanczos vector, and a subspace of 2000 vectors was built up. Diagonalizing $\mathbf{T}_{2000}$ (the tridiagonal representation of H) yields the eigenvalues corresponding to all 146 bound states, plus many duplicates thereof. Additionally, in the energy region less than D_e, there are some 10 spurious eigenvalues which do not match any of the true eigenvalues. The ghost eigenvalues appeared at 0.072272, 0.869976, 0.897207, 1.117298, 1.206483, 1.225578, 1.333112, 1.360057, 1.446329, and 1.453180 eV. These results are summarized in Figs. 1 and 2. In Fig. 1, the results are expressed in terms of stick spectra, where the heights of the sticks are scaled to reflect the dispersion associated with the corresponding eigenvector (in the case where duplicate eigenvalues occured, the *smallest* dispersion is plotted): a poorly converged eigenvector has a large dispersion and the height of the stick is reduced accordingly (see the figure caption). The upper frames of Figs. 1a and 1b indicate the eigenvalues obtained from the Lanczos diagonalization (solid lines represent true eigenvalues, while dotted lines represent spurious eigenvalues). For comparison we also performed two MINRES filter diagonalizations based on the same Lanczos subspace, the results of which are summarized in the lower frames of Figs. 1a and 1b. The MFD calculations in the first window (Fig. 1a) covered the energy region up to 1.1 eV and utilized $N_{\text{MFD}} = 400$ evenly spaced energy shifts to yield 62 true eigenvalues. The dispersions of the associated MFD eigenvectors were generally much smaller than those of the Lanczos eigenvectors, which had been degraded due to ghosting effects, and no ghost or duplicate eigenvalues arose from the MFD calculation. For the second window (Fig. 1b), covering energies up to threshold, $N_{\text{MFD}} = 500$ energy shifts were used in the region lying from 1.0 to 1.494 eV, yeilding 75 true eigenvalues. It is clear that for the simple Lanczos algorithm, the dispersions of eigenvectors associated with true eigenvales lying near the ghost states tend to be large. Figure 2 indicates the extent of duplication of the Lanczos eigenvalues for this subspace of 2000 basis vectors by plotting multiplicities as a function of the eigenenergy.



(a)



(b)

FIG. 1. Comparison of purity of eigenvalues (a) at low energies and (b) at high energies from the simple Lanczos and MINRES filter diagonalization (MFD) for a Lanczos subspace of 2000 vectors for one-dimensional Morse potential. Here, $Y = e^{-4.0*\mathrm{Dis}}$ with the dispersion (Dis/eV). The dashed lines refer to the spurious values.

We note that the estimates of dispersions are carried out within the Lanczos subspace using standard formulae. In principle, the dispersion is more precisely determined directly from the eigenvector in the primary representation, but this will obviously be inconvenient for problems with very large basis sets. However, estimates of such quantities based on the Lanczos subspace representation of H are generally quite reliable [22]. Deviations of the MFD eigenvalues from the analytical eigenvalues of Eq. (4) were less than 1.0×10^{-7} eV.

III. CONVERGENCE OF THE FILTERED STATES AND THE ELIMINATION OF GHOSTING

In this section, we examine the reason why ghost and spurious eigenvalues which appear in the Lanczos spectrum are eliminated by the MFD algorithm. The first clue as to how

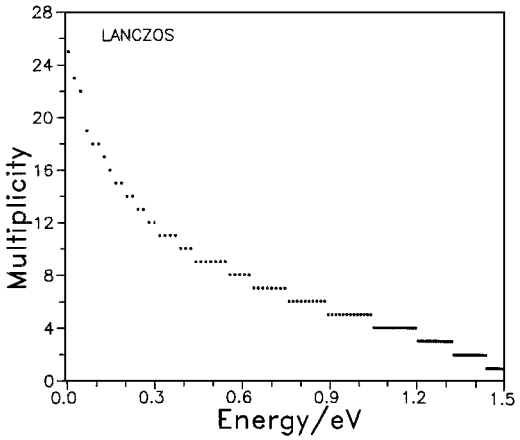


FIG. 2. Plot of the multiplicity of duplicated eigenvalues in the Lanczos spectrum for the Morse oscillator problem with a subspace of 2000 vectors.

this works is obtained by examining the projections of the filtered states onto the Lanczos basis vectors. Figure 3 plots the squares of the expansion coefficients in the Lanczos basis of four (renormalized) filtered states with mean energies at ca. 0.3, 0.6, 0.9, and 1.2 eV. It is apparent that solution of the MINRES equations yields filtered states with a bias toward the earlier part of the Lanczos subspace. For clarity of presentation, we have not shown the squares of the expansion coefficients beyond 450 Lanczos basis vectors: the remaining projections out to the full order of the subspace of 2000 vectors used in the Morse oscillator calculation are uniformly zero for all four filtered states. The reason for this is associated with the fact that the LQ decomposition of $\mathbf{T}_k$ proceeds iteratively from left to right across the columns of the matrix, with the solution to the linear system of equations defining the

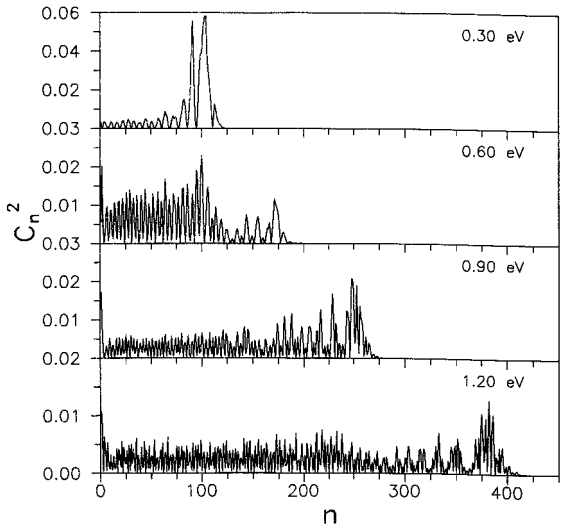


FIG. 3. Plot of the squares of the expansion coefficients of filtered states with respect to the Lanczos basis vectors for the Morse oscillator problem. The four filtered states shown were generated by solution of the MINRES equations with shift energies of 0.30, 0.60, 0.90, and 1.20 eV.

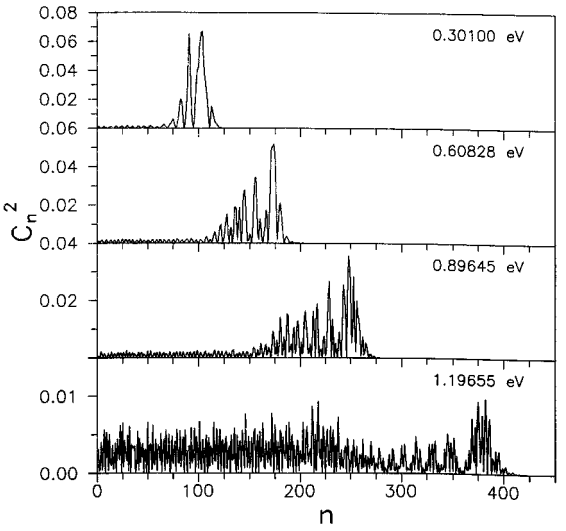


FIG. 4. Plot of the squares of the expansion coefficients of MFD eigenstates with respect to the Lanczos basis vectors. The four eigenstates occur at 0.30100, 0.60828, 0.89645, and 1.19655 eV.

"best" approximation to the action of the Green operator being updated correspondingly. As the residual norm for the linear system decreases, so the weighting of new Lanczos subspace vectors in the solution is decreased. Finally, when the residual norm for the linear system has dropped below machine ε, any further Lanczos basis vectors introduced are effectively ignored.

The practical importance of the above observation is that the solution of the linear system of equations defining the action of the Green operator $G(E)$ converges with approximately the same number of Lanczos iterations as do the eigenvalues in this region of the spectrum. As the Lanczos subspace is extended further, loss of orthogonality causes unwanted components in the direction of previously converged eigenvectors to be reintroduced into the subspace. The MINRES algorithm ignores these, but the regular Lanczos algorithm is not as discerning: straightforward diagonalization of $\mathbf{T}_k$ yields duplicate or ghost eigenvalues and eigenvectors containing amplitude throughout the Lanczos subspace. This bias of the MINRES algorithm toward the early part of the Lanczos subspace (without loss of accuracy) propagates through the singular value decomposition and diagonalization stages of the MFD algorithm, so that the final eigenvectors likewise contain amplitude only in that part of the Lanczos subspace that is required for an accurate solution. This is indicated in Fig. 4, where we plot the squares of the expansion coefficients of four MFD eigenstates in the Lanczos subspace, again corresponding to energies of approximately 0.3, 0.6, 0.9, and 1.2 eV. Hence, the MINRES algorithm provides a very convenient way of incorporating only that part of the Lanczos subspace required for accurate convergence of eigenstates in a given part of the spectrum.

Of course, the same final results can be achieved manually (and more laboriously) by progressively examining the Lanczos spectrum as a function of the number of iterations and picking out the true eigenvalues and eigenvectors as they converge, before the eigenvectors become corrupted due to ghosting. Our point, however, is to illustrate that the MFD algorithm appears to provide a very convenient means of reducing the amount of labor involved, and also the amount of user expertise required, to achieve results of at least the same accuracy.

IV. APPLICATION TO DENSE SPECTRA

As a further illustration of the utility of the MFD algorithm, we have applied it to a flexible model Hamiltonian first suggested by Wyatt [19] in order to test the layered iteration method for the calculation of interior eigenvalues of large matrices. It has also been utilized by Kouri and co-workers [14] in testing a filter diagonalization algorithm based on Chebychev expansion of the Green operator. The matrix exhibits N_b bands of eigenvalues with N_s states within each band. The zero-order diagonal energies are chosen to lie in the interval [0, 1], so that the average spacing between successive states is $1/(N_b N_s)$. Four parameters $(\Delta, \delta, C, n_{od})$ may be adjusted to control the effective coupling between states. The coupling within each band is specified to be relatively strong while the interband coupling is weaker. The Hamiltonian is defined by the diagonal elements $(i = i', j = j')$,

$$H_{ij,ij} = (i-1)\Delta + (j-1)\delta, \qquad \text{where } \delta \ll \Delta, \tag{6}$$

the intraband coupling terms $(i = i', j \neq j')$,

$$H_{ij,ij'} = C \exp(-|j - j'|), \tag{7}$$

and the interband coupling terms $(i \neq i', j \neq j')$,

$$H_{ij,i'j'} = \frac{C \exp(-|j - j'|)}{n_{od}[|i - i'| + 1]}, \tag{8}$$

where i denotes the band index, $i = 1, 2, \ldots, N_b$, and j denotes the substate index, $j = 1, 2, \ldots, N_s$. The parameters of Eqs. (6)–(8) are $N_b = 10$, $N_s = 200$, $\Delta = 0.10$, $\delta = 0.0001$, $C = 0.10$, and $n_{od} = 5$, forming a 2000×2000 matrix. The exact spectrum can be obtained by directly diagonalizing the Hamiltonian.

For the flexible model Hamiltonian described, we carried out 30,000 Lanczos iterations starting from a uniform initial vector. MFD calculations for several energy windows covering the spectrum were performed. In the interest of brevity, we present results only for a window in the middle of the spectrum (Figs. 5–7). The lower frame in Fig. 5 shows the stick spectrum obtained from an MFD calculation utilizing $N_{\mathrm{MFD}} = 400$ evenly spaced shifts spanning the eigenvalue range 0.4252 to 0.5050. This calculation yielded 169 true eigenvalues which correspond to the 931st through the 1099th eigenstates of the matrix. As in Fig. 1, the height of the sticks is indicative of the dispersion of the corresponding eigenvectors (the shorter the stick, the larger the dispersion). In the upper frame of Fig. 5, we have plotted only the 16 spurious eigenvalues obtained in this part of the spectrum from the Lanczos calculation (i.e., excluding the many copies of true eigenvalues). Note that the Y scale is different for the lower and upper frames of Fig. 5. The dispersions of the MFD eigenstates are illustrated quantitatively in Fig. 6 on a log scale. In Fig. 7 the multiplicities of duplicate eigenvalues obtained from the diagonalization of $\mathbf{T}_{30,000}$ are plotted. The figure illustrates well-understood Lanczos convergence properties: many more duplicate eigenvalues are obtained in the sparse parts of the spectrum, since the Lanczos algorithm converges these eigenstates more quickly [3]. Again, we stress that duplicate and spurious eigenvalues are completely eliminated in the MFD calculations.

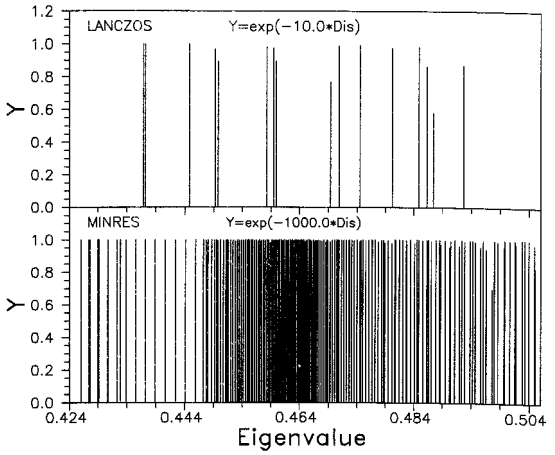


FIG. 5. Plot of eigenvalues at the middle region of the spectrum of the Wyatt test matrix calculated via the MFD technique (lower panel) and spurious states from the simple Lanczos method (upper panel). Shown are 169 states corresponding to the 931st through the 1099th eigenvalues of the full matrix. Both Lanczos and MFD calculations are based on a Lanczos subspace of order 30,000.

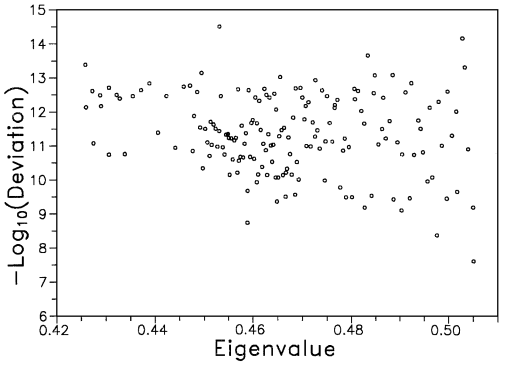


FIG. 6. Plot of the log deviations of eigenvalues calculated using the MFD technique relative to the eigenstates obtained by direct diagonalization of the Wyatt test matrix. The energy window is as in Fig. 5.

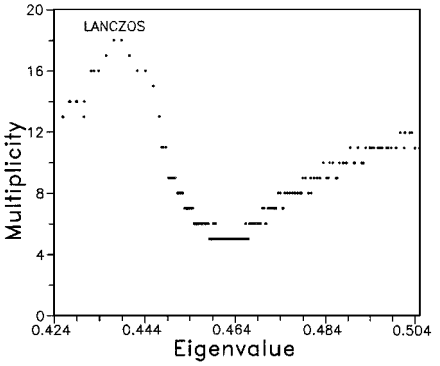


FIG. 7. Plot of the multiplicity of duplicated eigenvalues in the Lanczos spectrum for the Wyatt test matrix with a subspace of 30,000 vectors.

V. CONCLUSION

Clearly, the Lanczos subspaces which were generated in the two examples of this paper (order 2000 for the Morse oscillator and order 30,000 for the Wyatt test matrix) constitute overkill if one simply wishes to compute the eigenstates! With subspaces of this size, not only are all eigenvalues correctly obtained by the Lanczos algorithm, but many copies thereof as indicated in Figs. 2 and 7. We have illustrated in earlier work that a combination of MINRES spectral filtering [23] and filter diagonalization [17] does provide an extremely efficient method for extracting interior eigenvalues of a dense spectrum. Our focus in this paper, however, has been to explain the intriguing and potentially very useful fact that the MFD algorithm eliminates the spurious and duplicate eigenvalues which complicate the interpretation of a regular Lanczos spectrum. We have shown that this is principally due to the convergence properties of the MINRES equations which we use for constructing filtered states by approximating the action of the Green operator. Only that part of the Lanczos subspace which is required for convergence of the linear system of equations defining the action of the Green operator at the specified energy is incorporated into the solution, and the remaining Lanczos basis vectors are automatically ignored. This behavior stems from the iterative LQ factorization of the tridiagonal $\mathbf{T}_k$ in the Lanczos subspace which is used to solve the linear system [18].

For eigenvalue problems involving very large sparse Hermitian matrices, such as the calculation of high-lying rovibrational eigenstates of molecular Hamiltonians, the major computing cost in a Lanczos calculation is the matrix-vector multiples required to generate the subspace. Hence, the computational overhead associated with the MFD procedure is minimal. We believe that, due to its enhanced convergence properties and the elimination of the ghosting problem, the MFD technique has the potential to greatly facilitate such calculations in the future.

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