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Zero-temperature properties of the two-dimensional Heisenberg antiferromagnet: A numerical study

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Using a modified Lanczos method we have studied the two-dimensional Heisenberg antiferromagnetic model (at zero temperature) with lattices up to 24 sites. The ground-state and first-excited-state energies are evaluated. We show that the model is gapless in the thermodynamic limit in agreement with recent Monte Carlo simulations. Accurate results for the "square ladder" are also presented showing that this model is massive. The finite-size dependence of the results is discussed. In addition, we calculate the energy of a resonating-valence-bond state on finite lattices and its overlap with the exact ground state.

The discovery of superconductivity at high temperatures in some special oxide compounds[1] induced a considerable theoretical effort in the study of purely electronic models. This renewal of interest in old problems is due to the recent suggestion[2] that the CuO_2 planes of the new superconductors may be described by the two-dimensional (2D) Hubbard model (in the strong-coupling region) with a small fraction of holes. For the undoped case and with a strong Coulomb repulsion, the model reduces to the antiferromagnetic Heisenberg (AFH) model.

La_2CuO_4 has been studied experimentally[3] showing that it has two-dimensional antiferromagnetic properties at low temperature. On the theoretical side, not much is known about the AFH model in two dimensions. Is there long-range order at zero temperature? Spin-wave calculations[4] suggest the existence of Néel order. Or course, this method assumes that Néel order exists and the quantum fluctuations around it are studied. It is clear that better techniques are required. Besides, recently, the whole idea that the ground state of the two-dimensional 2D AFH model is Néel-like has been challenged by Anderson, Baskaran, Zou, and Hsu.[5] They suggested that a new state [resonating-valence bond (RVB)] may actually be the gound state of the theory at least when doping is added to the system.

We clearly need a better theoretical understanding of the 2D AFH model. Since there are no reliable analytical methods to study it, there is a great interest in the numerical analysis of this model. Oitmaa and Betts[6] did an exact calculation using finite lattices up to 16 sites finding antiferromagnetic order in the ground state. Recent Monte Carlo studies[7] also support this picture.

It is the purpose of this Rapid Communication to further analyze the 2D AFH model using a recently proposed modified Lanczos technique.[8] Using this method we can exactly study zero-temperature properties of the model with lattices up to 24 sites. This technique is complementary to the Monte Carlo (MC) methods that can attack larger systems than ours, but with statistical errors due to the stochastic importance sampling (besides some MC techniques have the problem that they are actually working at a small but finite temperature introducing an additional error in the calculation[7,9]).

The Hamiltonian of the 2D AFH model is defined as

$$H = 2J\sum_{\mathbf{x},\hat{l}} \mathbf{S}_{\mathbf{x}} \cdot \mathbf{S}_{\mathbf{x}+\hat{l}} . \tag{1}$$

where $\mathbf{S}_{\mathbf{x}}$ is a spin-$\frac{1}{2}$ operator at site $\mathbf{x}$ of a two-dimensional square lattice with periodic boundary conditions. $\hat{l}$ denotes unit vectors in the two directions. In this paper, we take $J=1$. For the ground-state energy, we will work in the subspace with total magnetization equal to zero.

The modified Lanczos method[8] that we use in this paper has proved to be a very efficient technique in the study of the spin-$\frac{1}{2}$ AFH chain. It has been recently successfully applied to the analysis of spin-1 and -$\frac{3}{2}$ chains, dynamical problems, and other systems.[10] The method starts with some initial state (that we take as a Néel state for simplicity; the only constraint is that the starting configuration needs a nonzero projection over the exact ground state). Applying the Hamiltonian to the initial state, we can construct a vector orthogonal to it and by diagonalizing the 2×2 Hamiltonian matrix in that subspace we improve the initial values of the energy and ground state as in a variational technique. We repeat this process many times until we achieve the required accuracy in the ground-state energy and wave function. We have measured observables with an accuracy of 10^{-7}. For more details, we refer the reader to Ref. 8.

In Table I, we present the results for the ground-state energy for different lattice sizes. To obtain a numerical estimation of the gound-state properties of the two-dimensional model in the thermodynamic limit we did the following: first we obtain results for lattices of $N\times L$ sites keeping fixed N and increasing L, and only at the end take the limit $N\rightarrow\infty$.

Following these ideas, first we study the case of lattices $2\times L$ and try to make the extrapolation $L\rightarrow\infty$. In this case, we can get the ground-state energy with great accuracy, since the results for L odd and even converge (to the same value) from above and from below, respectively, giving upper and lower bounds to the energy in the $L=\infty$ limit. In fact, from a simple inspection of the results for

TABLE I. Ground-state energy per site of the 2D AFH model on a $N \times L$ lattice (absolute value).

L/N	2	3	4
2	2.000000	1.666666	1.733583
3	1.666666		1.228036
4	1.733583	1.228036	1.403560
5	1.713657		1.330769
6	1.720471	1.175699	1.379376
7	1.718017		
8	1.718954	1.159269	
9	1.718587		
10	1.718735		
11	1.718673		
12	1.718699		

$L=11$ and 12 we obtain

$$E_{2\times\infty} = -1.718686 \pm 0.000013 . \quad (2)$$

Since for the $4\times L$ and $6\times L$ lattices we cannot reach such an accuracy by simple inspection, it is important to analyze the L dependence of the results. We fitted the data with a polynomial

$$E_{2\times L} = E_{2\times\infty} + \frac{a}{L^{\alpha}} . \quad (3)$$

a and $E_{2\times\infty}$ are obtained using a least-squares-fit subroutine for a fixed α. We choose the value of α that maximizes the correlation of the fit. For the special case of $2\times L$ lattice we found that the optimal α takes a large value ($\alpha=4$ if the results from $L=2$ to 12 are considered). This is not surprising since from Table I we observe that the convergence is very fast. (In fact, we found that we can also fit the data very well with an exponential, i.e., $E_{2\times L} = E_{2\times\infty} + ae^{-bL}$.) We explicitly checked that using the ground-state energy results for the one-dimensional AFH chain [see Ref. (8)] we correctly reproduced the well-known result that the optimal α is 2. Using the energies for L even between 2 and 12, we found an extrapolated energy -1.718 ± 0.003, in good agreement with the more accurate result Eq. (2).

Note that the $2\times L$ lattice can be thought of as a one-dimensional chain with two spin degrees of freedom per site and an involved nearest-neighbor interaction. The fact that there are no $1/L^2$ corrections to the ground-state energy tells us (from conformal invariance) that the theory is not critical and there should be a mass gap (we have checked below this prediction; however, note that our final result for the 2D model is that it is gapless). We believe that the crossover between critical and noncritical behavior for the "square ladder" deserves further study. A model with a coupling constant $\tilde{J}$ between the two chains can interpolate between a gapless theory ($\tilde{J}=0$) and a massive one ($\tilde{J}=J$) with probably a critical point in between.

In Table II we show the staggered correlation function

$$\omega_{\mathbf{y}} = \langle S^z_{\mathbf{x}} S^z_{\mathbf{x}+\mathbf{y}} \rangle , \quad (4)$$

for the $2\times L$ lattices. The results for $L=12$ can be approximated very well by an exponential fit, giving additional support to the idea that this model has a mass gap.

Now let us study the $4\times L$ and $6\times L$ lattices. For the case $4\times L$, we have only three numbers for the extrapolation to $L=\infty$ ($L=3,5$ are not very useful here). We found that they can be fit with the polynomial Eq. (3) again using $\alpha=4$. Our extrapolated ground-state energy is $E_{4\times\infty} = -1.37 \pm 0.02$. For the $6\times L$ system we assume that $\alpha=4$ works here as well as in the previous cases. The extrapolated result is $E_{6\times\infty} = -1.36 \pm 0.02$. We have repeated our analysis for the $N\times L$ lattices with $N=3$, 5. The best fits are obtained with $\alpha=2$ and 3, showing a slower convergence than for N even. The extrapolated results are $E_{3\times\infty} = -1.15 \pm 0.02$ and $E_{5\times\infty} = -1.28 \pm 0.03$.

With the knowledge of the energy for lattices $N\times\infty$, we can obtain a rough estimation of the ground-state energy in the bulk limit. In fact the energies for $N=2$, 4, and 6 can again be fit with an optimal $\alpha=4$. Our result is $E_{\infty\times\infty} = -1.35 \pm 0.02$. It compares well with the more accurate prediction of Barnes and Swanson[11] ($E_{\infty\times\infty} = -1.344 \pm 0.002$) using a random-walk technique. These results show that the previous estimation of Oitmaa and Betts ($E_{\infty\times\infty} = -1.31 \pm 0.01$) had too optimistic error bars.

In Table III, we show results for the square of the staggered magnetization in the ground state defined as

$$\langle \mathbf{M}^2 \rangle = \left\langle \left[\frac{1}{V} \sum_{\mathbf{x}} (-1)^{|\mathbf{x}|} \mathbf{S}_{\mathbf{x}} \right]^2 \right\rangle . \quad (5)$$

The Néel state has $\sqrt{\langle \mathbf{M}^2 \rangle} = 0.5$ in this notation. The results for the magnetization $\langle \mathbf{M}^2 \rangle$ of the $2\times L$ lattice can be extrapolated again using Eq. (3) with an optimal $\alpha=1$ (using $L=4,\ldots,12$). In the $L\to\infty$ limit, we obtain a result compatible with zero ($\simeq 0.008$) showing that the square ladder has a very small staggered magnetization. Next, we should try to obtain the bulk two-dimensional

TABLE II. Correlation functions ($\omega_{\mathbf{y}}$) for $2\times L$ lattices. $\mathbf{y}$ is along the long direction of the lattice.

$\mathbf{y}$	2×12	2×10	2×8	2×6	2×4	2×2
1	0.295221	0.295404	0.296313	0.301034	0.328604	0.666666
2	0.088943	0.089375	0.091522	0.102731	0.168020	
3	0.036816	0.037849	0.043116	0.072459		
4	0.015848	0.018176	0.030386			
5	0.007971	0.013302				
6	0.005877					

TABLE III. Ground-state expectation value of $\langle \mathbf{M}^2 \rangle$ as defined in Eq. (5) for lattices of size $N \times L$.

L/N	2	4
2	0.500000	0.203522
4	0.203522	0.276527
6	0.160385	0.0459
8	0.116915	
10	0.086530	
12	0.066751	

limit, hoping to find a good convergence as with the ground-state energy. However, we observed a peculiar behavior: The magnetization has a maximum for the square lattices ($N=L$). For example, the results for the 4×2 and 4×6 lattices are much smaller than for the 4×4 one, in spite of the fact that, intuitively, we would have expected the 4×6 lattice to be closer to the bulk limit. Then for the magnetization the order of the limits towards the two-dimensional bulk is very important. One-dimensional-like lattices probably do not have a spontaneous magnetization. The Néel order is a genuine two-dimensional effect, i.e., the bulk two-dimensional limit is very singular. These details deserve further study. Other calculations[7] support the idea that there is a staggered magnetization ($\sqrt{\langle \mathbf{M}^2 \rangle}$) in the 2D AFH with a value around 0.30.

In Table IV, we present our results for the mass gap defined as the difference in energy between the triplet and singlet states. As in the case of the ground state, special care must be taken with the quantum numbers of the first excited level. For both N and L even, the momentum is π in both directions. For lattices where N or L is odd, there are no general rules, but, for example, on a $2\times L$ and $3\times L$ we found that the momentum is 0 along the "even" direction and $\pi(N-1)/N$ in the "odd" direction (where N is the length in that direction).

As we did with the ground-state properties, let us first begin with the $2\times L$ lattice. In this case, we cannot get a very accurate result by simple inspection as we did in Eq. (2) for the ground-state energy, mainly because the L odd results converge very slowly (probably because in this case a Néel state does not fit correctly on the lattice). For this reason, we need to make some extrapolation. The results for L even follow the polynomial behavior Eq. (3) with $\alpha=3$ while for L odd we obtain that the optimal α is 1. Our best estimate for the mass gap (ΔE) comes from L even and gives $\Delta E_{2\times\infty}=2.561\pm0.002$. It is then clear that the "square ladder" has a finite mass gap as suggested by the analysis of the ground-state properties.

TABLE IV. Mass gap for lattices of size $N \times L$.

L/N	2	3	4
2	4.000000	3.725083	2.745559
3	3.725083		1.783380
4	2.745559	1.783380	1.157198
5	3.216230		1.395900
6	2.595551	1.223028	0.848042
7	2.952831		
8	2.569085		
9	2.814183		
10	2.563948		
11	2.735942		
12	2.562905		

Using again the L even results for the $4\times L$ and $6\times L$ lattices we obtain the extrapolated values $\Delta E_{4\times\infty}=0.62\pm0.01$ and $\Delta E_{6\times\infty}=0.27\pm0.02$ (for the $4\times L$ lattice the best extrapolation is obtained with $\alpha=2$; for the $6\times L$ lattice we assumed the same behavior). We can see that the mass gap decrease very quickly with the size N of the $N\times\infty$ lattice. In fact, we found that the results for $N=2$, 4, and 6 are fit very well by a polynomial with $\alpha=2$ and the extrapolated value is

$$\Delta E_{\infty\times\infty}=-0.02\pm0.02\,, \tag{6}$$

which is compatible with a gapless theory in the bulk two-dimensional limit. In Ref. 11, a similar result was found with lattices of 4×4, 6×6, and 8×8 sites. The approach to the bulk limit is very different in this paper (first one direction is sent to ∞ and then the other) from that in Ref. 11 (they approach the two-dimensional case with square lattices). It is remarkable that the conclusions of both are the same.

We have also evaluated the energy of the "resonating-valence-bond" (RVB) state that Anderson proposed some time ago as a candidate for the ground-state energy of a triangular lattice.[12] In the square lattice it is believed that this state may have an energy very close to that of the ground state. A small amount of frustration (through next-nearest-neighbor interactions or by the introduction of holes) may then induce a phase transition to a new regime where the RVB state is the exact ground state.

The RVB state is defined as

$$\psi_{\mathrm{RVB}}=\sum_{\alpha}|\alpha\rangle\,, \tag{7}$$

where the states $\{|\alpha\rangle\}$ are "dimer" coverings of the lattice (for details, see Ref. 13). Each dimer involves nearest-neighbor sites coupled in a singlet $(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle)/\sqrt{2}$. The state $|\alpha\rangle$ represents a product of singlets involving all the spins of the lattice. For a two-dimensional lattice, the number of coverings grows exponentially.[14–16]

We have measured the energy of the RVB state in a straightforward way: first we generate all the possible coverings and then we transform each covering into the S_z basis. With the help of the programs used to get the exact energy, we can now evaluate the RVB energy. Since in the RVB calculation, we have not implemented the symmetries used in the evaluation of the ground state, we have computer memory problems to go beyond a 4×4 or 2×8 lattice but these lattices are big enough to extract some qualitative information for the state. Special care must be taken on the boundary of the lattice with the sign of each bond singlet. The "orientation" of the bond must be the same as in the rest of the lattice.

In Table V, we present the energy of the RVB state. For a 2×2 lattice, it is the exact ground state. Increasing the size of the lattice the energy remains very close to the

TABLE V. Results for the RVB state for $N \times L$ lattices: E_{RVB} denotes the energy, N_d is the number of dimers of each state, $O_1 = |\langle \psi_{RVB} | \psi_{exact} \rangle|$ is the overlap with the exact wave function. $O_2 = |\langle \psi_{Néel} | \psi_{exact} \rangle|$ is the overlap between the Néel state defined in the text and the exact ground state.

	E_{RVB}		N_d		O_1 (%)		O_2 (%)	
L/N	2	4	2	4	2	4	2	4
2	2.000000	1.571429	2	9	100	75	82	55
4	1.571429	1.337274	9	272	75	57	55	41
6	1.630435		20	3108	71		36	
8	1.646139		49		60		23	

gound-state one. For example, for a 2×8 lattice the difference is only 4.24% and for a 4×4 4.72% (by the way note that the RVB energy for a 4×4 lattice has also been evaluated in Ref. 17). In Ref. 18, the RVB state energy for the $2\times L$ lattice has been estimated using a variational calculation but we cannot compare results since we used periodic boundary conditions (PBC's) in all directions while the authors of Ref. 18 used PBC's only along the longer direction.

In Table V, we also show the number of dimer coverings of each lattice. For the $2\times L$ system they grow like $e^{0.473L+0.111}$ (to get this asymptotic formula, we also used results not quoted in Table V, i.e., the number of dimers for 2×10 and 2×12 lattices are 125 and 324, respectively). Our lattices are not big enough to test the two-dimensional bulk prediction of Ref. 14. Note also that the number of dimers is greatly reduced if free boundary conditions are used.

Also in Table V, we present the overlap of the RVB state with the exact ground state defined as $|\langle \psi_{RVB} | \psi_{exact} \rangle|$ where both states are normalized to 1. The overlap is remarkable high and, at least for the $2\times L$ lattice, it may converge asymptotically to a nonzero constant. We have also evaluated the overlap between the exact ground state and a Néel state defined as the symmetric sum of the two states with staggered magnetization 0.5 in the z direction. The results are also shown in Table V. They are systematically smaller than the RVB overlaps but that does not mean that the exact state is "RVB-like." It simply means that the Néel state that we used represents just one of the possible directions in which the system can develop a staggered magnetization. Without the introduction of a staggered external field, each direction in spin space has equal probability (that goes to zero in the thermodynamic limit). So we can say that the ground state has Néel order (from the nonzero staggered magnetization result of Ref. 7) but it does not resemble what it is usually called, a Néel state. In fact, the exact ground state is a singlet so it would be more interesting to make a projection of the Néel state into that subspace and study its overlap. Recently, that state has been formally constructed[16] in terms of long-range dimers (with a length-independent weight).[19]

After completion of this work, we received a paper by Tang and Hirsch[20] where exact diagonalizations of finite lattices for the 2D AFH model are also presented.

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