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Two-dimensional Heisenberg antiferromagnet with next-nearest-neighbor coupling

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We study the two-dimensional $S=\frac{1}{2}$ antiferromagnet with next-nearest-neighbor antiferromagnetic coupling using a sublattice-symmetric spin-wave theory and exact diagonalization. For sufficiently large frustration the theory predicts a transition to a disordered state with an energy gap and exponentially decaying correlations, rather than to a gapless spin-liquid state. Comparison with exact results on finite lattices up to 26 sites indicates that the theory overestimates the disordering effect of the next-nearest-neighbor coupling, implying that the long-range antiferromagnetic order is surprisingly robust.

Recently, there has been great interest in two-dimensional quantum antiferromagnets[1-7] due to their possible relevance to high-T_c superconductivity. Much of it was generated by Anderson's suggestion[4] that a novel spin-liquid state may be the ground state of a two-dimensional quantum antiferromagnet.[5] However, recent numerical work[3,6] has conclusively established that the ground state of the $S=\frac{1}{2}$ Heisenberg antiferromagnet on a square lattice with nearest-neighbor coupling only possesses long-range order, close to but slightly larger than that predicted by spin-wave theory.

If a next-nearest-neighbor antiferromagnetic coupling J_2 is introduced in this system, however, the situation is less clear, and it has recently been suggested that the system could exhibit a spin-liquid ground state for sufficiently large J_2.[7] Besides its intrinsic interest, this model has been proposed to describe the spin degrees of freedom of the Hubbard model away from $\frac{1}{2}$ filling,[8] and a detailed understanding of it is desirable.

The Hamiltonian of interest is defined on a square lattice by

$$H=J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j+J_2\sum_{\langle i,i'\rangle}\mathbf{S}_i\cdot\mathbf{S}_{i'}, \tag{1}$$

where $\langle i,j\rangle$ denote nearest neighbors on different sublattices, and $\langle i,i'\rangle$ denote nearest neighbors on the same sublattice. We study this Hamiltonian using a sublattice-symmetric spin-wave theory (SSSW), recently introduced,[3,9] and exact diagonalization.

We diagonalize the Hamiltonian Eq. (1) within the spin-wave approximation and impose the additional constraint that the sublattice magnetization be zero. The resulting spin-wave spectrum has the form

$$\epsilon_k=\frac{zJ_s}{\bar{\eta}(k)}\sum\sqrt{1-\bar{\eta}(k)^2\gamma_k^2}\,, \tag{2}$$

with

$$\bar{\eta}_k(\eta)=\frac{\eta}{1+(J_2/J_1)\eta(\Gamma_k-1)}\,, \tag{3a}$$

$$\Gamma_k=\frac{1}{z}\sum_{\delta'}e^{i\mathbf{k}\cdot\boldsymbol{\delta}'}, \tag{3b}$$

$$\gamma k=\frac{1}{z}\sum_{\delta}e^{i\mathbf{k}\cdot\boldsymbol{\delta}}. \tag{3c}$$

Here, $\boldsymbol{\delta}(\boldsymbol{\delta}')$ are the lattice vectors connecting a site to its nearest neighbors on the other (same) sublattice, and z is the number of nearest neighbors. The parameter η is determined by the constraint equation

$$2S+1=\frac{1}{N}\sum_k\frac{1}{\sqrt{1-\bar{\eta}_k^2(\eta)\gamma_k^2}}\,. \tag{4}$$

On a finite lattice, Eq. (4) yields a solution with $\eta<1$, thus generating a gap for the spin-wave spectrum as appropriate for a finite lattice. As $N\rightarrow\infty$, Eq. (4) has a solution with $\eta=1-O(1/N^2)$ for J_2/J smaller than a critical value. The long-range order is given by[3,10]

$$m=\frac{1}{N}\frac{1}{\sqrt{1-\eta^2}}$$
$$=\frac{1}{2}\left[2S+1-\int\frac{d^dk}{(2\pi)^d}\frac{1}{\sqrt{1-\bar{\eta}_k^2(1)\gamma_k^2}}\right], \tag{5}$$

which is the same as predicted by ordinary spin-wave theory.[11] Beyond a critical value $(J_2/J)_c$ determined by

$$2S+1=\int\frac{d^dk}{(2\pi)^d}\frac{1}{\sqrt{1-\bar{\eta}_k^2(1)\gamma_k^2}}\,, \tag{6}$$

the long-range order disappears and Eq. (4) has a solution with $\eta<1$ in the limit $N\rightarrow\infty$ that generates a gap for spin-wave excitations. That is, the present theory predicts that when the long-range order disappears for sufficiently large J_2 the resulting phase is a disordered phase with massive spin waves as elementary excitations, rather than a gapless spin-liquid state.[7] For $S=\frac{1}{2}$, $(J_2/J)_c=0.38$. At $J_2/J=0.5$ the theory breaks down as the argument of the square root can become negative for $\mathbf{k}$ values close to $(\pi,0)$ and $(0,\pi)$. In the limit $S\rightarrow\infty$ the ground state of the Hamiltonian Eq. (1) crosses over between a Néel ordered state and a state where each sublattice is independently Néel ordered at $J_2/J=0.5$.

Next we solve the Hamiltonian Eq. (1) on finite square lattices of up to $N=26$ sites and compare spin-correlation functions with those predicted by SSSW:[3,9]

$$\langle \mathbf{S}_0 \cdot \mathbf{S}_R \rangle = |f(R)|^2 - |g(R)|^2 - \delta_{R,0}/4 , \quad (7a)$$

$$f(R) = \frac{1}{2N} \sum_k e^{i\mathbf{k}\cdot\mathbf{R}} \frac{1}{\sqrt{1-\bar{\eta}_k^2 \gamma_k^2}} , \quad (7b)$$

$$g(R) = \frac{1}{2N} \sum_k e^{i\mathbf{k}\cdot\mathbf{R}} \frac{\bar{\eta}_k \gamma_k}{\sqrt{1-\bar{\eta}_k^2 \gamma_k^2}} . \quad (7c)$$

We diagonalize the Hamiltonian using a Lanczos method. For $N=4$ and $N=8$, spin-spin correlations are independent of J_2 up to a critical value $(J_2/J)_c = 0.5$ (using boundary conditions such that each site has the same number of nearest and next-nearest neighbors). At that point there is a crossing of energy levels and the ground state becomes Néel ordered in each sublattice. It is easy to see that SSSW reproduces the behavior before the tran-

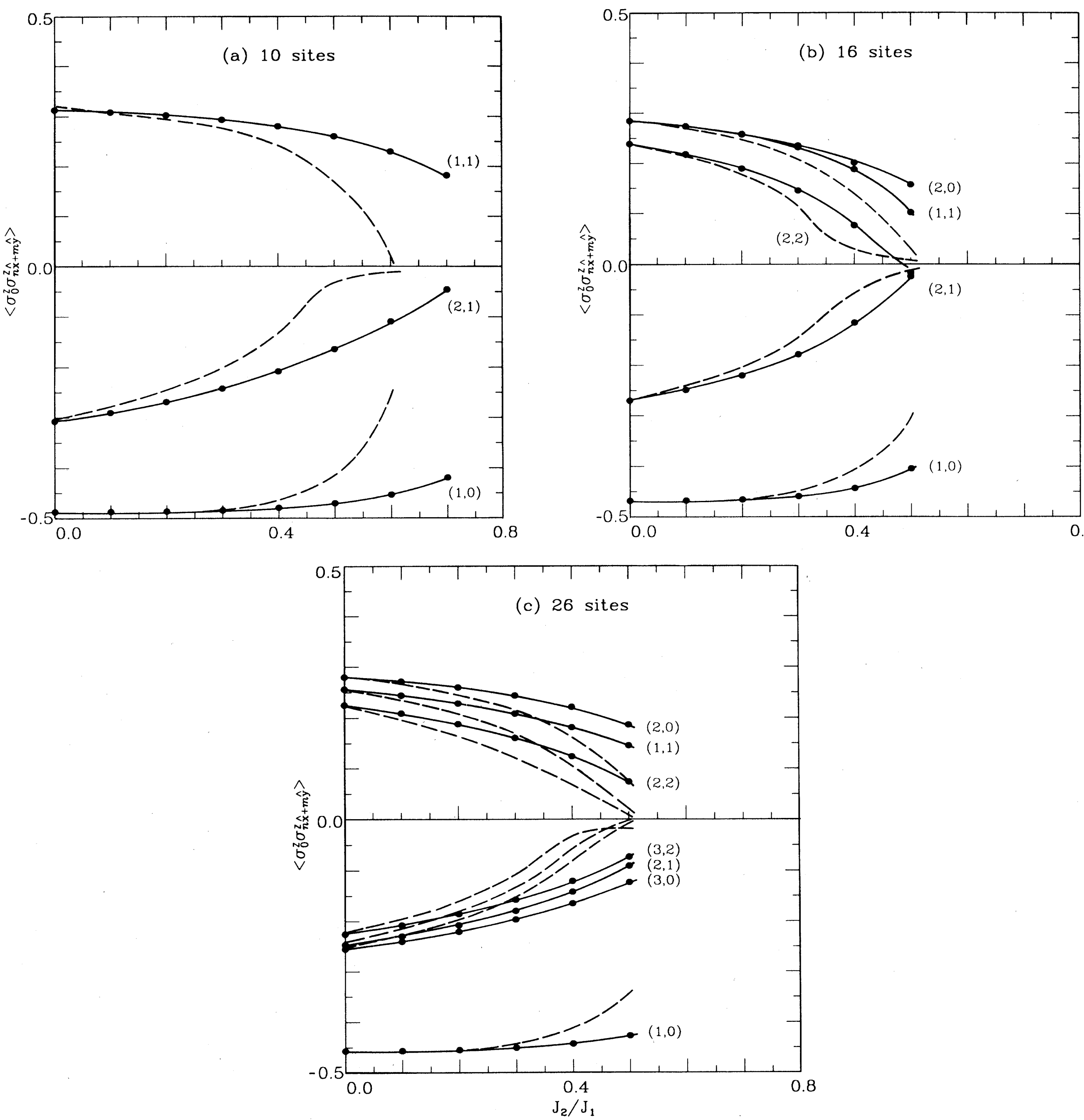

FIG. 1. Spin-spin correlations $\langle \sigma_0^z \sigma_{n\hat{x}+m\hat{y}}^z \rangle$ vs J_2 (in units where $J=1$) for lattices of (a) 10, (b) 16, and (c) 26 sites. Exact: solid lines, points. SSSW: dashed lines. The exact results are labeled by (n,m). The corresponding SSSW results are indistinguishable from the exact ones for $J_2=0$. For the 16-site lattice, the (2,0) and (1,1) correlations are identical within SSSW.

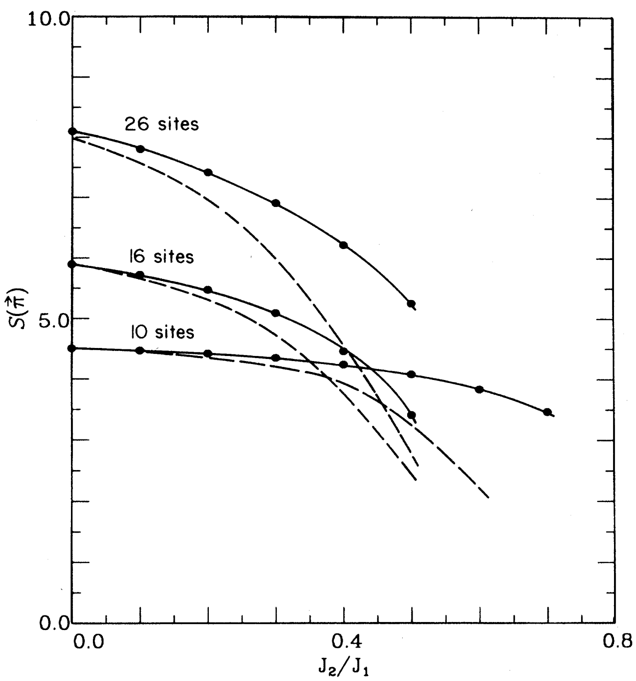

FIG. 2. Spin-structure factor $S(\boldsymbol{\pi})=\sum_{n\hat{x}+m\hat{y}}(-1)^{n+m}\times\langle\sigma_{\hat{0}}\sigma_{n\hat{x}+m\hat{y}}\rangle$ vs J_2 for lattices of 10, 16, and 26 sites. Exact: solid lines, points. SSSW: dashed lines.

sition *exactly*: for these lattices, Eqs. (4) and (7) predict spin correlations that are independent of J_2/J because $\Gamma_k=1$ for all k values for which $\gamma_k\neq 0$. In addition, the value of the spin correlations obtained from Eqs. (4) and (7) are exact.[3] However, SSSW does not see the transition point to the sublattice-ordered structure.

Results for spin correlations for lattices of size $N=10$, $N=16$, and $N=26$ are shown in Fig. 1, and $\mathbf{q}=\boldsymbol{\pi}$ structure factors for these cases in Fig. 2. Results for $N=18$ and $N=20$ are qualitatively similar and thus not shown. Note that SSSW consistently *overestimates* the effect of J_2 in destroying the antiferromagnetic correlations. This indicates that $J_2/J=0.38$ underestimates the value of J_2 at which the long-range antiferromagnetic order disappears.

In the Lanczos procedure, we started with a random initial vector and repeated the procedure several times to make sure we did not miss any level crossing. For $N=4$ and $N=8$ we found that there was a crossing of energy levels and a discontinuous change in spin-spin correlations, as discussed. For other values of N no level crossing was detected in the parameter range studied ($J_2/J\leq 1$).

In summary, we have studied the two-dimensional antiferromagnet with a frustrating next-nearest neighbor coupling J_2 using a sublattice-symmetric spin-wave theory and exact diagonalization. Comparison between these shows that the theory overestimates the effect of J_2, implying that the long-range order is surprisingly robust. In particular, for $S=\frac{1}{2}$ these results indicate that the long-range Néel order disappears at a value of J_2 that is larger than the spin-wave prediction $J_2/J=0.38$. The theory predicts a disordered phase with massive spin waves as elementary excitations for J_2/J greater than this critical value, and breaks down at $J_2/J=0.5$. These results suggest that the disordered state in this system is not a gapless spin-liquid state but rather a disordered state of the type described by the quantum disordered phase in the nonlinear σ model of Chakravarty, Halperin, and Nelson.[1]

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