Lanczos calculation for the $s=\frac{1}{2}$ antiferromagnetic Heisenberg chain up to $N=28$ spins

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Highly precise numerical calculations using a variation of the Lanczos method devised by Paige were performed for $s=\frac{1}{2}$ antiferromagnetic Heisenberg finite chains up to sizes $N=28$. Several interesting physical quantities, including the ground-state energy, the mass gap, and the spin-wave velocity, were computed and fitted for logarithmic finite-size corrections, as suggested by conformal invariance and Bethe ansatz calculations. A crossover size for a maximum of the spin-wave velocity is predicted for $N\sim 50$, well above the current available sizes in a typical Lanczos simulation. A list of our numerical results is given along with extrapolated values using standard algorithms.

The antiferromagnetic Heisenberg chain for spin $s=\frac{1}{2}$, in spite of being exactly solvable through the Bethe ansatz,[1] continues to be extensively studied by numerical calculations,[2] mainly due to the intricate character of the exact solution. Concerning finite-size effects, even Bethe ansatz methods must recur to numerical computations to test analytic asymptotic behavior for large systems.[3,4] In the whole critical region of the anisotropic XXZ model, finite-size corrections to the bulk behavior can be obtained by using the predictions of the conformal group.[5,6] At the Heisenberg point (isotropic case) both of the above methods yield logarithmic corrections to power-law dependence with size. This logarithmic behavior has an extremely slow convergence, and numerical finite-size scaling methods appear at first sight as hopeless for extrapolating the thermodynamic limit.

In this paper we would like to present new numerical exact results for finite chains for sizes not yet reported in the literature, $N=28$ being the largest size available in our calculation. In spite of the *scenario* described above, we will also show that some logarithmic corrections can be correctly accounted for in the cases treated here, including the ground-state energy, the scaled mass gap, and the spin-wave velocity.[7] This latter case is the most interesting, since previous reported data[8] (up to 18 spins in the chain) show a monotonic increase over the known exact result for the infinite system.[9] A crossover size to yield the correct limit is expected well above the size available in numerical simulations. In this contribution we make predictions for the value of this characteristic size. The Hamiltonian used in our calculation is

$$H=J\sum_m [S_x(m)S_x(m+1)+S_y(m)S_y(m+1) +S_z(m)S_z(m+1)] , \quad (1)$$

where $J>0$, and S_x, S_y, and S_z are the usual spin operators for $s=1/2$. In (1) we have assumed periodic boundary conditions. Only even values of N have been calculated to avoid frustration at the chain boundaries.

Our computer work was based on the Lanczos[10] method, using a powerful variant introduced by Paige.[11] This efficient algorithm does not require reorthogonalization of vectors at every step of the computation. Moreover, since only two vectors are stored in the iteration process, less memory is needed and larger sizes can be reached. It has also been shown by Paige that numerical accuracy is better when compared to standard Lanczos calculations and good convergence can be achieved even for very close eigenvalues.

Time inversion symmetry implies that the ground and first excited states are, respectively, symmetric and antisymmetric if $N/2$ is even and conversely if it is odd.[12] This type of symmetry can be implemented in a computer to save memory, since, for translational invariants, only one representative state is stored for computation. The *hashing* technique[13] has also been used to process a large number of states. This type of consideration allows one to calculate sizes of the order of $N=28$ in a VAX 11/785 with standard Fortran double precision for the ground and first excited levels. Concerning the spin-wave velocity, we have used the Lanczos method to determine the smallest energy for a state of momentum $p=2\pi/N$ in the manifold of $S_z=1$ without specifying the full symmetry, thus limiting our calculation to the maximum size of $N=22$ for this case.

In Table I we display the exact numerical values obtained through the Lanczos process with a convergence precision of the order of 10^{-14}. Extrapolated values using the Vanden Broeck-Schwartz (VBS) algorithm[14] are also shown, together with the known exact analytic results for the infinite system.[1,9,15] It is worth mentioning that the extrapolated value for the ground-state energy coincides with the exact value within seven figures. The other quantities, due to stronger logarithmic corrections, extrapolate to values which differ within 5% from the exact results. A different procedure must be adopted in this case for efficient extrapolation. We have fitted our numerical results for small systems requiring that the exact value for the infinite system must be reached.

Several least-squares fits were attempted for logarithmic corrections as functions of size. Some of these were suggested by Bethe ansatz solutions[4] and conformal-invariance arguments.[5] We would like to note that the

TABLE I. Values for the ground-state energy *per spin* $E^{(0)}(N)$, the scaled mass gap $G(N)=N^2[E^{(1)}(N)-E^{(0)}(N)]$, and the spin-wave velocity $V(N)=N^2[E^{(p)}(N)-E^{(0)}(N)]/2\pi$ for various values of size N. High-precision calculations were done up to 14 significant figures. For space reasons, we only display our results with the first 7 figures (complete results will be given by the authors upon request). Extrapolated values obtained using the VBS algorithm (Ref. 14) are compared with known analytical results for the infinite limit, i.e., $E^{(0)}(\infty)=-\ln 2+\frac{1}{4}$ (Ref. 1), $G(\infty)=\pi^2/2$ (Ref. 15), and $V(\infty)=\pi/2$ (Ref. 9).

N	$-E^{(0)}(N)$	$G(N)$	$V(N)$
4	0.500 000 0	4.000 000 0	1.273 239 5
6	0.467 129 3	4.108 449 6	1.453 402 4
8	0.456 386 7	4.181 395 2	1.518 153 7
10	0.451 544 6	4.232 390 0	1.547 251 2
12	0.448 949 2	4.270 161 6	1.562 295 5
14	0.447 396 4	4.299 475 6	1.570 829 8
16	0.446 393 5	4.323 020 8	1.575 987 8
18	0.445 708 3	4.342 507 2	1.579 251 9
20	0.445 219 3	4.358 920 0	1.581 377 9
22	0.444 858 2	4.372 988 4	1.582 796 6
24	0.444 583 9	4.385 260 8	
26	0.444 370 7	4.396 095 6	
28	0.444 201 7	4.405 766 4	
Ext.	0.443 147 2	4.745 376 4	1.585 582 8
Exact	0.443 147 2	4.934 802 2	1.570 796 3

above theories differ slightly in their predictions for higher-order terms. Best fits were obtained for the expressions shown below:

$$-12N^2(E_N^{(0)}-E_\infty)/\pi^2=1+a_1(\ln N)^{-3}+a_2(\ln N)^{-4}\ , \tag{2a}$$

$$2N^2(E_N^{(1)}-E_N^{(0)})/\pi^2=1+b_1(\ln N)^{-1}+b_2(\ln N)^{-2}\ , \tag{2b}$$

$$N^2(E_N^{(p)}-E_N^{(0)})/\pi^2=1+c_1(\ln N)^{-2}+c_2(\ln N)^{-3}\ , \tag{2c}$$

where E_∞ is the Hulthén value for the ground-state energy *per spin* for the infinite system, $E_N^{(0)}$ is the ground-state energy of the finite system (size N), $E_N^{(1)}$ is the energy for the first excited state, and $E_N^{(p)}$ is the minimum energy for states of momentum $p=2\pi/N$. Functional forms for size corrections in (2a) and (2b) are the same as those obtained by Cardy.[5] The energy difference in expression (2c) determines the spin-wave velocity in the limit of large N (the infinite-size limit yields the value $\pi/2$ for the spin-wave velocity[9]). To the authors' knowledge, no analytic derivation of the logarithmic corrections of (2c) is available in the literature.

In Table II we display the various coefficients which optimize our fits through expressions (2). Both fits and simulation results are shown in the Fig. 1. The most remarkable result is the size dependence of the quantity given by (2c), related to the spin-wave velocity behavior. A maximum appears for sizes of the order $N\sim 54$, but slow logarithmic behavior develops a *plateau* in a rather

TABLE II. Different coefficients used for the least-squares fits of simulation results after formulas (2).

	1	2
a	0.109 51	0.321 64
b	−0.423 40	0.220 73
c	0.505 70	−1.340 40

broad region, as can be seen in the inset of Fig. 1. This size marks the beginning of the regime, also of slow convergence, of decreasing values in direction to the thermodynamic limit. We believe that this predicted crossover size is a good approximation, since our fits work up to sizes $N\approx 200$. This conclusion has been obtained from comparisons with isolated values for the ground-state energy and the mass gap calculated via Bethe ansatz.[3,4] For very large sizes our fits will deviate from the asymptotic behavior due to contribution of small-size values.

For the ground-state energy, the specific scaling law with corrections proportional to $(\ln N)^{-3}$ yields excellent convergence even for small sizes. This illustrates a typical case where common extrapolation algorithms work properly. On the other hand, the dominant $(\ln N)^{-1}$

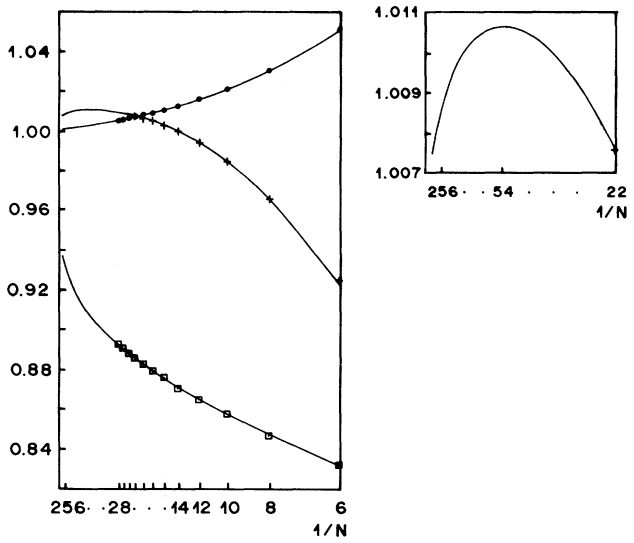

FIG. 1. Plot of the finite-size correction for the ground-state energy, the scaled mass gap, and the spin-wave velocity as function of the inverse of size. Solid circles refer to exact numerical values for corrections to the ground-state energy, open squares are for the scaled mass gap, and crosses are for the spin-wave velocity. All three quantities are normalized to their dominant asymptotic behavior, i.e., they assume the value 1 at the infinite-size limit. Continuous lines are used for depicting our least-squares fits according to formulas (2) with the coefficients given in Table II. Simulation values are calculated within high precision and error bars are much smaller than the symbols which we are using for visual purposes. In the inset we show, in a different scale, a magnified view of the spin-wave velocity behavior close to the maximum, which happens around the value $N=54$. The values plotted are $1/N$, where N is indicated on the scale.

correction for the scaled mass gap makes any extrapolation based on small system values extremely difficult. This latter behavior contrasts with the one observed in the anisotropic Heisenberg-Ising system (*XXZ* model),[16,17] where a dominant exponential dependence with size for the mass gap is obtained.

We finally conclude that an unambiguous analysis of finite-size scaling must usually be complemented by theoretical arguments, especially when only small sizes are available for numerical computations. This fact should be taken into account in calculations for higher values of spin, as well as in higher dimensions. *Naive* extrapolation procedures may lead to wrong conclusions for the thermodynamic limit, particularly when we are close to an essential singularity.

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