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LETTER TO THE EDITOR

The method of moments and the Lanczos representation

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Abstract. Given the moments of the Hamiltonian of a system, the problem is to find a prescription for the matrix elements in the tridiagonal Lanczos representation in a form suitable for numerical calculation. In this letter a sequence of reductions of the moments is described, whereby the redundant information contained in the higher moments is progressively removed, leading to a numerically stable algorithm for the Lanczos matrix elements.

For an arbitrary initial state $|1\rangle$, we define the moments of the Hamiltonian of a system by

$$\mu_{n,0} = \langle 1|H^n|1\rangle .$$

The Lanczos process (Lanczos 1950) generates the states of the tridiagonal Lanczos representation, $|n\rangle$ $(n \geq 1)$ where $H = L_0 + L_+ + L_-$ such that the only non-zero matrix elements are

$$\langle n|L_0|n\rangle = L_{n,n}$$
$$\langle n+1|L_+|n\rangle = L_{n+1,n}$$
$$\langle n|L_-|n+1\rangle = L_{n,n+1} .$$

Working in the Lanczos representation it is convenient to describe the contributions to the moments in terms of diagrams

e.g. $\mu_{2,0} = \langle L_- L_+\rangle_1 + \langle L_0^2\rangle_1$  + 

where sloping lines represent matrix elements of L_+, L_-, and horizontal lines L_0.

The problem of writing the Lanczos matrix elements in terms of the moments $\mu_{n,0}$ has been solved in terms of determinants (Akhiezer 1965, Whitehead and Watt 1978, Fletcher 1980), but these determinants are unsuitable for numerical computation as they involve taking differences of rapidly increasing numbers. This difficulty arises because the high-order moments contain many contributions involving repetitions of lower-order terms. In this letter we devise a sequence of reductions to progressively remove the repetitions, ultimately leading to the irreducible moments, u_n, where

$$u_{2n} = \langle L_-^n L_+^n\rangle_1$$
$$u_{2n+1} = \langle L_-^n L_0 L_+^n\rangle_1 .$$

The Lanczos matrix elements are given by

$$L_{n,n} = u_{2n-1} u_{2n-2}^{-1}$$
$$|L_{n,n+1}|^2 = u_{2n} u_{2n-2}^{-1} .$$

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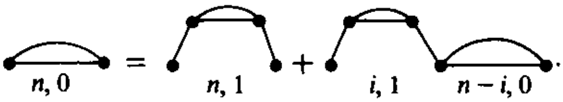
The first reduced moments, $\mu_{n,1}$, involve no intermediate returns to state $|1\rangle$. Thus, moments involving intermediate returns to $|1\rangle$ can be factorized into two parts, the first factor being $\mu_{i,1}$, therefore

$$\mu_{n,0} = \mu_{n,1} + \sum_{i=1}^{n-1} \mu_{i,1}\mu_{n-i,0} \qquad \text{for } n > 1$$

$$\mu_{1,0} = \mu_{1,1}$$

or diagrammatically

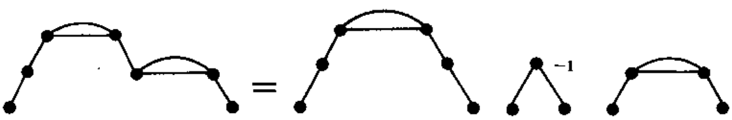


The first reduced moments can then be found by the sequence of equations

$$\mu_{n,1} = \mu_{n,0} - \sum_{i=1}^{n-1} \mu_{i,1}\mu_{n-i,0} \qquad \text{for } n > 1.$$

This first reduction was given by Whitehead and Watt who pointed out that it was of little help in numerical calculation. We now show that this reduction can be repeated indefinitely, leading to the irreducible moments u_n.

The second reduced moments, $\mu_{n,2}$, involve no intermediate returns to state $|2\rangle$. The contributions to the first reduced moment involving intermediate returns to state $|2\rangle$ can be factorized by introducing a factor u_2^{-1}.



$$= \mu_{i,2}u_2^{-1}\mu_{j,1}.$$

Thus we can write

$$\mu_{n,1} = \mu_{n,2} + \sum_{i=3}^{n-1} \mu_{i,2}u_2^{-1}\mu_{n-i+2,1} \qquad \text{for } n > 3$$

and

$$\mu_{n,1} = \mu_{n,2} \qquad \text{for } n < 4.$$

The second reduced moments are given by

$$\mu_{n,2} = \mu_{n,1} - u_2^{-1} \sum_{i=3}^{n-1} \mu_{i,2}\mu_{n-i+2,1} \qquad \text{for } n > 3.$$

The process can be repeated as often as necessary, giving the pth reduced moments in terms of the $(p-1)$th by the general equations

$$\mu_{n,p} = \mu_{n,p-1} - u_{2p-2}^{-1} \sum_{i=2p-1}^{n-1} \mu_{i,p}\mu_{(n-i+2p-2)(p-1)} \qquad \text{for } n > 2p-1$$

and

$$\mu_{n,p} = \mu_{n,p-1} \qquad \text{for } n < 2p.$$

Inspection shows that $\mu_{n,p}$ is irreducible in $n \leqslant 2p+1$ and hence

$$\mu_{n,p} = u_n \qquad \text{if} \qquad n \leqslant (2p+1).$$

Thus the irreducible moments and the Lanczos matrix elements can be found by the successive reduction of the moments. If the first m moments are known, the first m matrix elements can be calculated by not more than $m/2$ reductions.

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