Ground-state staggered magnetization of the antiferromagnetic Heisenberg model

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Using helical boundary conditions, we present exact-diagonalization results for two-dimensional spin-$\frac{1}{2}$ antiferromagnetic Heisenberg systems. Energy and staggered magnetization for an infinite system are obtained by extrapolation from finite square systems. Comparisons with the results obtained for periodic boundary conditions are made.

I. INTRODUCTION

Antiferromagnetic ordering in two-dimensional planes at low temperatures has been discovered in La_2CuO_4,[1] which becomes a high-T_c superconductor upon doping with Ba or Sr.[2] There have been various attempts to find out whether the behavior of stoichiometric La_2CuO_4 can be associated with the ground-state properties of the antiferromagnetic Heisenberg (AFH) model.[3] The observation of interest, which measures the antiferromagnetic ordering in the ground-state, is the expectation value of the "staggered magnetization,"

$$m^{\dagger}(N)=\left[\langle 0|\left[\frac{1}{N}\sum_{x=1}^{N}(-1)^{x}\mathbf{S}(x)\right]^{2}|0\rangle\right]^{1/2}, \tag{1.1}$$

where N is the number of spins.

Exact computations of this quantity on small lattices have been performed by Oitmaa and Betts[4] and later by Dagotto and Moreo[5] and Schulz and Ziman.[6] The results on a 4×4 and 6×6 lattice are as follows:

$$m^{\dagger}(4\times4)=0.5258\ , \tag{1.2}$$

$$m^{\dagger}(6\times6)=0.458\ . \tag{1.3}$$

The extrapolation to the thermodynamical limit from a 4×4 and a 6×6 lattice has been performed by Schulz and Ziman; their result is

$$m^{\dagger}=0.2765\ . \tag{1.4}$$

The staggered magnetization is a highly sensitive quantity, changing strongly with dimension, size, geometry, and boundary conditions of the system. E.g., it is known that in the thermodynamical limit $N\to\infty$, the dependence on the dimension is

$$\lim_{N\to\infty} m^{\dagger}(N)=\begin{cases}0 & \text{for } d=1\\ \neq 0 & \text{for } d\geq 3\ .\end{cases} \tag{1.5}$$

The situation in two dimensions ($d=2$) is not so obvious: Spin-wave calculations,[7] Monte Carlo simulations,[8] and series expansions[9] suggest a nonvanishing limit,

$$\lim_{N\to\infty} m^{\dagger}(N)\approx 0.3 \quad \text{for } d=2\ , \tag{1.6}$$

whereas the Anderson RVB state (with nearest-neighbor spin-0 couplings) would predict a vanishing value of this quantity.

In this paper, we want to present results of an exact computation of the ground-state properties of the AFH Hamiltonian with $N=8,10,\ldots,26$ sites and helical boundary conditions.

II. THE AFH MODEL WITH HELICAL BOUNDARY CONDITIONS

The AFH Hamiltonian with helical boundary conditions,

$$\mathcal{H}=\sum_{x=1}^{N}[\mathbf{s}(x)\mathbf{s}(x+1)+\mathbf{s}(x)\mathbf{s}(x+k)]\ , \tag{2.1}$$

can be considered as one dimensional with two couplings: between nearest neighbors, and between sites x and $x+k$, which are k sites apart.

In order to implement Marshall's sign rule,[10] we restrict N to be even and k to be odd. The geometry of the corresponding two-dimensional lattices $\mathcal{L}(N,k)$ is shown in Fig. 1 for $N=26$ and $k=5$. Depending on the values of N and k, the shape of these two-dimensional lattices is more or less like a square. Square lattices with helical boundary conditions are realized for

$$N=k^2+1,\quad k=3,5,7,\ldots,\qquad N=10,26,50,\ldots\ . \tag{2.2}$$

For lattices of the type

$$N=k^2-1,\quad k=3,5\ , \tag{2.3}$$

the sites, which are identified due to the helical boundary conditions, form a parallelogram generated by nonperpendicular vectors l_1 and l_2 of equal length. The ground state on the square lattice $\mathcal{L}(N=10,\ k=3)$ has been cal-

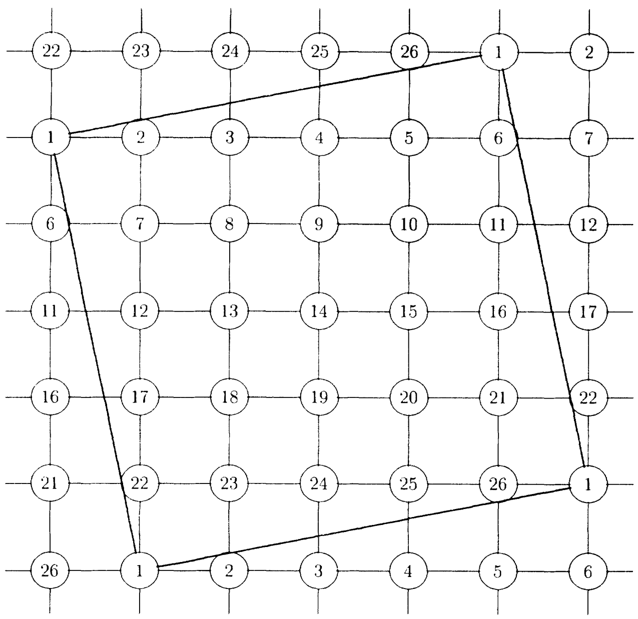

FIG. 1. Lattice $\mathcal{L}(N=26,\ k=5)$.

culated analytically by Saito.[11] For lattices $\mathcal{L}(N,k)$ with N and k different from (2.2) and (2.3), let us introduce an asymmetry parameter

$$A(N,k)=\frac{l_1-l_2}{l_1+l_2} . \tag{2.4}$$

l_1 is the longer, l_2 the shorter length of the lattice $\mathcal{L}(N,k)$. In Table I we list the asymmetry parameters $A(N,k)$ for the lattices $\mathcal{L}(N,k)$ with $N=8,10,\ldots,26$ and $k=1,3,5,7,9,11,13$.

The ground-state energies (per site) $\varepsilon(N,k)$ and the ground-state staggered magnetization $m^\dagger(N,k)$ on these lattices are listed in Tables II and III. There is an apparent correlation between the asymmetry parameter $A(N,k)$, the ground-state energy $\varepsilon(N,k)$, and the staggered magnetization $m^\dagger(N,k)$:

(a) For fixed N, $\varepsilon(N,k)$ and $m^\dagger(N,k)$ are monotonically decreasing with $A(N,k)$.

(b) On systems with vanishing or small asymmetry,

$$\begin{aligned} &A(N=8,\ k=3)=0 ,\\ &A(N=10,\ k=3)=0 ,\\ &A(N=18,\ k=5)=0.03 ,\\ &A(N=22,\ k=5)=0.07 ,\\ &A(N=24,\ k=5)=0 ,\\ &A(N=26,\ k=5)=0 , \end{aligned} \tag{2.5}$$

we find the largest values for the ground-state energies $\varepsilon(N,k)$ and the staggered magnetizations $m^\dagger(N,k)$.

(c) For fixed k, $\varepsilon(N,k)$ $[m^\dagger(N,k)]$ are monotonically increasing (decreasing) with increasing N.

III. THE THERMODYNAMICAL LIMIT OF SQUARE SYSTEMS

If we try to extract from the finite lattice results the behavior in the thermodynamical limit $N\to\infty$, we have to disentangle here two effects on $\varepsilon(N,k)$ and $m^\dagger(N,k)$. The first one arises from the finiteness of the lattice (finite N), the second one from its asymmetry $A(N,k)$. Therefore, we first concentrate on the lattices (2.5) which are almost squarelike. For these systems, we make the following finite-size ansatz:

$$\varepsilon(N,A=0)=\varepsilon(N\to\infty)+a/N^\alpha , \tag{3.1}$$

$$m^\dagger(N,A=0)^2=m^\dagger(N\to\infty)^\dagger+\frac{b_1}{N^{\beta_1}}+\frac{b_2}{N^{\beta_2}} . \tag{3.2}$$

We took the spin-wave exponents for finite-size scaling of square Heisenberg systems,[9,12]

$$\alpha=\tfrac{3}{2},\quad \beta_1=\tfrac{1}{2},\quad \beta_2=1 .$$

Best fits were obtained for

$$a=-1.8918,\quad b_1=0.635\,75,\quad b_2=0.459\,36 .$$

Figure 2 shows the modulus of the ground-state energy versus $N^{-3/2}$. The extrapolation to the thermodynamical limit in this case is extracted from the square systems $\mathcal{L}(N=10,\ k=3)$ and $\mathcal{L}(N=26,\ k=5)$. This procedure yields

TABLE I. Asymmetry parameters for various lattices $\mathcal{L}(N,k)$.

N \ k	Asymmetry 1	3	5	7	9	11	13
8	1.000 000	0.000 000					
10	1.000 000	0.000 000	0.436 542				
12	1.000 000	0.116 963	0.286 422				
14	1.000 000	0.234 436	0.234 436	0.559 037			
16	1.000 000	0.234 436	0.234 436	0.428 571			
18	1.000 000	0.309 718	0.026 334	0.026 334	0.638 185		
20	1.000 000	0.381 966	0.120 784	0.381 966	0.523 987		
22	1.000 000	0.381 966	0.065 497	0.381 966	0.065 497	0.693 378	
24	1.000 000	0.433 399	0.000 000	0.142 857	0.197 017	0.592 263	
26	1.000 000	0.439 626	0.000 000	0.250 000	0.482 343	0.131 884	0.734 014

TABLE II. Ground-state energy per site for helical lattices $\mathcal{L}(N,k)$.

N \ k	Energy 1	3	5	7	9	11	13
8	0.912 000	0.750 000					
10	0.903 089	0.730 007	0.861 817				
12	0.897 899	0.717 142	0.718 119				
14	0.894 793	0.709 206	0.709 206	0.859 681			
16	0.892 787	0.704 737	0.704 737	0.708 560			
18	0.891 417	0.701 676	0.693 957	0.693 957	0.859 398		
20	0.890 439	0.699 545	0.693 337	0.699 545	0.704 706		
22	0.889 716	0.698 009	0.688 226	0.698 009	0.688 226	0.859 355	
24	0.889 168	0.696 859	0.685 914	0.686 454	0.686 453	0.702 898	
26	0.888 741	0.695 978	0.684 452	0.684 729	0.695 978	0.684 729	0.859 347

$$\varepsilon(N\rightarrow\infty)=-0.670\ ,$$

which is very close to the estimate of Huse and Elser.[13] Higher-order corrections (in N^{-1}) might be responsible for the deviation of $\varepsilon(N=8, A=0)$. We have also included in Fig. 2 the ground-state energy on a 4×4 and a 6×6 lattice with periodic boundary condition.[4,6] One one hand, the result[6] on the 6×6 lattice is exactly on our extrapolation curve, on the other hand, the result[4] on the 4×4 lattice turns out to be a little bit higher than what we expect from our fit.

Figure 3 shows the staggered magnetization versus $N^{-1/2}$ together with two extrapolations to the thermodynamical limit:

(i) The first one is based on a quadratic fit ($N^{-1/2}$ and N^{-1}) to the data points on the systems (2.5) and yields for the staggered magnetization,

$$m^{\dagger}(N\rightarrow\infty)=0.304\ .$$

(ii) The second one is a linear extrapolation between the square systems $\mathcal{L}(N=10,\ k=3)$ and $\mathcal{L}(N=26,\ k=5)$ and yields for the staggered magnetization,

$$m^{\dagger}(N\rightarrow\infty)=0.253\ .$$

It should be noted that the staggered magnetization of the 4×4 lattice is somewhat below the fit, which might be due to the periodic boundary condition. The fit to the finite lattice results is very sensitive to the selection of data points.

IV. CONCLUSIONS

A nonvanishing staggered magnetization in the ground state of the two-dimensional antiferromagnetic Heisenberg model, found in spin-wave calculations,[7] Monte Carlo simulations,[8] and series expansions,[9] is by now established as well in exact computations on finite systems:[14,15]

(a) A linear extrapolation of the results (1.2) and (1.3) obtained on a 4×4 and 6×6 lattice with periodic boundary conditions[4,6] yields the value (1.4) in the thermodynamical limit.

(b) Depending on the extrapolations of the results—obtained on the lattices with helical boundary conditions, listed in Eq. (2.5)—the estimate of the thermodynamical limit is found in the interval

$$m^{\dagger}=0.25\text{–}0.3\ .$$

Therefore, all the approaches to determine the staggered magnetization of the two-dimensional AFH model agree with each other within 20%. It is crucial that the

TABLE III. Ground-state staggered magnetization for helical lattices $\mathcal{L}(N,k)$.

N \ k	Staggered magnetization 1	3	5	7	9	11	13
8	0.568 040	0.612 372					
10	0.527 390	0.581 413	0.506 187				
12	0.495 709	0.558 506	0.557 575				
14	0.470 009	0.539 755	0.539 755	0.432 014			
16	0.448 555	0.522 916	0.522 916	0.517 171			
18	0.430 253	0.508 211	0.518 312	0.518 312	0.381 778		
20	0.414 374	0.495 081	0.503 268	0.495 081	0.484 373		
22	0.400 407	0.483 227	0.498 615	0.483 227	0.498 615	0.345 479	
24	0.387 985	0.472 452	0.491 194	0.490 014	0.490 016	0.456 449	
26	0.376 832	0.462 581	0.483 631	0.482 853	0.462 581	0.482 853	0.317 824

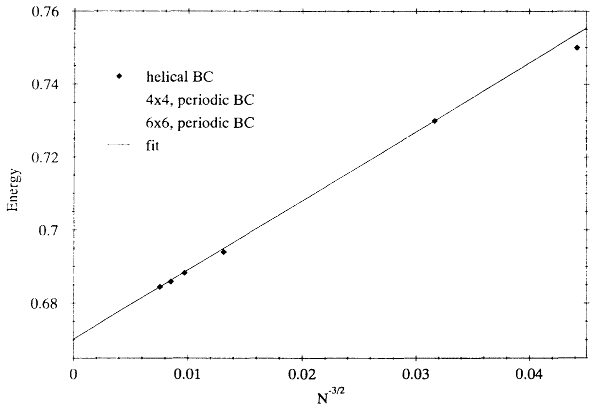

FIG. 2. Energy per site for square and nearly square Heisenberg systems.

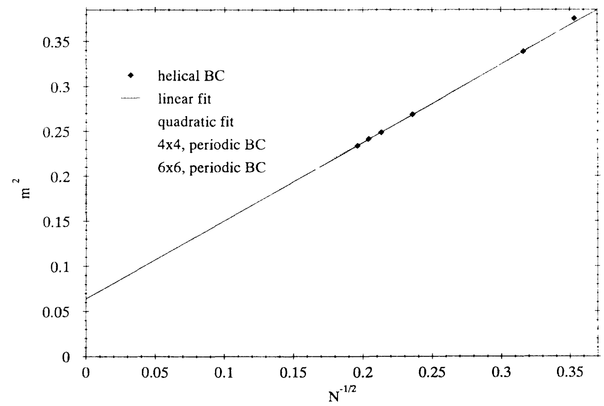

FIG. 3. Staggered magnetization for square and nearly square Heisenberg systems.

extrapolation to the thermodynamical limit starts from squarelike or almost squarelike systems.

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