A method of finding the predominant states of an interacting system

1980 J. Phys. A: Math. Gen. 13 2029

(http://iopscience.iop.org/0305-4470/13/6/025)

J. Phys. A: Math. Gen. **13** (1980) 2029–2033. Printed in Great Britain

A method of finding the predominant states of an interacting system

J R Fletcher

Department of Physics, University of Nottingham, University Park, Nottingham NG7 2RD, England

Received 24 August 1979, in final form 19 November 1979

Abstract. A transformation of the representation of an arbitrary Hamiltonian is described such that, for any initial state $|1\rangle$, the matrix elements of $\mathcal{H}$ between the states $|i\rangle (i \geq 1)$ obey the condition $\mathcal{H}_{i,j} = 0$ when $|i-j| > 1$. All the matrix elements are given in terms of $\langle 1|\mathcal{H}^n|1\rangle$. This leads to simplification of complicated interacting systems.

1. Introduction

The aim of the method is to transform the representation of the Hamiltonian $\mathcal{H}$ of a system in such a way that, for any choice of an initial state $|1\rangle$, a hierarchy of new states $|i\rangle (i > 1)$ is generated in which the matrix elements $\mathcal{H}_{ij}$ obey the condition

$$\mathcal{H}_{ij} = 0 \qquad \text{for } |i-j| > 1. \tag{1}$$

This means that the new states are so ordered that the states predominating in the interaction with the initial state are taken in first and those less involved in the interaction are taken in later.

Once the initial state has been chosen, the method gives explicit expressions for the hierarchy of states, without the need for an iterative process. However, if only the eigenvalues of $\mathcal{H}$ are required, only the matrix elements of $\mathcal{H}$ in the new representation are needed. These matrix elements are given in terms of the expectation values of powers of $\mathcal{H}$ within the initial state.

This method of calculation is the analytical analogue of the Lanczos process (Lanczos 1950, Rosser *et al* 1951). The Lanczos process is a numerical method for transforming a matrix into tri-diagonal form. At each step the nth state is related to the previous two states, but not given directly in terms of the initial state. Thus the new states and matrix elements are not given explicitly by the Lanczos process; they are given by an iterative process suitable for numerical calculations.

2. Construction of the orthonormal states

The second state $|2\rangle$ is coupled in first order to the initial state $|1\rangle$ and orthogonal to it. Taking the form

$$|2\rangle = C_{2,1}\mathcal{H}|1\rangle + C_{2,0}|1\rangle$$

0305-4470/80/062029+05$01.50

gives the conditions

$$\langle 1|2\rangle = C_{2,1}E_1 + C_{2,0} = 0$$

and

$$\langle 2|2\rangle = C_{2,1}^2 E_2 + 2C_{2,1}C_{2,0}E_1 + C_{2,0}^2 = 1,$$

where

$$E_n = \langle 1|\mathscr{H}^n|1\rangle.$$

Thus

$$C_{2,1} = (E_2 - E_1^2)^{-1/2}$$

and

$$C_{2,0} = -E_1(E_2 - E_1^2)^{-1/2}.$$

Generalising this for the nth state,

$$|n\rangle = \sum_{r=0}^{n-1} C_{n,r}\mathscr{H}^r|1\rangle \qquad \text{with } C_{n,r} \text{ real.} \tag{2}$$

This state is to be orthogonal to all the previous states. Therefore

$$\langle 1|n\rangle = \sum_{r=0}^{n-1} \langle 1|C_{n,r}\mathscr{H}^r|1\rangle = 0,$$

and therefore

$$\sum_{r=0}^{n-1} C_{n,r}E_r = 0.$$

Also, $\langle 2|n\rangle = 0$, and therefore

$$(\langle 1|C_{2,1}\mathscr{H} + \langle 1|C_{2,0})|n\rangle = 0.$$

So

$$C_{2,1}\langle 1|\mathscr{H}|n\rangle = 0.$$

$C_{2,1}$ is never zero, and

$$\langle 1|\mathscr{H}|n\rangle = \sum_{r=0}^{n-1} C_{n,r}E_{r+1} = 0.$$

Continuing in this way gives the set of equations

$$\sum_{r=0}^{n-1} C_{n,r}E_{r+j} = 0 \qquad \text{for } 0 \leqslant j \leqslant n-2. \tag{3a}$$

Normalisation

$$\langle n|n\rangle = \sum_{p=0}^{n-1} C_{n,p}\langle 1|\mathscr{H}^p|n\rangle = C_{n,n-1}\langle 1|\mathscr{H}^{n-1}|n\rangle = C_{n,n-1}\sum_{r=0}^{n-1} C_{n,r}E_{r+n-1}.$$

Therefore

$$C_{n,n-1}\sum_{r=0}^{n-1} C_{n,r}E_{r+n-1} = 1. \tag{3b}$$

Defining an $n \times n$ matrix M_n with elements $(M_n)_{i,j} = E_{i+j-2}$, and writing $D_n = \det M_n$, equations (3) give

$$|C_{n,n-1}|^2 = (M_n^{-1})_{n,n} = D_{n-1}D_n^{-1}. \tag{4}$$

Choosing the phase of $|n\rangle$ so that $C_{n,n-1}$ is real, all the coefficients of (2) are determined:

$$C_{n,r} = C_{n,n-1}^{-1}(M_n^{-1})_{(r+1),n}. \tag{5}$$

3. Matrix elements of $\mathscr{H}$

In the orthonormal basis constructed above, the general matrix element of $\mathscr{H}$ is given by substituting into (2):

$$\langle n|\mathscr{H}|n+q\rangle = \sum_{p=0}^{n-1} \langle 1|C_{n,p}\mathscr{H}^{p+1} \sum_{r=0}^{n+q-1} C_{n+q,r}\mathscr{H}^r|1\rangle = \sum_{p=0}^{n-1} C_{n,p} \sum_{r=0}^{n+q-1} C_{n+q,r}E_{p+r+1}. \tag{6}$$

From (3*a*) the second summation is zero if $p \leqslant (n+q-3)$ and the matrix element is zero when $q \geqslant 2$. Thus condition (1) is satisfied.

Taking $q = 1$ gives the non-vanishing off-diagonal matrix elements. The only contributions from (6) arise when $p = n-1$, giving

$$\langle n|\mathscr{H}|n+1\rangle = C_{n,n-1} \sum_{r=0}^{n} C_{n+1,r}E_{n+r}.$$

Using equations (3*b*) and (4),

$$\langle n|\mathscr{H}|n+1\rangle = C_{n,n-1}/C_{n+1,n} = (D_{n-1}D_{n+1})^{1/2}D_n^{-1}. \tag{7}$$

For the diagonal elements $q = 0$, and contributions from (6) arise when $p = n-1$ and $n-2$. Therefore

$$\langle n|\mathscr{H}|n\rangle = C_{n,n-1} \sum_{r=0}^{n-1} C_{n,r}E_{n+r} + C_{n,n-2} \sum_{r=0}^{n-1} C_{n,r}E_{n+r-1}$$

$$= C_{n,n-1} \sum_{r=0}^{n-1} C_{n,r}E_{n+r} + C_{n,n-2}C_{n,n-1}^{-1},$$

using equation (3*b*)

$$= \sum_{r=0}^{n-1} (M_n^{-1})_{(r+1),n}E_{n+r} + (M_n^{-1})_{n-1,n}C_{n,n-1}^{-2},$$

using equation (5)

$$= F_nD_n^{-1} - F_{n-1}D_{n-1}^{-1}, \tag{8}$$

where $F_n = \det W_n$ and W_n is an $n \times n$ matrix having elements

$$(W_n)_{i,j} = \begin{pmatrix} E_{(i+j-2)} & 1 \leqslant j < n \\ E_{(i+j-1)} & j = n \end{pmatrix} 1 \leqslant i \leqslant n.$$

4. Completeness

The above procedures appear at first sight to be capable of generating an infinite sequence of states and matrix elements, whatever the Hamiltonian and initial state may be. This is clearly inappropriate if the Hamiltonian only operates within a finite set of states. The escape from this apparent contradiction follows from the following considerations. Suppose that $\mathcal{H}$ operates within a Hilbert space of dimension g. Then $\mathcal{H}$ can have at most g distinct eigenvalues. Only the first g expectation values of $\mathcal{H}^n$ can be independent, and E_n for $n \geqslant g$ is a linear combination of the values of E_n for $0 \leqslant n < g$.

It follows for $n > g$ that the columns of the matrices M_n and W_n are not independent and their determinants D_n and F_n vanish. From equation (8) the diagonal matrix elements are indeterminate for the spurious states with $n > g$, but from equation (7) $\langle g|\mathcal{H}|g+1\rangle$ vanishes and the spurious states are not coupled to the physical states. The spurious states can be ignored, and from the way in which the first g states have been constructed they give an equivalent representation of the Hamiltonian. No approximation is involved.

5. Example

In the following paper (Fletcher *et al* 1980) the method is applied to the Jahn–Teller interaction, but in order to illustrate the features of the method consider the following system. For spin $S = 1$ and Hamiltonian

$$\mathcal{H} = \lambda S_x$$

take initial state

$$|1\rangle = |M_S = 0\rangle.$$

Firstly we evaluate

$$E_n = \langle M_S = 0|\mathcal{H}^n|M_S = 0\rangle.$$

By time reversal $E_{2n+1} = 0$ and

$$\begin{aligned} E_{2n} &= (\lambda/2)^{2n}\langle M_S = 0|(S_+ + S_-)^{2n}|M_S = 0\rangle \\ &= (\lambda/2)^{2n}[\langle M_S = 0|(S_+ + S_-)^2|M_S = 0\rangle]^n \\ &= \lambda^{2n}. \end{aligned}$$

Thus

$$\begin{aligned} &D_0 = D_1 = 1, && D_2 = \lambda^2, \\ &D_n = 0 && n > 2, \\ &F_n = 0 && n \geqslant 0. \end{aligned}$$

Using equations (7) and (8) these values give a 2×2 matrix:

$$\mathcal{H} = \begin{pmatrix} 0 & \lambda \\ \lambda & 0 \end{pmatrix}.$$

The eigenvalues are $+\lambda$ and $-\lambda$ as expected for the two states $|S_x = \pm 1\rangle$. The third state from $S = 1$ is $|S_x = 0\rangle$, having energy zero. This state has been omitted by the procedure as the Hamiltonian does not couple $|S_x = 0\rangle$ to the initial state $|S_z = 0\rangle$. It is characteristic of this method that it only generates states that are coupled by the Hamiltonian to the initial state, and all other states are omitted. It is this feature which leads to useful simplifications in complicated interacting systems such as the defect–phonon interaction.

6. Conclusion

A prescription is given for finding a representation of any Hamiltonian in which only the matrix elements on the diagonal or adjacent to it are non-zero. The uses of this transformation apear to be as follows:

(*a*) This form of matrix is convenient for the numerical calculation of eigenvalues.

(*b*) If the initial state is an approximate eigenstate of the Hamiltonian, e.g. a variational state, the application of this method will give an improved energy and wavefunction without the necessity of explicitly constructing a complete orthonormal set containing the initial state.

(*c*) A complicated Hamiltonian is transformed into a simpler form which may be already familiar. This is the case in the following paper (Fletcher *et al* 1980) where the method is applied to the Jahn–Teller interaction.

(*d*) In a complicated interacting system the initial state may be directly coupled to a large number of states, each of which is again coupled to a large number of states, etc. The procedure replaces this by a simpler system in which each state is only coupled to the immediately preceding and following single states.

References

Fletcher J R, O'Brien M C M and Evangelou S N 1980 *J. Phys. A: Math. Gen.* **13**
Lanczos C 1950 *J. Res. NBS* **45** 255–82
Rosser J B, Lanczos C, Hestenes M R and Karush W 1951 *J. Res. NBS* **47** 291–7