The Lanczos representation for the density of states

1991 J. Phys. A: Math. Gen. 24 L719

(http://iopscience.iop.org/0305-4470/24/13/003)

J. Phys. A: Math. Gen. 24 (1991) L719–L720. Printed in the UK

LETTER TO THE EDITOR

The Lanczos representation for the density of states

J R Fletcher

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

Received 12 April 1991, in final form 17 May 1991

Abstract. It is shown that the previously described reduction process for tridiagonal matrix elements can be used for calculation of the density of states of a system for which the traces of powers of the Hamiltonian are known. The result is particularly simple for a system of spins.

The Lanczos procedure generates a representation of a quantum system in which the matrix of the Hamiltonian operator is tridiagonal. The form of the representation is dependent on a choice of an initial state, and in the case of systems with symmetry, states differing in symmetry from the initial state are omitted from the Lanczos representation. The purpose of this letter is to show that there is a similar representation for the total density of states of a system with bounded energy, that does not depend on an arbitrary choice of initial state.

Define the normalized density of states for a system with D states by

$$\rho(E) = D^{-1} \sum_{i=1}^{D} \delta(E - E_i)$$

and the moments of the Hamiltonian by

$$\mu_{p,o} = \int E^p \rho(E)\, dE = D^{-1} \operatorname{tr} H^p. \tag{1}$$

We now introduce a set of states $|n\rangle$ ($n \geq 1$) in which the Lanczos operator L takes the tridiagonal form. The moments of L within the first state, $|1\rangle$ are to be equal to the moments of the Hamiltonian, i.e.

$$\mu_{p,o} = \langle 1|L^p|1\rangle.$$

The matrix elements of L in this basis can be found by the reduction process previously described (Fletcher 1991). L can always be chosen to be Hermitian, and its eigenstates form a complete set within the basis $|n\rangle$.

Let $|\lambda j\rangle$ be an eigenstate of L with eigenvalue λ_j. Therefore

$$\begin{aligned}\mu_{p,o} &= \sum_{j,k} \langle 1|\lambda j\rangle\langle \lambda j|L^p|\lambda k\rangle\langle \lambda k|1\rangle \\ &= \sum_j \lambda_j^p |\langle 1|\lambda j\rangle|^2. \end{aligned} \tag{2}$$

Comparing (1) and (2) gives

$$\rho(E) = \sum_j |\langle 1|\lambda j\rangle|^2 \delta(E - \lambda_j). \tag{3}$$

0305-4470/91/130719+02$03.50

Thus diagonalizing the Lanczos matrix may give a useful route to the density of states. The potential advantage of this process is that the order of the Lanczos matrix is equal to the number of energy levels of the system, and may be much less than the number of states, as in the following example.

As an illustrative example, consider a collection of N non-interacting spins, $S=\frac{1}{2}$ in an external magnetic field, with Hamiltonian

$$H=2W\sum_{i=1}^{N} S_z^{(i)}.$$

It is straightforward to calculate the non-vanishing even moments, and thus find the irreducible moments

$$u_{2p}=\frac{p!N!}{(N-p)!}W^{2p}.$$

Thus the diagonal elements of L vanish and

$$L_{n,n+1}=W\sqrt{n(N-n+1)} \qquad \text{for } 1\leqslant n\leqslant N+1.$$

The order of the Lanczos matrix is $N+1$. This suggests the introduction of a fictitious spin $\hat{S}=N/2$. Identifying the state $|p\rangle$ with the fictitious spin state with $M_s=p-N/2-1$, we find the simple form

$$L=2W\hat{S}_x.$$

The eigenvalues of L are $2WM$ with $-N/2\leqslant M\leqslant N/2$.

The matrix element required in (3) for the density of states is $|\langle\hat{S}_z=\frac{1}{2}N|\hat{S}_x=M\rangle|^2$. Manipulating the spin states brings this into the form $2^{-N}C_{(N/2-M)}$. Thus the density of states takes the expected form

$$\rho(E)=2^{-N}\sum_{j=o}^{N} NC_j\delta(E-WN+2Wj).$$

Reference

Fletcher J R 1991 *J. Phys. A: Math. Gen.* **24** L7-9