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An efficient method for obtaining the eigenvectors of a ring system

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Abstract. A method for calculating the eigenvectors of a ring system is developed. The system can be one chain or many coupled chains. A sample calculation demonstrates that this method is accurate, efficient and can be used to handle large systems.

1. Introduction

To solve the eigenvalue equation is the basic problem in physics. Standard programs such as TRED2 and TQL2 [1] can deal with matrices of dimensions up to 600×600 on a VAX computer. The Dean method [2] can be used to find some eigenvalues and corresponding eigenvectors. The Lanczos method can transform the matrix to the tridiagonal form [3]. In recent years Wu and Zheng developed a new integrated method for obtaining the eigenvalues and eigenvectors of an unusually large size tridiagonal matrix [4, 5]. Zheng also developed a method for obtaining the eigenvectors of a block tridiagonal Hamiltonian up to $N = 10^4$-10^5, where N is the number of diagonal elements of the matrix [6].

In some cases we need to study a system with a periodic boundary condition. In this work a method for obtaining the eigenvalue and eigenvectors of a ring system is developed. The sample calculation demonstrates that this method is accurate and more efficient.

2. Formulation of the method

The Hamiltonian of many-coupled-chain ring systems has the form:

$$H = \begin{pmatrix} A_{1,1} & A_{1,2} & & & & & A_{1,m} \\ A_{2,1} & A_{2,2} & A_{2,3} & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & & & A_{m-1,m-2} & A_{m-1,m-1} & A_{m-1,m} \\ A_{m,1} & & & & & A_{m,m-1} & A_{m,m} \end{pmatrix} \tag{1}$$

where the $A_{i,j}$ are $n \times n$ submatrices, $i, j = 1, 2, \ldots, m$, and the dimension of H is $N = n \times m$. H is real and symmetric. The Dean method can be used to calculate the

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eigenvalue. The main steps of the Dean method are the calcultion of the number of real negative eigenvalues of H.

If $\eta(x)$ denotes the number of real negative eigenvalues of matrix X then we can derive the following results:

$$\eta(H - xI) = \sum_{i=1}^{m} \eta(U_i) \tag{2}$$

where

$$\begin{aligned} &U_1 = A_{11} - xI \\ &U_i = A_{ii} - xI - A_{i,i-1} U_{i-1}^{-1} A_{i-1,i} \qquad i = 2, 3, \ldots, m-1 \\ &U_m = A'_{m,m} - xI - A'_{m,m-1} U_{m-1}^{-1} A'_{m-1,m} \end{aligned} \tag{3}$$

and where I is the $n \times n$ unit matrix and

$$\begin{aligned} &A'_{m-1,m} = A_{m-1,m} + S_{m-1} \qquad A'_{m,m-1} = A_{m,m-1} + S_{m-1}^{\mathrm{T}} \\ &A'_{m,m} = A_{m,m} - \sum_{i=1}^{m-1} S_i^T U_i^{-1} S_i \\ &S_1 = A_{1m} \qquad S_1^{\mathrm{T}} = A_{m1} \\ &S_i = -A_{i,i-1} U_{i-1}^{-1} S_{i-1} \\ &S_i^{\mathrm{T}} = -S_{i-1}^{\mathrm{T}} U_{i-1}^{-1} A_{i-1,i} \qquad i = 2, 3, \ldots, m-1. \end{aligned}$$

This means that these U_i, $i \leqslant m-1$, are the same as the U_i of fixed boundary conditions ($A_{1m} = A_{m1} = 0$). Only U_m should be calculated by equation (3). The number of eigenvalues of matrix H which are smaller than X can be found from the U_i, $i = 1, 2, \ldots, m$. Hence it can be used to determine the Jth eigenvalue to the desired degree of accuracy by bisection [2].

For the Jth eigenvalue E_j the eigenvector $\boldsymbol{U}_j$ is determined by

$$H\boldsymbol{U}_j = E_j \boldsymbol{U}_j \tag{4}$$

where

$$\boldsymbol{U}_j = \begin{pmatrix} \boldsymbol{b}_1 \\ \boldsymbol{b}_2 \\ \vdots \\ \boldsymbol{b}_m \end{pmatrix} \qquad \boldsymbol{b}_i = \begin{pmatrix} b_{i1} \\ b_{i2} \\ \vdots \\ b_{in} \end{pmatrix}.$$

For $\boldsymbol{b}_{k \neq 0}$ equation (4) can be expressed as the following equations (5) and (6), by changing the positions of $\boldsymbol{b}_i$ arising from the nature of ring systems:

$$\begin{pmatrix} A_{k+1,k+1} - E_j I & A_{k+1,k+2} & & & & & & & & \\ A_{k+2,k+1} & A_{k+2,k+2} - E_j I & A_{k+2,k+3} & & & & & & & \\ & \ddots & \ddots & \ddots & & & & & & \\ & & & A_{m,m-1} & A_{m,m} - E_j I & A_{m,1} & & & & \\ & & & & A_{1,m} & A_{1,1} - E_j I & A_{1,2} & & & \\ & & & & & \ddots & \ddots & A_{k-2,k-3} & & \\ & & & & & & & A_{k-2,k-2} - E_j I & A_{k-2,k-1} & \\ & & & & & & & A_{k-1,k-2} & A_{k-1,k-1} - E_j I & \end{pmatrix}$$

$$\times \begin{pmatrix} \boldsymbol{b}_{k+1} \\ \boldsymbol{b}_{k+2} \\ \vdots \\ \boldsymbol{b}_m \\ \boldsymbol{b}_1 \\ \vdots \\ \boldsymbol{b}_{k-2} \\ \boldsymbol{b}_{k-1} \end{pmatrix} = \begin{pmatrix} -A_{k+1,k}\boldsymbol{b}_k \\ 0 \\ \vdots \\ 0 \\ 0 \\ \vdots \\ 0 \\ -A_{k-1,k}\boldsymbol{b}_k \end{pmatrix} \tag{5}$$

and

$$A_{k,k-1}\boldsymbol{b}_{k-1} + (A_{k,k} - E_j I)\boldsymbol{b}_k + A_{k,k+1}\boldsymbol{b}_{k+1} = 0. \tag{6}$$

Equation (5) can be expressed simply by

$$\boldsymbol{A}\boldsymbol{b} = \boldsymbol{d}$$

so that

$$\boldsymbol{b} = \boldsymbol{b}' + \boldsymbol{b}'' \tag{7}$$

$$\boldsymbol{d} = \boldsymbol{d}' + \boldsymbol{d}'' \tag{8}$$

where

$$\boldsymbol{d}' = \begin{pmatrix} -A_{k+1,k}\boldsymbol{b}_k \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix} \qquad \boldsymbol{d}'' = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ -A_{k-1,k}\boldsymbol{b}_k \end{pmatrix}$$

and

$$\boldsymbol{A}\boldsymbol{b}' = \boldsymbol{d}' \tag{9}$$

$$\boldsymbol{A}\boldsymbol{b}'' = \boldsymbol{d}''. \tag{10}$$

By using the same method as in [5, 6] the relations between $\boldsymbol{b}_k$ and $\boldsymbol{b}_i$, $i \neq k$, can be obtained.

From equation (9) we obtain

$$\boldsymbol{b}' = \begin{pmatrix} \boldsymbol{b}'_{k+1} \\ \boldsymbol{b}'_{k+2} \\ \vdots \\ \boldsymbol{b}'_m \\ \boldsymbol{b}'_1 \\ \vdots \\ \boldsymbol{b}'_{k-2} \\ \boldsymbol{b}'_{k-1} \end{pmatrix} \qquad \text{where} \qquad \begin{aligned} \boldsymbol{b}'_{k+1} &= -\Delta^+_{k+1}A_{k+1,k}\boldsymbol{b}_k \\ \boldsymbol{b}'_{k+2} &= -\Delta^+_{k+2}A_{k+2,k+1}\boldsymbol{b}'_{k+1} \\ &\vdots \\ \boldsymbol{b}'_m &= -\Delta^+_m A_{m,m-1}\boldsymbol{b}'_{m-1} \\ \boldsymbol{b}'_1 &= -\Delta^+_1 A_{1,m}\boldsymbol{b}'_m \\ &\vdots \\ \boldsymbol{b}'_{k-2} &= -\Delta^+_{k-2}A_{k-2,k-3}\boldsymbol{b}'_{k-3} \\ \boldsymbol{b}'_{k-1} &= -\Delta^+_{k-1}A_{k-1,k-2}\boldsymbol{b}'_{k-2} \end{aligned} \tag{11}$$

and where

$$\Delta^+_{k-1} = \frac{1}{A_{k-1,k-1} - E_j I} \qquad \Delta^+_m = \frac{1}{A_{m,m} - E_j I - A_{m,1}\Delta^+_1 A_{1,m}}$$

$$\Delta^+_i = \frac{1}{A_{i,i} - E_j I - A_{ii+1}\Delta^+_{i+1}A_{i+1,i}} \qquad i = k-2, \ldots, 1, m+1, \ldots, k+1.$$

From equation (10) we obtain

$$\boldsymbol{b}'' = \begin{pmatrix} \boldsymbol{b}''_{k+1} \\ \boldsymbol{b}''_{k+2} \\ \vdots \\ \boldsymbol{b}''_m \\ \boldsymbol{b}''_1 \\ \vdots \\ \boldsymbol{b}''_{k-2} \\ \boldsymbol{b}''_{k-1} \end{pmatrix} \qquad \text{where} \qquad \begin{aligned} \boldsymbol{b}''_{k-1} &= -\Delta^-_{k-1}A_{k-1,k}\boldsymbol{b}_k \\ \boldsymbol{b}''_{k-2} &= -\Delta^-_{k-2}A_{k-2,k-1}\boldsymbol{b}''_{k-1} \\ &\vdots \\ \boldsymbol{b}''_1 &= -\Delta^-_1 A_{1,2}\boldsymbol{b}''_2 \\ \boldsymbol{b}''_m &= -\Delta^-_m A_{m,1}\boldsymbol{b}''_1 \\ &\vdots \\ \boldsymbol{b}''_{k+2} &= -\Delta^-_{k+2}A_{k+2,k+3}\boldsymbol{b}''_{k+3} \\ \boldsymbol{b}''_{k+1} &= -\Delta^-_{k+1}A_{k+1,k+2}\boldsymbol{b}''_{k+2} \end{aligned} \tag{12}$$

and where

$$\Delta_{k+1}^{-}=\frac{1}{A_{k+1,k+1}-E_jI} \qquad \Delta_1^{-}=\frac{1}{A_{1,1}-E_jI-A_{1,m}\Delta_m^{-}A_{m,1}}$$

$$\Delta_i^{-}=\frac{1}{A_{i,i}-E_jI-A_{i,i-1}\Delta_{i-1}^{-}A_{i-1,i}} \qquad i=k+2,\ldots,m,2,3,\ldots k-1.$$

From the above formulations, the $\boldsymbol{b}_i$, $i=k+1,\ldots,m,1,2,\ldots k-1$, can be calculated by equations (11), (12) and (7) after the $\boldsymbol{b}_k$ have been determined by the following method.

From equations (6) and (7) we have

$$A_{k,k-1}(\boldsymbol{b}'_{k-1}+\boldsymbol{b}''_{k-1})+(A_{k,k}-E_jI)\boldsymbol{b}_k+A_{k,k+1}(\boldsymbol{b}'_{k+1}+\boldsymbol{b}''_{k+1})=0. \tag{13}$$

From equations (11) and (12)

$$\begin{aligned}
\boldsymbol{b}'_{k+1}&=-\Delta_{k+1}^{+}A_{k+1,k}\boldsymbol{b}_k\\
\boldsymbol{b}''_{k+1}&=-\Delta_{k+1}^{-}A_{k+1,k+2}\ldots(-1)\Delta_{k-1}^{-}A_{k-1,k}\boldsymbol{b}_k\\
\boldsymbol{b}'_{k-1}&=-\Delta_{k-1}^{+}A_{k-1,k-2}\ldots(-1)\Delta_{k+1}^{+}A_{k+1,k}\boldsymbol{b}_k\\
\boldsymbol{b}''_{k-1}&=-\Delta_{k-1}^{-}A_{k-1,k}b_k.
\end{aligned} \tag{14}$$

Substituting (14) into (13) we obtain

$$C\boldsymbol{b}_k=0$$

or

$$\sum_{j=1}^{n}C_{ij}\boldsymbol{b}_{kj}=0 \qquad i=1,2,\ldots,n \tag{15}$$

where C is an $n\times n$ matrix.

For $b_{kl}\neq 0$ we choose $b_{kl}=1$ and can then obtain the b_{ki}, $i=1,2,\ldots,l-1,\ l+1,\ldots,n$, by solving equation (15) for those $(n-1)$ values of i. The eigenvalues E_j calculated by Dean's method are in error by $\Delta E_j=|E_j-\lambda_j|$ where λ_j is the accurate jth eigenvalue.

If $\Delta E_j=0$ we can choose any values of k and l for the pivoting. If $\Delta E_j\neq 0$ the choice made for the pivoting values of k and l is of central importance in this method. In this case the unsolved equation in (15) $(i=l)$ which is not used to determine the b_{ki}, $i=1,2,\ldots,l-1,\ l+1,\ldots,n$, is not equal to zero

$$\Delta E_{kl}=\left|\sum_{j=1}^{n}C_{lj}b_{kj}\right|\neq 0. \tag{16}$$

The ΔE_{kl} are the indicators of the error in the calculation when k and l are the pivoting values and they depend on those values. Thus the ΔE_{kl} can be used to find the pivoting values and to check the accuracy.

The conclusion is that we should choose the values of k and l so that the error indicator ΔE_{kl} is minimal.

The procedure of this method is summarised as follows.

(i) Calculation of the eigenvalue E_j by the Dean method. The number of real negative eigenvalues can be found by equations (2) and (3).

(ii) Choosing the values at k and l so that the error indicator ΔE_{kl} is minimal.

(iii) Determination of $\boldsymbol{b}_k$ by equation (15).

(iv) Calculation of $\boldsymbol{b}_i$, $i=k+1,\ldots,m,1,\ldots,k-1$, by equations (11), (12) and (7).

3. Example of calculation and discussion

As an example we calculate the eigenvalue and eigenvector of a tight-bonding Hamiltonian with periodic boundary conditions on a plane

$$H = \sum_i t_i |i\rangle\langle i| + \sum_{i \neq j} V_{ij} |i\rangle\langle j| \tag{17}$$

with potential $V_{i,j} = 1$ for first nearest neighbours and $V_{i,j} = 0$ for others, and where t_i are random numbers distributed uniformly in the range $-\frac{1}{2}W < t_i < \frac{1}{2}W$. We choose $W = 1$.

The system can be a one-chain ring system ($n = 1$) or a many-coupled-chains ring system ($n = 2, 5$). We used the standard programs TRED2 and TQL2 and the new program based on the above method. For $N \leqslant 500$ all eigenvalues and eigenvectors have been calculated. The results calculated by the two methods are the same to six significant figures. The CPU times are listed in table 1.

Table 1. CPU time on the VAX computer. For $N = 100$, 200, 500 all eigenvalues and eigenvectors have been calculated. For $N > 500$ only one eigenvalue and eigenvector have been calculated. n is the number of coupled chains.

n	N	TRED2, TQL2	New method
1	100	1 min 24.84 s	30.75 s
1	200	8 min 49.63 s	1 min 21.99 s
1	500	2 h 22 min 18.72 s	9 min 59.39 s
2	100	1 min 26.19 s	3 min 12.63 s
2	200	8 min 44.18 s	10 min 15.51 s
2	500	2 h 31 min 11.47 s	60 min 24.14 s
2	2 000	—	26.05 s
2	20 000	—	6 min 32.82 s
5	5 000	—	12 min 40.44 s

For a one-chain ring system the efficiency of the new method is clearly seen from table 1. For example, for $N = 500$ the new method only took about 10 min of CPU time while the standard programs needed about 2h 22 min.

For a two-coupled-chains ring system when $N \leqslant 200$ the new method is not more efficient than the standard program. But for $N = 500$ the new method only took about 60 min while the standard program took about 2h 31 min. When the number of coupled chains increases the CPU time of this new method increases quickly.

There are two aspects to this. On the one hand, the new method needs to calculate the $\Delta_i^{\pm}$, which involves calculating m times the inverse matrix ($n \times n$) for ring systems. When the number of coupled chains increases the dimension of $\Delta_i^{\pm}$ increases and the calculation of the inverse matrix demands more computer time.

But on the other hand, in the new method all calculations involve only the non-zero elements of the matrix. So when the N increases the CPU time increases slowly. The CPU time of the standard program is proportional to N^3. So when N is large the new method is more efficient than the standard program.

Because the nature of our method it is possible to calculate eigenvalue and eigenvector for a particular state. This method can handle large systems up to $N = 10^4$-10^5.

For $N > 600$, the standard programs cannot be used on a VAX computer but the new method continues to calculate easily. The CPU times are 26.05 s for $n = 2$, $N = 2000$, 6 min 32.82 s for $n = 2$, $N = 20\,000$ and 12 min 40.44 s for $n = 5$, $N = 5000$.

4. Conclusions

A method for calculating the eigenvectors of a many-coupled-chains ring system has been developed. A calculated example demonstrates that this method is accurate, efficient and can be used to handle large systems. The key point of this method is to choose the pivoting value so that the error indicator is minimal. The principle and the formulations of this method can be applied to more general submatrices $A_{i,j}$ that are $ni \times nj$ matrices.

This method has the following advantages.

(i) It is efficient when N is large.

(ii) Its accuracy can be checked easily by the error indicator.

(iii) It can calculate particular states in which we are interested.

By using this method we can undertake amplitude analysis of many-chain ring systems such as, for example, a many-coupled ring system in a magnetic field.

In some disordered systems the statistic distributions have unusual properties. One example is the low frequency AC conductivity [7]. In order to obtain the correct ensemble average value, hundreds of configurations were previously needed. The new method can be used instead.

This method can also be used to study one-dimensional ring systems with many-neighbour interactions.

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References

[1] Fox L 1965 *An Introduction to Numerical Linear Algebra* (Oxford: Oxford University Press)
[2] Dean P 1972 *Rev. Mod. Phys.* **44** 127
[3] Yoshino S and Okazaki M 1976 *Solid State Commun.* **20** 81
[4] Wu S Y and Zheng Z B 1981 *Phys. Rev.* B **24** 4787
[5] Wu S Y, Zheng Z B and Wong J P 1985 *J. China Univ. Sci. Tech.* **15** 150
[6] Zheng Z B 1986 *J. Phys. C: Solid State Phys.* **19** L689
[7] Alber R C and Gubernatis J E 1978 *Phys. Rev.* B **17** 4487