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Determination of Eigenstates via Lanczos-Based Forward Substitution and Filter-Diagonalization

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A filter-diagonalization scheme based on the Lanczos tridiagonalization algorithm is proposed for the determination of highly excited eigenstates in a prespecified energy range. Filtered states localized in the energy domain can be generated during the Lanczos iteration by forward substitution which formally corresponds to a Green function filter. Eigenstates in the energy range of interest are then obtained by diagonalizing a small Hamiltonian matrix in a subspace spanned by the filtered states. It is shown that the accuracy of this approach is affected neither by the loss of orthogonality among the Lanczos states nor by the instability in the forward substitution. Since the filtered states are assembled while the Lanczos states are generated, no storage of the Lanczos states is needed. The computational savings can be significant in calculating high energy eigenstates of large systems. The proposed scheme is shown numerically to have comparable accuracy with the basic Lanczos method.

I. INTRODUCTION

Since its introduction nearly a half century ago, the Lanczos algorithm [1] has been extensively used to solve eigneproblems in a wide range of applications, including in chemistry and physics. For a given $N \times N$ real symmetric (or Hermitian) matrix $\mathbf{H}$, Lanczos showed that it can be reduced to a $M \times M$ symmetric tridiagonal matrix ($\mathbf{T}$) via an iterative scheme. The iteratively generated orthonormal Lanczos states (*vida infra*) can be shown to span the Mth Krylov subspace $\{|\phi_1\rangle, \mathbf{H}|\phi_1\rangle, \mathbf{H}^2|\phi_1\rangle, ..., \mathbf{H}^{M-1}|\phi_1\rangle\}$ in exact arithmetic, where $|\phi_1\rangle$ is an arbitrary starting vector. So, the Lanczos iteration terminates with $M \leq N$ and the eigenproblem of $\mathbf{H}$ can thus be reduced to the less expensive diagonalization of $\mathbf{T}$, In fact, some eigenvalues start to converge even when $M \ll N$. A major advantage of the Lanczos approach is that no modifications of $\mathbf{H}$, such as direct diagonalization or factorization, are required in the iteration. The only major operation involved is a vector–matrix multiplication. Thus, it is particularly suited for solving eigenproblems of large and sparse matrices. Its early history has been surveyed by Golub and O'Leary [2] and several excellent books provide discussions of the original algorithm and its variants, as well as their numerical applications [3–6]. In chemical physics, its application ranges from the solution of eigen-problems [7–9] to the calculation of generalized transition amplitudes [10] and the construction of temporal propagators [11].

However, it is well known that the numerical behavior of the Lanczos algorithm in finite precision arithmetic is different from that in exact arithmetic. The global orthonormality of the Lanczos states deteriorates with the increasing number of iterations due to roundoff errors. In fact, the Lanczos states may even become linearly dependent with large M. Consequently, the Lanczos iteration does not terminate at N steps and spurious eigenvalues emerge even when $M < N$. The emergence of the spurious eigenvalues is actually related to the convergence of some eigenvalues [12, 13]. A solution to this problem is some form of forced global reorthogonalization, which can be computationally demanding. An alternative procedure proposed by Cullum and Willoughby (CW) identifies the spurious eigenvalues without the expensive reorthogonalization [4, 14]. This is done by diagonalizing a submatrix $\mathbf{T}'$ which is derived by deleting the first row and first column of the tridiagonal Lanczos matrix $\mathbf{T}$. The common eigenvalues of the two matrices are identified as spurious and discarded. The CW identification test is possible because of the so-called Lanczos phenomenon, which essentially states that in finite precision arithmetic all the eigenvalues of $\mathbf{H}$ will eventually appear in $\mathbf{T}$ for a large enough M [14]. The CW approach is efficient, accurate, and reliable. It has been successfully applied to calculate a few or all the eigenvalues of matrices with ranks above 10^3.

Because the Lanczos states are constructed in the Krylov subspace, the Lanczos algorithm tends to converge first to extremal and/or widely-spaced eigenvalues. Hence, this method is often used to extract eigenvalues near the edges of a spectrum. There is, however, nothing preventing it from being used to extract the entire spectrum, thanks to the Lanczos phenomenon. To improve the efficiency of the Lanczos algorithm in the interior of the spectrum where the separation of two adjacent eigenvalues may be small, many researchers used spectral transformation [15–18].

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In this approach, the Lanczos states are generated by a transformed matrix $\mathbf{H}' = f(\mathbf{H})$, which should be appropriately chosen to ''amplify'' a certain range of the spectrum. This generally requires two nested loops; the inner loop provides an accurate evaluation of the action of $\mathbf{H}'$ while the outer loop updates the Lanczos states. Compared with the basic Lanczos iteration, evaluating the action of $\mathbf{H}'$ at each Lanczos step typically requires many more computational resources. However, when storage is of primary concern, this method may be more advantageous because of the smaller number of Lanczos states. Roy and Carrington [19] compared the efficiency of the basic Lanczos method to that of a (Gaussian) spectral transform Lanczos approach and a guided Lanczos scheme in which the initial state is prefiltered in the spectral range of interest. Interestingly, their numerical results favor the basic Lanczos method without any spectral transform or prefiltering. There is apparently some trade-offs for spectral transform, which may depend on system and on implementation.

When only the eigenvalues of $\mathbf{H}$ are desired, the CW version of the Lanczos algorithm is apparently the method of choice. It requires minimal memory because the Lanczos states are not stored, except the ones generated in the last two steps. The diagonalization of a tridiagonal matrix is considered trivial. If one is interested in eigenstates, however, more computational resources are needed. In order to construct the approximate eigenstate (Ritz vector), the Lanczos states have to be regenerated after the convergence of eigenvalues. Alternatively, one may elect to store all the Lanczos states in the first iteration, which may require unmanageably large memory if $N \times M$ is large. For highly excited states in large systems, both strategies can be costly.

In this paper, we propose an efficient method based on the Lanczos method to calculate the eigenstates in a spectral range of interest. This method involves two steps: the construction of filtered states via the Lanczos iteration and the subsequent diagonalization in a subspace spanned by the filtered states. Thus, the strategy is in a spirit similar to the filter-diagonalization method proposed by Neuhauser [20–22] and others [23–27]. In earlier versions of filter-diagonalization, however, the filtered states are calculated via the evolution of the wave packet in the time domain or via the (Chebyshev) polynomial expansion, which is basically the evolution of the Chebyshev order domain [28, 29]. The filtered states can also be obtained via matrix factorization [15] and via iterative methods [17]. The distinguishing feature of the method proposed here is that we use the forward substitution in the Lanczos iteration to accumulate the filtered states. There are two advantages associated with this approach. First, the Lanczos states are generated only once and they need not be stored. Second, many filtered states in the energy range of interest can be calculated with the same set of Lanczos states. Thus, this method is considered global in energy. Although the forward substitution is known to be numerically unstable [30], we show that this deficiency is irrelevant if a final diagonalization of a small Hamiltonian matrix is introduced. In the next section, we present a short review of the filter-based methods, which serves as a prelude to the Lanczos-based filtering. The forward substitution method based on the Lanczos iteration is outlined in Section III. The numerical result for a one-dimensional Morse oscillator is presented in Section IV and the conclusion is given in Section V.

II. FILTER-BASED METHODS IN SOLVING EIGENPROBLEMS

If one is interested in finding the eigenvalues and eigenstates of a Hermitian operator, say $\mathbf{H}$, he is confronted with the equation

$$\mathbf{H}|E_n\rangle = E_n|E_n\rangle, \quad n = 1, 2, ..., N. \tag{1}$$

For simplicity, we assume that $\mathbf{H}$ is a Hermitian Hamiltonian which has a discrete spectrum, although the discussion is applicable to other operators. The Hamiltonian is defined in some physical space as an abstract operator which can be represented on a specific basis as a matrix. If a physical state can be represented as a state vector in the Hilbert space which has N variables, there exist, in general, N orthonormal eigenstates and the corresponding eigenvalues for the Hamiltonian. When N is large ($>10^4$), it becomes impractical to solve the whole eigenproblem because of constraints in computer speed and memory. Note that the conventional variational approach typically scales as $O(N^3)$ in arithmetic operations and $O(N^2)$ in memory. Thus, there is a need for theoretical methods designed to solve the eigenproblem in a narrow energy range in the spectrum, $[E_{\text{low}}, E_{\text{up}}]$, rather than the whole spectrum. This divide-and-conquer strategy has worked well in many problems because it typically requires many fewer computational resources [17, 19, 20].

Equation (1) can be formally considered as a special case of the inhomogenous time-independent Schrödinger equation,

$$(\mathbf{H} - E\mathbf{I})|\Psi\rangle = |\Phi\rangle, \tag{2}$$

where $\mathbf{I}$ is the unit operator and state $|\Phi\rangle$ can be chosen arbitrarily, provided it has nonzero overlaps with the eigenstates of interest. The formal solution to Eq. (2) is $|\Psi\rangle = (\mathbf{H} - E\mathbf{I})^{-1}|\Phi\rangle$, where the operator $(\mathbf{H} - E\mathbf{I})^{-1}$ is the Green, or resolvent operator. When the energy parameter (E) of the Green operator is close to an eigenvalue, the corresponding eigenstate is effectively amplified relative to others and picked up from the trial vector $|\Phi\rangle$.

The above discussion underscores the importance of a

generalized filter operator, $F(\mathbf{H}|E)$, whose corresponding scalar function $F(H|E)$ is usually chosen to be negligibly small except for a small region near E. When the filter operator is applied to an arbitrary trial wave function $|\Phi\rangle$, a filtered state is obtained, $|\varphi(E)\rangle = F(\mathbf{H}|E)|\Phi\rangle$. It can be shown that the filtered state is mainly composed of the eigenstates near E. In other words, the eigenstates far away are efficiently suppressed [27]. The Green operator $(\mathbf{H} - E\mathbf{I})^{-1}$ [31–34] and the Dirac delta operator $\delta(\mathbf{H} - E\mathbf{I})$ [35, 36] are two widely used filter operators. We have shown recently that a finite-width filter, such as the Gaussian filter $e^{-(\mathbf{H}-E\mathbf{I})^2/2\sigma^2}$, may have some advantages [27, 29]. Other examples include the relaxation operator $(e^{-\mathbf{H}\tau})$, which has been used to extract the lowest eigenstates [37–39].

One can expand the operator function $F(\mathbf{H}|E)$ by using a complete set of basis functions (the normalization of $\mathbf{H}$ is assumed),

$$F(\mathbf{H}|E) \approx \sum_k a_k(E) T_k(\mathbf{H}), \tag{3}$$

where $T_k(\mathbf{H})$ can be orthogonal polynomials, typically the Chebyshev polynomials, and $a_k(E)$, the expansion coefficients. The filtered state is a coherent sum of the Chebyshev states $|\psi_k\rangle = T_k(\mathbf{H})|\Phi\rangle$,

$$|\varphi(E)\rangle = \sum_k a_k(E) T_k(\mathbf{H})|\Phi\rangle = \sum_k a_k(E)|\psi_k\rangle, \tag{4}$$

where the Chebyshev states can be obtained using a recurrence relationship. The elementary operation in this approach involves the evaluation of the action of the Hamiltonian operator on a vector. In grid-based methods, one does not even need to store the full $\mathbf{H}$ matrix because of efficient transformation methods such as the discrete variable representation (DVR) and/or the fast Fourier transform (FFT) [40, 41]. Because of the uniformity and stability [42], the Chebyshev polynomials have been widely used for approximating operator functions [27, 31, 33–36, 43]. Since the Chebyshev polynomials ($\{T_k(\mathbf{H}), k = 0, 1, 2, ...\}$) are global in energy (i.e., independent of E), only one set of Chebyshev states $T_k(\mathbf{H})|\Phi\rangle$ is needed for all the energy parameters.

It has been noted that the number of Chebyshev terms in the expansion is inversely proportional to the spectrum resolution and the convergence is considered to be slow. In addition, the truncation of the polynomial expansion can introduce further errors due to the Gibbs phenomenon [20, 28, 29, 36]. To circumvent the slow convergence, it was proposed that variational methods can be used to resolve the spectrum in a subspace spanned by the filtered states [20]. Since the number of filtered states is usually small ($\sim 10^2$), a direct diagonalization of a local Hamiltonian matrix can be done with relative ease. Very recently, it has been shown that the Hamiltonian and overlap matrices can be efficiently and accurately obtained from the correlation functions without calculating the filtered states explicitly [44–46]. This so-called filter-diagonalization scheme has been shown to be effective in many bound and scattering problems [20–27, 44–46].

A. *Forward Substitution in the Lanczos Algorithm*

In the Lanczos algorithm [1] a series of orthonormal Lanczos states $|\phi_m\rangle$, $m = 1, 2, ..., M$, are generated iteratively from an arbitrary initial vector $|\phi_1\rangle$,

$$\beta_{m+1}|\phi_{m+1}\rangle = \mathbf{H}|\phi_m\rangle - \alpha_m|\phi_m\rangle - \beta_m|\phi_{m-1}\rangle, \tag{5a}$$

where

$$\alpha_m = \langle\phi_m|\mathbf{H}|\phi_m\rangle, \tag{5b}$$

$$\beta_{m+1} = \|\mathbf{H}|\phi_m\rangle - \alpha_m|\phi_m\rangle - \beta_m|\phi_{m-1}\rangle\|, \quad \text{with } \beta_1 = 0. \tag{5c}$$

The Hamiltonian is thus iteratively transformed to a tridiagonal matrix on the Lanczos basis:

$$\mathbf{T}_M = \begin{bmatrix} \alpha_1 & \beta_2 & \cdots & 0 \\ \beta_2 & \alpha_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \alpha_M \end{bmatrix} = \mathrm{trid}_M[\beta, \alpha, \beta]. \tag{6}$$

Here M is the total number of the Lanczos states, i.e., the dimension of the Lanczos tridiagonal matrix. The Lanczos states are in fact the orthogonalized Krylov states $\{|\phi_1\rangle, \mathbf{H}|\phi_1\rangle, \mathbf{H}^2|\phi_1\rangle, ..., \mathbf{H}^{M-1}|\phi_1\rangle\}$ via the Gram–Schmidt procedure. In exact arithmetic, the Lanczos iteration terminates when $M \le N$ because of the inherent orthogonality of the Lanczos basis and all the eigenvalues of $\mathbf{H}$ can be found in $\mathbf{T}$. In finite precision arithmetic, however, the global orthogonality of the Lanczos states cannot generally be maintained. As a result, the Lanczos iteration can be performed for $M \gg N$ and there is no guarantee that all the eigenvalues will appear when $M = N$.

It has been shown [4] that for sufficiently large M, the eigenvalues of $\mathbf{H}$ will appear in $\mathbf{T}_M$, even when no forced reorthogonalization is implemented (Lanczos phenomenon). Spurious eigenvalues emerged along the way can be identified by the CW procedure and removed. Practically, the diagonalization of $\mathbf{T}_M$ yields approximate eigenvalues for $\mathbf{H}$,

$$\mathbf{A}^{-1}\mathbf{T}_M\mathbf{A} = \mathbf{E}, \tag{7}$$

where $\mathbf{E}$ is a diagonal matrix containing all the eigenvalues of the Lanczos matrix $\mathbf{T}_M$ and $\mathbf{A} \equiv [\mathbf{A}_1, \mathbf{A}_2, ..., A_M] \equiv [\mathbf{A}_{nm}]$ is a transformation matrix with its orthonormal columns

representing the eigenvectors of the tridiagonal matrix $\mathbf{T}_M$. An approximate eigenstate of the Hamiltonian is thus expressed as a linear superposition of the Lanczos states:

$$|E'_n\rangle = \sum_{m=1}^{M} A_{nm}|\phi_m\rangle. \tag{8}$$

For a given eigenvalue E'_n, Eq. (7) can be written as

$$(\mathbf{T}_M - E'_n\mathbf{I})\mathbf{A}_n = 0, \tag{9}$$

where the corresponding eigenvector is the nth column of the transformation matrix: $\mathbf{A}_n = [A_{n1}, A_{n2}, \cdots, A_{nM}]^{\mathrm{T}}$. The matrix elements, A_{nm}, are usually obtained only after the diagonalization process which yields the corresponding eigenvalue E'_n. This, in turn, becomes available after the M Lanczos states and Lanczos tridiagonal matrix are calculated. Thus, one has to either store the Lanczos states, or regenerate these states after the eigenvalues are determined. In the above iteration, M should be large enough to converge the eigenvalue E'_n which may or may not be at the edges of the spectrum.

One could argue that if A_{nm} are known during the Lanczos iteration, Eq. (8) can then be used to update an eigenstate. In fact, these coefficients can be obtained iteratively due to the fact that $\mathbf{T}_M$ is tridiagonal. To illustrate the forward substitution procedure, we rewrite the eigenequation (Eq. (9)) in the inhomogeneous form,

$$(\mathbf{T}_M - E\mathbf{I})\mathbf{A} = \mathbf{B}, \tag{10}$$

where E is the energy parameter and $\mathbf{B}$ is the inhomogeneity which is in principle arbitrary. The subscript n is dropped because the solution of Eq. (10) is not necessarily an eigenstate of $\mathbf{T}_M$. Formally, the vector $\mathbf{A}$ can be written as

$$\mathbf{A} = \frac{1}{\mathbf{T}_M - E\mathbf{I}}\mathbf{B}. \tag{11}$$

When the energy parameter E is sufficiently close to an eigenvalue E'_n, the vector $\mathbf{A}$ converges to $\mathbf{A}_n$. In other words, $\mathbf{A}$ can be regarded as a filtered vector generated by a Green function filter defined by a tridiagonal Hamiltonian matrix. The filtered state at this energy can be subsequently formed with $\mathbf{A}$ and the Lanczos states, according to Eq. (8). The above equation can be expressed explicitly in terms of the Lanczos matrix elements,

$$\beta_m A_{m-1} + \tilde{\alpha}_m A_m + \beta_{m+1} A_{m+1} = B_m, \quad m = 1, 2, ..., M, \tag{12}$$

where $\tilde{\alpha}_m = \alpha_m - E$ and $\beta_1 = 0$. Note that at the mth step in the Lanczos iteration and a given energy E, the coefficients (β_m, $\tilde{\alpha}_m$, and β_{m+1}) are known. The above equation typically has only three unknowns: A_{m-1}, A_m, and A_{m+1}. For the first equation ($m = 1$), there are only two variables because $\beta_1 = 0$. Hence, the solution to the inhomogeneous equation (Eq. (12)) can in principle be found iteratively within an arbitrary constant factor,

$$\begin{aligned} A_{m+1} &= (B_m - \beta_m A_{m-1} - \tilde{\alpha}_m A_m)/\beta_{m+1} \\ &= B'_m - \beta'_m A_{m-1} - \alpha'_m A_m, \end{aligned} \tag{13a}$$

where

$$B'_m = B_m/\beta_{m+1}, \quad \beta'_m = \beta_m/\beta_{m+1}, \quad \alpha'_m = \tilde{\alpha}_m/\beta_{m+1}. \tag{13b}$$

Note that the coefficient A_m is energy dependent. The first coefficient A_1 is related to the normalization of the filtered states, so it can be chosen arbitrarily. A similar iterative relation has been suggested for calculating eigenstates, but not the filtered states [47, 48].

Since we assume no prior knowledge of the spectrum, L points can be chosen at E_l, $l = 1, 2, ..., L$, in the energy range of interest $[E_{\mathrm{low}}, E_{\mathrm{up}}]$ to construct the filtered states. The distribution of E_l can be rather arbitrary, although typically a uniform grid is used. The number of filtered states (L) has to be larger than the number of eigenstates in the range of interest. A filtered state at E_l can thus be expressed as

$$|\varphi(E_l)\rangle = \sum_{m=1}^{M} A_m(E_l)|\phi_m\rangle. \tag{14}$$

Since the expansion coefficients and the Lanczos states are generated iteratively, the filtered states can be assembled along with the iteration. The Lanczos-based forward substitution proceeds as follows:

(1) Choose an arbitrary initial vector $|\phi_1\rangle = |\Phi\rangle$; let $|\varphi^{(1)}(E_l)\rangle$ be zero and $A_l(E_l) = 1$.

(2) Generate the next Lanczos state $|\phi_m\rangle$, $m = 2, 3, ...$, and the corresponding Lanczos matrix elements α_m and β_{m+1} according to Eq. (5).

(3) Calculate the overlap between the initial vector and the Lanczos state, $B_m = \langle\Phi|\phi_m\rangle$, and the coefficients $A_m(E_l)$ using Eq. (13).

(4) Update the filtered states: $|\varphi^{(m)}(E_l)\rangle \Leftarrow |\varphi^{(m-1)}(E_l)\rangle + A_m(E_l)|\phi_m\rangle$, $l = 1, 2, ..., L$.

(5) Exit if m equals to M; otherwise go to (2).

The filtered states are finally normalized after the iteration. It is not difficult to see that the computational demand

in the aforementioned scheme is much smaller than in the basic Lanczos method, in which all the Lanczos states have to be stored or regenerated. The number of filtered states is typically much smaller than the total Lanczos steps for highly excited eigenstates.

We point out that the filtering based on the Lanczos iteration is similar in spirit to that based on the Chebyshev polynomial expansion. To this end, note that the filtered states in both schemes, Eqs. (4) and (14), are expressed as linear combinations of iteratively generated bases. While the coefficients can be calculated *a priori* in the Chebyshev expansion, those for the Lanczos filter have to be obtained iteratively. In the Chebyshev approach, we have shown that the basis (Chebyshev states) is essentially the evolution state in the order domain of the Chebyshev propagator ($T_k = \cos(k \arccos(\mathbf{H}))$) [28]. A parallel can thus be drawn between the evolution of a wave packet in the Chebyshev order domain and that in the time domain. A filtered state in Eq. (4) can be regarded as a convoluted Fourier transform of the order-dependent wave packet. Similar statements can also be made here for the filtering based on the Lanczos iteration. Although an analytical expression for the Lanczos ''propagator'' cannot be identified, the Krylov sequence can certainly be viewed as an equivalent of the Chebyshev states. In other words, a formal linear transformation must exist between the two because these states are generated by some polynomials of $\mathbf{H}$ up to the mth order. Of course, the Lanczos iteration does not possess the same level of stability as the Chebyshev recursion and errors can cause significant contamination in the filtered states. This point is addressed below.

B. *Stability of Forward Substitution and Filter-Diagonalization*

The forward substitution described above is easy to understand and to implement. Theoretically, the superdiagonal element of the Lanczos matrix, β_{m+1}, will inevitably become zero when the Lanczos states completely span the Krylov subspace of interest. Since the forward substitution (Eq. (13)) requires β_{m+1} in the denominator, the iteration eventually breaks down in exact arithmetic. In practical applications, however, the Lanczos states do not remain orthonormal due to the numerical instability of the finite precision Lanczos algorithm. Because of the linear dependence of these states, the overlap, β_{m+1}, never becomes exactly zero. In fact, it may not even be very small. Although this is usually considered as a disadvantage of the Lanczos algorithm, it is this feature that makes the forward substitution possible for large M. However, construction of eigenvectors with forward substitution is known to be unstable [30]. The lack of stability in the procedure, despite its simplicity in exact arithmetic, is probably the reason that it has not seen many applications. As we show below, however, this procedure, coupled with diagonalization of the Hamiltonian matrix spanned by the filtered states, can yield accurate eigenvalues and eigenstates.

From Paige's analysis [4, 12], loss of the orthogonality of the Lanczos states is closely related to the convergence of some eigenvalues and the corresponding eigenstates, typically at the edges of the spectrum. Copies of converged eigenvalues emerge in further Lanczos propagation. As a result, later Lanczos states become contaminated by these converged eigenstates. Formally, one can view the Lanczos states in finite precision arithmetic as the exact Lanczos states plus some combination of the converged states. In forward substitution, this implies that the filtered states can be contaminated by converged eigenstates as well. In other words, the filtered states obtained in finite precision arithmetic may not be completely localized in the energy domain. Consequently, it is generally not possible to obtain the eigenstates directly from filtering via forward substitution. To this end, the filtering via forward substitution based on the Lanczos iteration is inferior to other stable filtering methods, such as the ones based on the Chebyshev expansion.

Although the loss of orthogonality of the Lanczos states is certainly a numerically unpleasant feature, its effects on the final results can often be managed effectively. This point has been demonstrated by earlier work on eigenproblems [4] and on other properties [10]. In this work, we show that this difficulty of the Lanczos algorithm can be greatly alleviated or even eliminated if filter-diagonalization is employed. This can be understood by examining the subspace spanned by the filtered states. When an eigenstate $|E_i'\rangle$ is converged at certain Lanczos step m, the Lanczos states generated afterward may be contaminated by this state. A contaminated Lanczos state for $m' > m$ can be written as a sum of the converged eigenstates and the corresponding exact Lanczos state, which can only be obtained with exact arithmetic:

$$|\phi_{m'}^{\text{finite}}\rangle = |\phi_{m'}^{\text{exact}}\rangle + \sum_i c_{im'}|E_i'\rangle. \tag{15}$$

The deviation of the finite precision Lanczos states from the exact ones causes the filtered states to be inaccurate:

$$|\varphi(E_l)^{\text{finite}}\rangle = |\varphi(E_l)^{\text{exact}}\rangle + \sum_i d_{im'}|E_i'\rangle. \tag{16}$$

Thus, the subspace spanned by $\{|\varphi(E_l)^{\text{finite}}\rangle\}$ is composed of that spanned by $\{|\varphi(E_l)^{\text{exact}}\rangle\}$ and the converged eigenstates $\{|E_i'\rangle\}$. It is important to realize that this subspace is complete, or invariant, under the system Hamiltonian, provided a sufficiently large number of filtered states are included. In other words, any vector in this subspace can be mapped by $\mathbf{H}$ to a linear combination of vectors spanning

the subspace. Consequently, the eigenvalues and eigenstates within the specified energy region $[E_{\text{low}}, E_{\text{up}}]$ can be accurately determined variationally, i.e., by diagonalization of a small Hamiltonian matrix. The contamination, even when severe, has little influence on the accuracy of the final results.

III. NUMERICAL TEST

To illustrate the method, we solve the eigenproblem for a one-dimensional Morse oscillator. Testing of this method in larger systems will be published elsewhere. The potential of the oscillator with a reduced mass of 1.0 au is

$$V = 1000(e^{-0.3x} - 2e^{-0.15x}), \tag{17}$$

where the parameters are adopted from an earlier work by Neuhauser [20]. This Morse potential accomendates 298 bound states. The Hamiltonian is discretized in a uniform grid of 512 points and the action of the kinetic energy operator is evaluated via 1D FFT. The initial wave packet is chosen as

$$\Phi(x) = \frac{1}{1 + e^{-\sigma(x-x_1)}} - \frac{1}{1 + e^{-\sigma(x-x_2)}}. \tag{18}$$

Roughly speaking, the initial wave packet is nearly constant in $[x_1, x_2]$ and decreases to zero outside this range, with the variation width characterized by σ. Two sets of parameters are chosen. The first set (Φ_1) with the parameters $x_1 = 13$, $x_2 = 20$, $\sigma = 2$ has very small overlaps with the lowest states, but considerable overlaps with the states higher than -300 au. The second set (Φ_2) is much broader ($x_1 = -13$, $x_2 = 120$, $\sigma = 2$) and it overlaps with all the bound states.

We are interested in the eigenstates in the energy range $[E_{\text{low}}, E_{\text{up}}]$ in which L filters are evenly distributed: $E_l = E_{\text{low}} + (l - 0.5)\cdot\Delta E$, $l = 1, 2, ..., L$, with $\Delta E = (E_{\text{up}} - E_{\text{low}})/L$. The filtered states are constructed by forward substitution as described above. In order to determine the quality of the filtered states, we first analyze its spectral composition under various conditions. Following our earlier work [28], we propagate a filtered state in the Chebyshev order domain with 8192 Chebyshev terms. The autocorrelation function in the order domain is then Fourier (cosine) transformed to the angle domain for the energy spectrum. For details of this method, the readers are referred to the original publication [28].

We concentrate on the filtered state at $E_l = -105.3333$ au. In Fig. 1, we display a semi-log plot of the spectra of the filtered state constructed from two different initial wave functions. Five hundred Lanczos states are used to construct the filtered state. It is obvious that even for such a not-so-large M, the effect of the filter operator is obvious:

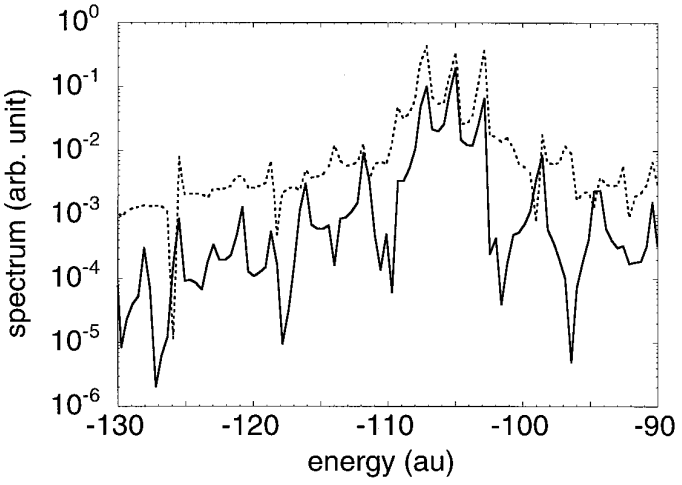

FIG. 1. Spectra of the filtered state at $E_l = -105.3333$ au obtained from two initial wave packets (solid line Φ_1 and dashed lines for Φ_2). 500 Lanczos steps are used.

The spectrum is dominated by eigenstates near E_l. This result shows that it is possible to construct filtered states via forward substitution. It is also interesting to notice that drastically different initial states resulted in little difference in the outcome of the filtering.

One would naively expect that the quality of the filtered states should increase with the number of Lanczos steps M. This is certainly the case in filtering based on stable Chebyshev recursion [27]. However, we should also bear in mind that the instability inherent in the forward substitution introduces contamination in the filtered states. Our primary concern here is whether the instability in the forward substitution will destroy its attractive characteristics. To illustrate the competition between the two factors, we give in Fig. 2 the spectra of the same filtered state obtained by using $M = 500$, 750, and 1000 Lanczos states from the second initial wave packet. The spectra are normalized at $E_l = -105.3333$ au and the details near this energy are given in the upper panel. From the figure, we observe that the quality of the filtered state does improve with increasing M. For $M = 500$, the filtered state is mainly composed of three eigenstates corresponding to eigenenergies close to E_l. For $M = 750$, the peaks near 107 au and 103 au are suppressed, compared to the peak near 105 au. For $M = 1000$, the filtered state is mainly composed of the eigenstate corresponding to the eigenvalue nearest to E_l.

In the lower panel in Fig. 2, it can be seen that the background for the filtered state obtained with $M = 1000$ is significantly higher than that from $M = 750$, due to the instability in the forward substitution. For the problem examined here, this instability is not severe even for M as large as $2N$. However, whether the instability will affect the accuracy of the filtered states in large systems requires

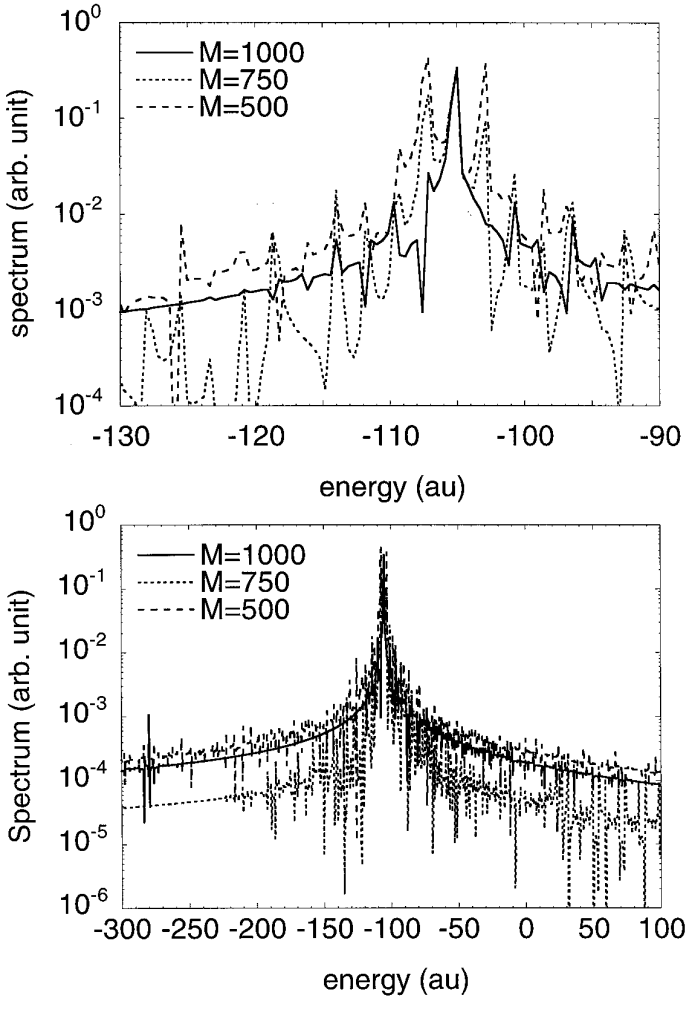

FIG. 2. Spectra of the filtered state at $E_l = -105.3333$ au obtained with three different numbers of Lanczos iterations. The upper panel gives detailed spectral features near E_l. The second set of parameters for the initial wave packet is used.

further investigations. This indicates that the Lanczos-based forward substitution may not be applied for a very large M.

Once the filtered states are constructed, one has to remove their linear dependence. This can be carried out by either the singular value decomposition (SVD) or the Gram–Schmidt orthogonalization scheme [49]. The orthogonalized vectors are then used to construct a local Hamiltonian matrix, which is finally diagonalized using conventional EISPACK routines. The first question that we try to answer is whether the forward substitution filter-diagonalization (FSFD) method introduces additional errors other than those already in the basic Lanczos method. In other words, are the results from the FSFD method less accurate? To this end, we performed a calculation with $M = 1000$ iterations for both basic and FSFD Lanczos methods and 30 filtered states. Under such conditions, the eigenvalues of the Lanczos matrix in the range [−130 au, −90 au] have not yet converged to the true eigenvalues, as shown in Table I. Nevertheless, it can be readily seen from the table that the agreement between the eigenvalues obtained from the FSFD and the basic Lanczos scheme is extremely good, despite of poor agreement with exact values. This indicates that the unstable forward subsitution, when followed by filter-diagonalization, does not introduce additional errors, except for those inherited from the basic Lanczos algorithm.

At lower energies, the eigenvalues are well converged for 1000 Lanczos iterations. Table II displays the eigenvalues obtained from both the FSFD and basic Lanczos calculations in the energy range [−170 au, −130 au]. Similar to the results presented at higher energies, the agreement between the FSFD and basic Lanczos is excellent. Their agreement with the exact results is also extremely good. The convergence of the corresponding eigenstates should be good, since for variational calculations the error in the eigenvalue is proportional to the square of the error in the eigenstate.

IV. CONCLUDING REMARKS

We have introduced a filter-diagonalization scheme based on the forward substitution in the Lanczos iteration. This method has conceptual and practical significance. First, when the Lanczos states are generated in the Lanczos algorithm, the filtered states can be constructed on-the-fly via forward substitution. The filter is the Green function

TABLE I

Comparison of the Eigenvalues in [−130 au, −90 au] Obtained from the FSFD and Basic Lanczos Algorithms

n	E'_n (FSFD)	E'_n (basic Lanczos)	E_n (exact)
7	−127.9351930846054	−127.9351930846055	−127.9417594263708
8	−125.5460511609613	−125.5460511609614	−125.5535554938715
9	−123.1525484616846	−123.1525484616845	−123.1878515613721
10	−120.8096613259043	−120.8096613259043	−120.8446476288728
11	−118.3846363721996	−118.3846363721996	−118.5239436963734
12	−116.1077390980454	−116.1077390980454	−116.2257397638740
13	−113.5507421620933	−113.5507421620933	−113.9500358313746
14	−111.3965855439493	−111.3965855439493	−111.6968318988753
15	−108.6094281048649	−108.6094281048648	−109.4661279663759
16	−106.6156176730321	−106.6156176730319	−107.2579240338765
			−105.0722201013771
17	−103.6474367962876	−103.6474367962875	−102.9090161688778
18	−101.6309875062529	−101.6309875062530	−100.7683122363784
19	−98.8215105854005	−98.8215105854006	−98.6501083038791
20	−96.3306429354566	−96.3306429354564	−96.5544043713797
21	−94.0570103159452	−94.0570103159451	−94.4812004388803
22	−91.0774364353989	−91.0774364354059	−92.4304965063809
			−90.4022925738816

TABLE II

Comparison of the Eigenvalues in [−170 au, −130 au] Obtained from the FSFD and Basic Lanczos Algorithms

n	E'_n (FSFD)	E'_n (basic Lanczos)	E_n (exact)
6	−169.2130223488259	−169.2130223489205	−169.2130223463607
7	−166.4648184171008	−166.4648184171007	−166.4648184138614
8	−163.7391144852315	−163.7391144852315	−163.7391144813620
9	−161.0359105536108	−161.0359105536106	−161.0359105488626
10	−158.3552066186402	−158.3552066186401	−158.3552066163633
11	−155.6970026847810	−155.6970026847812	−155.6970026838639
12	−153.0612986974404	−153.0612986974405	−153.0612987513646
13	−150.4480947258207	−150.4480947258209	−150.4480948188652
14	−147.8573900311168	−147.8573900311169	−147.8573908863658
15	−145.2891855985935	−145.2891855985935	−145.2891869538665
16	−142.7434725958204	−142.7434725958203	−142.7434830213670
17	−140.2202635071893	−140.2202635071892	−140.2202790888677
18	−137.7194670277229	−137.7194670277233	−137.7195751563683
19	−135.2412204088172	−135.2412204088172	−135.2413712238690
20	−132.7847290161098	−132.7847290161098	−132.7856672913696
21	−130.3512636771011	−130.3512636776135	−130.3524633588702

operator. Second, this method requires fewer computational resources than the basic Lanczos method in dealing with highly excited eigenstates, without sacrificing accuracy. This is due to the fact that the filtered states are updated along with the Lanczos iteration so that the Lanczos states need not be stored nor regenerated. Numerical results indicate that this method is efficient and as accurate as the basic Lanczos method. It can be very useful for the determination of highly excited eigenstates in large systems. An implication of this paper is that if prudently implemented, the forward substitution can be used to calculate the eigenstates corresponding to eigenvalues in a prespecified energy range. Further works in large systems and the effect of different modification to the basic algorithm presented here are underway.

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