Aust. J. Phys., 1992, **45**, 717–24

Hamiltonian Moments and the Lanczos Method in the Heisenberg Model

Lloyd C. L. Hollenberg and Christopher J. Griffin

Research Centre for High Energy Physics, School of Physics, University of Melbourne, Parkville, Vic. 3052, Australia.

Abstract

The connected Hamiltonian moments $\langle H^n \rangle_c$ of the one-dimensional $s = \frac{1}{2}$ Heisenberg model with respect to the Néel state are calculated up to $n = 17$. Subsequent calculation of the Hamiltonian moments $\langle H^n \rangle$ allows the first nine iterations of the Lanczos diagonalisation to be determined analytically for arbitrary lattice size.

1. Introduction

Given the recent renewed interest in the Hamiltonian formalism of field theories, in particular the light-cone Hamiltonian approach (Pauli and Brodsky 1985*a*, 1985*b*), it is timely to review and study methods of calculating energy eigenvalues for large systems. Traditionally the Lanczos method for tri-diagonalisation of matrices has been used extensively in the numerical diagonalisation of Hamiltonian systems with a large number of degrees of freedom (Lanczos 1950). The particular suitability of the Lanczos method for such problems is due to the fast convergence to the first few eigenvalues and only linear computer memory requirements. Typically, the lowest eigenvalues can be obtained *precisely* for basis sizes of the order 10^6 or more, depending on the character of the matrix being studied.

In these numerical applications of the Lanczos method, the limitation of the size of the basis which can be handled is the storage of at least two vectors at each iteration. Once the storage requirement has been met any number of Lanczos iterations can in principle be carried out, thereby giving precise values for the desired eigenvalues. In some instances it might be desirable to sacrifice the accuracy of the eigenvalues one obtains from the Lanczos method for a gain in the number of degrees of freedom of the system under consideration.

One can limit the number of Lanczos iterations (i.e. the accuracy of the eigenvalues) and work in an arbitrarily large basis by applying the Lanczos method directly to the operator form of the Hamiltonian, thereby avoiding the Hamiltonian matrix representation altogether. This method has been used in both solid state (Mancinia and Mattis 1983, 1984, 1985) and field theory (Duncan and Roskies 1985; Duncan 1985; Choe *et al.* 1988) contexts.

The Lanczos tri-diagonal matrix representation is constructed from the Hamiltonian by calculation of Hamiltonian moments, $\langle H^n \rangle$, with respect to some suitably chosen trial state. The major advantage of this approach is that

0004-9506/92/060717$05.00

expressions for a sufficient number of moments may be calculated, thereby giving the first few Lanczos iterations analytically for arbitrary basis size. Also, it is quite possible that some insight may be gained by the analytic form of the truncated Lanczos tri-diagonal matrix.

As a clear illustration of the method we present the application of the Lanczos approach in operator form to the one-dimensional $s = \frac{1}{2}$ Heisenberg model for which exact results have been obtained for lattices with up to $N = 28$ sites (Medeiros and Cabrera 1991) and the infinite lattice energy density is known analytically. The bulk of the work involves the calculation of the connected Hamiltonian moments $\langle H^n \rangle_c$ for this model; we have computed $\langle H^n \rangle_c$ up to $n = 17$. These quantities may at some stage also prove useful when using the Heisenberg model as a test of similar analytical techniques. Expressions for $\langle H^n \rangle$, $n \leq 17$, can be derived recursively from the connected moments which subsequently give the first nine Lanczos iterations with respect to the Néel state for arbitrarily large lattices.

This paper is organised as follows. In Section 2 the analytic application of the Lanczos method is outlined. The Heisenberg model is introduced in Section 3 together with the calculation of the Hamiltonian moments, $\langle H^n \rangle$, and the results obtained for the corresponding Lanczos iterations on various lattices are given in Section 4.

2. The Lanczos Method

To find the first few states of a Hamiltonian, H, using the Lanczos procedure one starts with a normalised state $|v_1\rangle$, which is arbitrary up to the condition that it has a nonzero overlap with the true ground state. The Hamiltonian is cast into tri-diagonal form by the following construction:

$$\begin{aligned} H|v_1\rangle &= \alpha_1|v_1\rangle + \beta_1|v_2\rangle, \\ H|v_2\rangle &= \beta_1|v_1\rangle + \alpha_2|v_2\rangle + \beta_2|v_3\rangle, \\ H|v_3\rangle &= \beta_2|v_2\rangle + \alpha_3|v_3\rangle + \beta_3|v_4\rangle, \qquad \text{etc.}, \end{aligned} \tag{1}$$

where the $|v_i\rangle$ are orthonormal and the α_i and β_i are thus given by

$$\alpha_i = \langle v_i | H | v_i \rangle, \qquad \beta_i = \langle v_{i+1} | H | v_i \rangle. \tag{2}$$

In the basis $\{|v_i\rangle\}$, H is tri-diagonal due to hermiticity; i.e.

$$H \rightarrow \mathbf{H} = \begin{pmatrix} \alpha_1 & \beta_1 & & & & & \\ \beta_1 & \alpha_2 & \beta_2 & & & & \\ & \beta_2 & \alpha_3 & & \beta_3 & & \\ & & \ddots & & \ddots & & \ddots \\ & & & \ddots & & \ddots & \end{pmatrix}. \tag{3}$$

The remarkable feature of the Lanczos construction is that the eigenvalues of the upper left $p \times p$ submatrix of $\mathbf{H}$ rapidly converge to those of H—the lowest eigenvalues converging first. Hence, in order to find the lowest eigenvalues one need not complete the full construction of the tri-diagonal basis $\{|v_i\rangle\}$, instead one can terminate the construction at a point where convergence in the required eigenvalues has been reached.

In the application of the Lanczos procedure to matrix diagonalisations one usually stores the vectors $|v_i\rangle$ and $|v_{i-1}\rangle$ at the ith iteration and computes the corresponding values of α_i and β_{i-1}. However, rather than realise the basis $\{|v_i\rangle\}$ one can compute the α_i and β_i directly from Hamiltonian moments with respect to the state $|v_1\rangle$. For example, the 2×2 submatrix of $\mathbf{H}$ (the second iteration) is given in terms of Hamiltonian moments as

$$\begin{aligned} \alpha_1 &= \langle H \rangle , \\ \beta_1 &= [\langle H^2 \rangle - \langle H \rangle^2]^{1/2} , \\ \alpha_2 &= \frac{\langle H^3 \rangle - 2\langle H \rangle \langle H^2 \rangle + \langle H \rangle^3}{\langle H^2 \rangle - \langle H \rangle^2} , \end{aligned} \tag{4}$$

where $\langle H^n \rangle \equiv \langle v_1 | H^n | v_1 \rangle$. Therefore, in casting the Hamiltonian into tri-diagonal form, the limits on basis size associated with the construction of the basis $\{|v_i\rangle\}$ can be avoided by computing moments with respect to some trial state $|v_1\rangle$. For well behaved Hamiltonians of finite systems the moments are given by analytic functions of the number of degrees of freedom. One can obtain expressions for the elements of the tri-diagonal representation of H which can then be computed for any number of degrees of freedom. Thus, calculating Hamiltonian moments up to a certain order on a small system yields the corresponding information for larger systems.

In practice, since Hamiltonian moments are in general difficult to calculate beyond the lowest orders, one selects $|v_1\rangle$ so that convergence is optimised. To

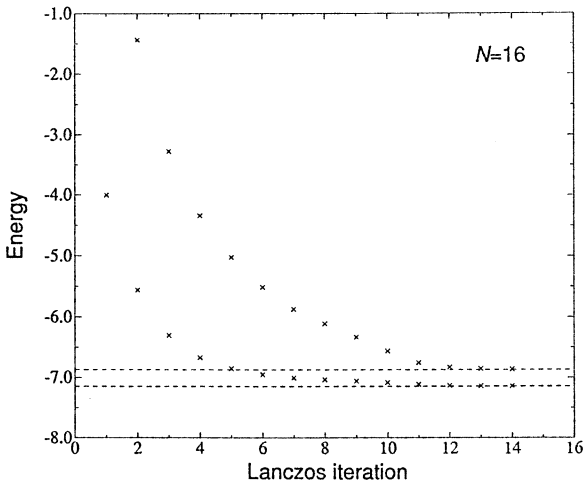

Fig. 1. Convergence of the ground and first excited states for $N = 16$ with the Néel state as the trial state. The exact values of the ground and first excited states are shown as dashed lines. Hamiltonian moments were computed numerically.

obtain the lth Lanczos iteration one requires $\langle H^n \rangle$ up to $n = 2l-1$. Convergence can be further improved by combining the Lanczos method with a variational approach by choosing a trial state with adjustable parameters (Dagotto and Moreo 1985).

In this paper we study the convergence properties of this method by applying it to the case of the one-dimensional Heisenberg antiferromagnetic spin chain for $s = \frac{1}{2}$. We sacrifice the accuracy of the spectrum of this model by restricting the size of the Lanczos submatrix to 9×9 and find upper bounds on the ground state and first excited state of systems whose matrix representation is too large to handle by conventional means.

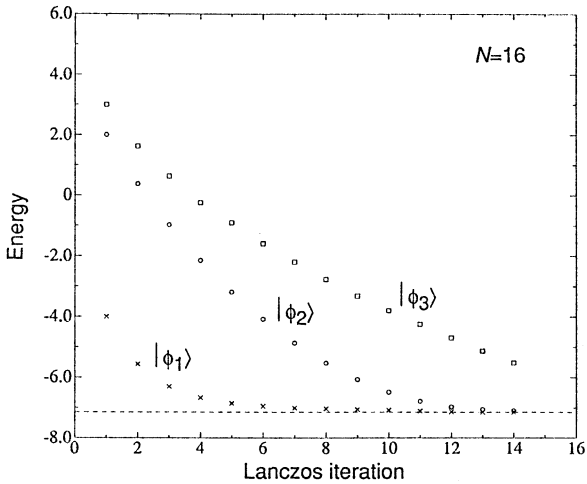

Fig. 2. Convergence of the ground-state energy ($N = 16$) for various trial states used in the Lanczos procedure. The curves correspond to the trial states $|\phi_1\rangle = |\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\rangle$ (Néel state), $|\phi_2\rangle = |\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\rangle$ and $|\phi_3\rangle = |\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\rangle$. Hamiltonian moments were computed numerically.

3. The Heisenberg Model

The Hamiltonian for the Heisenberg model is defined on a chain of N spins as

$$H = \sum_{i=1}^{N} \vec{S}(i) \cdot \vec{S}(i+1), \tag{5}$$

where $\vec{S}(i)$ is the spin operator at the lattice site i and we assume periodic boundary conditions. In the infinite lattice limit the ground-state energy density E_0/N is determined from the Bethe ansatz to be

$$\lim_{N\to\infty} \frac{E_0}{N} = -\ln 2 + \tfrac{1}{4} \approx -0{\cdot}443147. \tag{6}$$

A suitable choice for the trial state with respect to which we compute Hamiltonian moments is the Néel state

$$|\phi_{\text{Néel}}\rangle \equiv |\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\cdots\rangle. \tag{7}$$

On a relatively small lattice one can generate large orders of $\langle H^n \rangle$ on a computer. As an illustration we have performed the computations to large order for $N = 16$ and in Fig. 1 we present the results, using the Néel state as the trial state. Of course for $N = 16$ the actual Hamiltonian matrix can be diagonalised exactly since the basis size is only 65536. The importance of the choice of trial state is shown in Fig. 2 where various trial states have been used.

For small orders ($n \lesssim 4$) expressions for $\langle H^n \rangle$ with respect to the Néel state can be derived by hand. One finds in general that $\langle H^n \rangle$ is simply a polynomial in the number of lattice sites. To evaluate the moments for larger orders we compute $\langle H^n \rangle$ for the Néel state directly on specific lattices ($N > n$). Rather than calculate the polynomial for $\langle H^n \rangle$ it is considerably easier to calculate the *connected* Hamiltonian moments $\langle H^n \rangle_c$ which are related to the $\langle H^n \rangle$ by (Horn and Weinstein 1984)

$$\langle H^n \rangle_c = \langle H^n \rangle - \sum_{p=0}^{n-2} \binom{n-1}{p} \langle H^{p+1} \rangle_c \langle H^{n-1-p} \rangle \,. \tag{8}$$

The connected moments are proportional to the volume

$$\langle H^n \rangle_c \equiv c_n N \,, \tag{9}$$

and so on a given lattice one is able to calculate all c_n up to $n = N-1$ (c_N will suffer from boundary effects).

Table 1. Connected moments of the Heisenberg model, $\langle H^n \rangle_c \equiv c_n N$, up to $n = 17$

n	c_n	n	c_n	n	c_n
1	$-\frac{1}{4}$	7	$\frac{105}{8}$	13	$\frac{13808933}{8}$
2	$\frac{1}{4}$	8	$\frac{1583}{16}$	14	$\frac{86136239}{16}$
3	$\frac{1}{4}$	9	$\frac{85}{2}$	15	$-\frac{1946437647}{16}$
4	$-\frac{1}{8}$	10	-3313	16	$-\frac{48648668001}{32}$
5	$-\frac{3}{2}$	11	$-\frac{75049}{4}$	17	$\frac{4956065233}{2}$
6	$-\frac{21}{8}$	12	$\frac{1238205}{16}$		

We have in this manner calculated the connected Hamiltonian moments for the Heisenberg model up to $n = 17$; the values of c_n are given in Table 1. The corresponding expressions for the first few Hamiltonian moments with respect to the Néel state are

$$\begin{aligned}
\langle H \rangle &= -\tfrac{1}{4}N \,, \\
\langle H^2 \rangle &= (\tfrac{1}{4})^2(N^2 + 4N) \,, \\
\langle H^3 \rangle &= -(\tfrac{1}{4})^3(N^3 + 12N^3 - 16N) \,, \\
\langle H^4 \rangle &= (\tfrac{1}{4})^4(N^4 + 24N^3 - 16N^2 - 32N) \,, \\
\langle H^5 \rangle &= -(\tfrac{1}{4})^5(N^5 + 40N^4 + 80N^3 - 800N^2 + 1536N) \,,
\end{aligned}$$

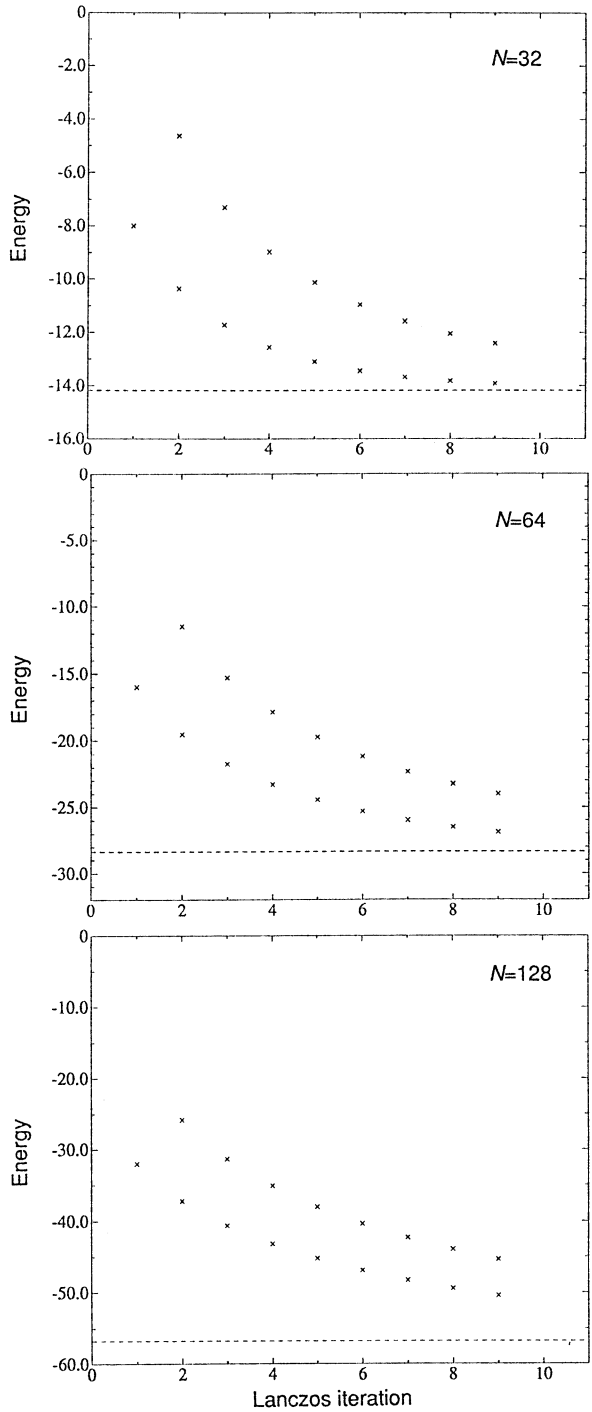

Fig. 3. Ground and first excited states from nine Lanczos iterations with respect to the Néel state using the $\langle H^n \rangle$ polynomials up to $n = 17$, for $N = 32$, $N = 64$ and $N = 128$. The dashed line in each case corresponds to the infinite lattice result for the ground-state energy.

$$\begin{aligned}
\langle H^6\rangle &= (\tfrac{1}{4})^6(N^6+60N^5+400N^4-3360N^3+9856N^2-10752N)\,,\\
\langle H^7\rangle &= -(\tfrac{1}{4})^7(N^7+84N^6+1120N^5-7840N^4+9856N^3+71680N^2\\
&\qquad -215040N)\,,\\
\langle H^8\rangle &= (\tfrac{1}{4})^8(N^8+112N^7+2464N^6-11200N^5-84224N^4+1053696N^3\\
&\qquad -4264960N^2+6483968N)\,,
\end{aligned} \tag{10}$$

leading to the following analytic expressions for α_i and β_i:

$$\begin{aligned}
\alpha_1(N) &= -\frac{N}{4}\,,\\
\alpha_2(N) &= -\frac{N}{4}+1\,,\\
\alpha_3(N) &= -\frac{N^2-11N+32}{4(N-3)}\,,\\
\alpha_4(N) &= -\frac{3N^5-81N^4+871N^3-4443N^2+10498N-9064}{4(3N^3-36N^2+151N-226)(N-3)}\,,\\
\beta_1(N) &= \tfrac{1}{2}\sqrt{N}\,,\\
\beta_2(N) &= \tfrac{1}{2}\sqrt{2(N-3)}\,,\\
\beta_3(N) &= \tfrac{1}{2}\frac{\sqrt{3N^3-36N^2+151N-226}}{N-3}\,, \qquad \cdots \text{etc.}
\end{aligned} \tag{11}$$

4. Results

Expressions for $\langle H^n\rangle$ up to $n=17$ enable us to compute the first nine Lanczos iterations, with respect to the Néel state, for *any* lattice size $N>18$. Of course, as N gets large the convergence properties become increasingly worse. However, one can still achieve reasonable accuracy for large lattices which are beyond any direct matrix diagonalisation (the number of basis states is 2^N). In Fig. 3 we have plotted the convergence of the lowest two states for $N=32$, $N=64$ and $N=128$. For $N \gtrsim 32$ the ground-state energy of the Heisenberg model is known to be very close to the infinite lattice result and hence one can use this fact as a guide to how close the ninth order Lanczos iteration is to the true result. For the lattices $N=32$, 64 and 128 the ninth order Lanczos iteration is within about 2%, 6% and 11% respectively of the infinite lattice result. One would hope that this level of accuracy would persist for other physically relevant Hamiltonians cast into this form.

Acknowledgments

The authors thank N. Witte for helpful discussions. This project was supported by the ARC Small Grants Scheme. CJG acknowledges the support of the A. O. Cappell scholarship.

References

Choe, J. W., Duncan, A., and Roskies, R. (1988). *Phys. Rev.* D **37**, 427.
Dagotto, E., and Moreo, A. (1985). *Phys. Rev.* D **31**, 865.
Duncan, A. (1985). *Nucl. Phys.* B **258**, 125.
Duncan, A., and Roskies, R. (1985). *Phys. Rev.* D **31**, 364.
Horn, D., and Weinstein, M. (1984). *Phys. Rev.* D **30**, 1256.
Lanczos, C. (1950). *J. Res. Natl Bur. Stand.* **45**, 255.
Mancini, J. D., and Mattis, D. C. (1983). *Phys. Rev.* B **28**, 6061.
Mancini, J. D., and Mattis, D. C. (1984). *Phys. Rev.* B **29**, 6988.
Mancini, J. D., and Mattis, D. C. (1985). *Phys. Rev.* B **31**, 7440.
Medeiros, D., and Cabrera, G. G. (1991). *Phys. Rev.* B **43**, 3703.
Pauli, H. C., and Brodsky, S. J. (1985*a*). *Phys. Rev.* D **32**, 1993.
Pauli, H. C., and Brodsky, S. J. (1985*b*). *Phys. Rev.* D **32**, 2001.

Manuscript received 10 June, accepted 10 November 1992