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LETTER TO THE EDITOR

A numerical method for computing eigenvectors of a large matrix

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Abstract. We introduce a new numerical method to determine eigenvectors of a Hamiltonian matrix. The method is particularly useful for matrices of large dimension. The essence of the method is to determine each phase in the expansion of an eigenvector by computing the projection weight to the eigenvector on a trial function with an arbitrary phase. The trial function depends on the unknown phase in the expansion of the eigenvector, and we show that the weight takes its maximum value if the phase in the trial function takes the correct value of the phase in the expansion of the eigenvector.

Many numerical methods have been developed for obtaining eigenvectors of a matrix. However, most standard methods require very large memory space when the dimension of the matrix becomes large.

The Hamiltonian operator of a physical system can, in general, be expressed in the form of a square matrix H. The Lanczos algorithm [1] can bring the matrix H on tridiagonal form. The eigenvalues of the resulting tridiagonal matrix can be obtained by using the negative eigenvalue method of Dean and Martin [2]. The recursion method of Haydock *et al* [3] or the Nex quadrature method [4] can be used to find the weight, i.e. square of the absolute value of the overlap, of an eigenvector on the original basis functions. We will here demonstrate a new method which can be used to obtain the remaining unknown quantities, the phases in the expansion of the eigenvector.

We first summarize the basic formulae in the Lanczos, Haydock and Nex methods. (For the negative eigenvalue method of Dean and Martin, see a review given by Dean [5].) In the Lanczos method [1], the matrix H is given in tridiagonal form by using the recursion relation

$$b_{n+1}|u_{n+1}\rangle = H|u_n\rangle - a_n|u_n\rangle - b_n|u_{n-1}\rangle. \tag{1}$$

Here $|u_{-1}\rangle$ is taken as zero and $|u_0\rangle$ is any linear combination of a set of original basis functions $\{|\phi_\alpha\rangle, \alpha = 1, \ldots, N\}$, assumed orthonormal. In the basis set $\{|u_n\rangle\}$ the matrix

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thus takes the form

$$H = \begin{pmatrix} a_0 & b_1 & & & & & \\ b_1 & a_1 & b_2 & & & & \\ & b_2 & a_2 & b_3 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & b_{N-3} & a_{N-3} & b_{N-2} & \\ & & & & b_{N-2} & a_{N-1} & b_{N-1} \\ & & & & & b_{N-1} & a_{N-1} \end{pmatrix} \tag{2}$$

where $\{a_n\}$ and $\{b_n\}$ are called recursion coefficients. The set $\{|u_n\rangle\}$ is also orthonormal. The Hamiltonian matrix in (2) obviously depends on the choice of $|u_0\rangle$. If $u_0\rangle$ is orthogonal to an eigenvector, that eigenvector does not appear as a solution. This can be used to advantage by cutting out solutions of a symmetry that is not of interest.

In the recursion merhod of Haydock *et al* [3], the diagonal matrix element of the Green function $G(E) \equiv (E-H)^{-1}$ corresponding to the starting vector $|u_0\rangle$ is expressed in terms of the recursion coefficients $\{a_n\}$ and $\{b_n\}$ in the form of a continued fraction:

$$G_{00}(E) \equiv \langle u_0|G(E)|u_0\rangle = \cfrac{1}{E-a_0-\cfrac{b_1^2}{E-a_1-\cfrac{b_2^2}{E-a_2-\cfrac{b_3^2}{E-\cdots}}}}. \tag{3}$$

The poles of $G_{00}(E)$ give the eigenvalues of H, and the imaginary part of $G_{00}(E+\mathrm{i}\varepsilon)$ is related to the local density of states (LDOS) ρ_0 corresponding to the starting vector $|u_0\rangle$ by the following equation:

$$\rho_0(E) \equiv \sum_{i=1}^{N} |\omega_{i0}|^2 \delta(E-E_i) = -\frac{1}{\pi} \lim_{\varepsilon \to \infty} \operatorname{Im} G_{00}(E+\mathrm{i}\varepsilon) \tag{4}$$

where $\omega_{i0} \equiv \langle u_0|\varphi_i\rangle$ and $|\varphi_i\rangle$ is an eigenvector. Equation (4) makes it clear that for eigenstates whose eigenvectors have zero projection on the starting vector $|u_0\rangle$, the eigenvalues cannot be obtained by solving the eigenequation of the tridiagonal Hamiltonian matrix given in (2). Equation (4) also gives an explicit way for computing the $|\omega_{i\alpha}|$, i.e. the absolute values of the overlaps of the eigenvectors on all the original basis functions $|\phi_\alpha\rangle$, by setting successively the different basis functions as the starting vector $|u_0\rangle$. One numerical difficulty to obtain $|\omega_{i\alpha}|$ by this method is that one has to integrate the Green function $G_{00}(E)$ which contains many δ-function peaks.

The quadrature method introduced by Nex [4] can be used to compute the projection $|\omega_{i0}|$ directly from the recursion coefficients $\{a_n\}$ and $\{b_n\}$, which often is an advantage, and thus the difficulty in the Haydock method associated with the integration of the δ-functions can be overcome. In this method, the projection weight $|\omega_{i0}|^2$ is expressed by the following equation:

$$|\omega_{i0}|^2 = (q_{N-1}(E_i))/(p'_N(E_i)) \tag{5}$$

where $p_N(E_i)$ and $q_{N-1}(E_i)$ are two polynomials calculated from recurrence relations

$$p_{n+1}(E_i) = (E_i - a_n)p_n(E_i) - b_n^2 p_{n-1}(E_i) \tag{6a}$$

$$q_{n+1}(E_i) = (E_i - a_{n+1})q_n(E_i) - b_{n+1}^2 q_{n-1}(E_i) \tag{6b}$$

with the initial conditions $p_{-1}(E_i) = q_{-1}(E_i) = 0$, $p_0(E_i) = 1$ and $q_0(E_i) = b_0^2 = 1$.

In this paper, a new method is developed for computing the eigenvectors of a large square matrix H. We will now show how (the phases in) the expansion of an eigenvector can be obtained.

We first calculate the eigenvalues E_i and the projections $|\omega_{i\alpha}|$ on the basis functions $|\phi_\alpha\rangle$, using a numerical procedure as described above. For the ith eigenstate, the eigenvector $|\varphi_i\rangle$ can be expressed in terms of the projections $|\omega_{i\alpha}|$:

$$|\varphi_i\rangle = \sum_{\alpha=1}^{N} \exp(i\theta_{i\alpha})|\omega_{i\alpha}||\phi_\alpha\rangle \tag{7}$$

where $\exp(i\theta_{i\alpha})$ are phase factors, and $\theta_{i\alpha}$ ($0 \leq \theta_{i\alpha} < 2\pi$) are unknown phaseshifts. The projections $|\omega_{i\alpha}|$ satisfy the normalization condition

$$\sum_{\alpha=1}^{N} |\omega_{i\alpha}|^2 = 1. \tag{8}$$

Since only relative phaseshifts have effect on physical results, we choose, without loss of generality, $\theta_{i1} = 0$ and rewrite (7) as

$$|\varphi_i\rangle = |\omega_{i1}||\phi_1\rangle + \sum_{\alpha=2}^{N} \exp(i\theta_{i\alpha})|\omega_{i\alpha}||\phi_\alpha\rangle. \tag{9}$$

We begin with the determination of θ_{i2} in (9) by defining the following normalized test function:

$$|\tilde{\varphi}_2(\tilde{\theta}_{i2})\rangle = \frac{1}{(|\omega_{i1}|^2 + |\omega_{i2}|^2)^{1/2}}[|\omega_{i1}||\phi_1\rangle + \exp(i\tilde{\theta}_{i2})|\omega_{i2}||\phi_2\rangle] \tag{10}$$

with a trial phaseshift $\tilde{\theta}_{i2}$. Remember that we have assumed that the basis functions $\{|\phi_\alpha\rangle, \alpha = 1, \ldots, N\}$ are all orthonormal. The projection weight $|\tilde{\omega}_{i2}(\tilde{\theta}_{i2})|^2$ of the ith eigenvector $|\varphi_i\rangle$ on the test function is given by

$$|\tilde{\omega}_{i2}(\tilde{\theta}_{i2})|^2 \equiv |\langle\tilde{\varphi}_2(\tilde{\theta}_{i2})|\varphi_i\rangle|^2 = \left|\frac{|\omega_{i1}|^2 + |\omega_{i2}|^2 \exp[i(\theta_{i2} - \tilde{\theta}_{i2})]}{(|\omega_{i1}|^2 + |\omega_{i2}|^2)^{1/2}}\right|^2. \tag{11}$$

It is very easy to show that $|\tilde{\omega}_{i2}(\tilde{\theta}_{i2})|^2$ is bounded by $(|\omega_{i1}|^2 \pm |\omega_{i2}|^2)^2/(|\omega_{i1}|^2 + |\omega_{i2}|^2)$, i.e. the following inequality holds:

$$(|\omega_{i1}|^2 - |\omega_{i2}|^2)^2/(|\omega_{i1}|^2 + |\omega_{i2}|^2) \leq |\tilde{\omega}_{i2}(\tilde{\theta}_{i2})|^2 \leq |\omega_{i1}|^2 + |\omega_{i2}|^2. \tag{12}$$

When and only when the trial phaseshift $\tilde{\theta}_{i2}$ is equal to the true phaseshift θ_{i2} in (9), the weight $|\tilde{\omega}_{i2}(\tilde{\theta}_{i2})|^2$ takes its maximum value, i.e.

$$|\tilde{\omega}_{i2}|^2 = |\omega_{i1}|^2 + |\omega_{i2}|^2 \qquad \text{if } \tilde{\theta}_{i2} = \theta_{i2}. \tag{13}$$

This suggests a numerical procedure for the determination of the relative phaseshift θ_{i2} in (9) as follows. We first construct a normalized test function of the form given in (10) from the calculated weights $|\omega_{i1}|^2$ and $|\omega_{i2}|^2$ with an arbitrarily trial phaseshift, and calulate the weight $|\tilde{\omega}_{i2}|^2$ of the eigenvector on the test function using, for example, the quadrature method. We then vary the trial phaseshift and repeat the calculations, until we find a value of the trial shift which gives the maximum $(|\omega_{i1}|^2 + |\omega_{i2}|^2)$ of the

projection weight $|\tilde{\omega}_{i2}|^2$. This value is the true value of the relative phaseshift θ_{i2} presented in (9). Here, we note that this procedure is very easy to implement, because the projection weight $|\tilde{\omega}_{i2}|^2$ is a cosine function of the trial phaseshift.

Using exactly the same procedure, we can determine the values for all the relative phaseshifts $\{\theta_{i\alpha}\}$ in (9), and the eigenvector of the ith eigenstate is then obtained.

Our numerical method becomes very simple if the matrix of the Hamiltonian H is real. In this case, all the relative phaseshifts $\{\theta_{i\alpha}\}$ can only have the values 0 and π. Therefore, we only have two test functions for each relative phaseshift.

Let us make the following notes about our numerical method. (i) A very useful feature of the method is that it can be used to calculate the eigenvector for any eigenstate without having any information about other eigenstates. (ii) The method does not require storage of the matrix of the unitary transformation generated by the Lanczos scheme or any other scheme. Therefore, the eigenequation of a large Hamiltonian matrix can be solved on ordinary workstations or even personal computers. (iii) In order to derive (9), we have chosen $\theta_{i1} = 0$ and left all other relative phaseshifts to be determined. However, we can choose any one of the phaseshifts in (7) to be zero and compute all others relative to this one. (iv) Only the phaseshifts for the terms where the eigenvector has non-zero projection weight need to be computed. This observation is very useful in study of eigenstates which are localized and/or have specific symmetry. (v) The accuracy of the method depends on how accurately the eigenvalues and the projections of the eigenvectors are determined. (It is worth mentioning that the Lanczos scheme and the negative eigenvalue and the quadrature methods can be used to determine the eigenvalues and the projection weights to arbitrarily high accuracy, at least for some eigenstates.) (vi) The present numerical procedure is applicable to both real and complex Hamiltonian matrices, provided they are represented in an orthonormal basis.

In summary, we have presented a new numerical method for computing eigenvectors of large square Hamiltonian matrices. The method does not require storage of unitary transformation matrices and, therefore, the eigenequations of large Hamiltonian matrices can be solved on ordinary work stations or even personal computers. An application of the method can be found in our earlier publication [6] where a Hamiltonian matrix of dimension $10\,648 \times 10\,648$ was treated. Further applications and the generalization of the method in order to compute eigenvectors represented in a non-orthogonal basis are in progress.

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