The Spin-1 Heisenberg Magnet with Uniaxial (S_z^2) Anisotropy

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We report results of theoretical studies of a spin-1 Heisenberg antiferromagnet with easy-axis or easy-plane anisotropy, for the two-dimensional square lattice, at zero temperature. A quantum phase transition is identified, separating a magnetically ordered phase, with gapless excitations, from a gapped paramagnetic phase.

1. Introduction

Spin-1 magnetic systems have been studied for many years. They have become of interest again recently through the novel material $NiGa_2S_4$ [1] which is believed to have a 'spin-nematic' phase, molecular oxygen adsorbed on graphite [2], the prediction of a supersolid phase in such systems [3] and the possibility of creating a Mott insulating phase of S = 1 bosonic atoms in optical lattices [4].

Our current series expansion techniques [5] allow reliable calculations of both ground state and finite temperature properties of spin-1 systems, as well as excitation spectra and structure factors, which are measurable by neutron scattering.

Specifically we consider the Hamiltonian

$$H = J \sum_{<ij>} S_i \bullet S_j - D \sum_i (S_i^z)^2 \qquad (1)$$

D > 0 (< 0) corresponds to an easy axis (easy plane) system, and the ordered state will be 'Ising like', with no continuous symmetry, or 'X-Y like' with a residual continuous O(2) symmetry in the easy plane. We assume antiferromagnetic exchange (J > 0). In our work to date we have focused on the two-dimensional square lattice, but there is also interest in the triangular lattice [1], and the triangular bilayer system $Ba_3Mn_2O_8$ [6].

The phase diagram of the model, as a function of D/J, is shown schematically in Figure 1.

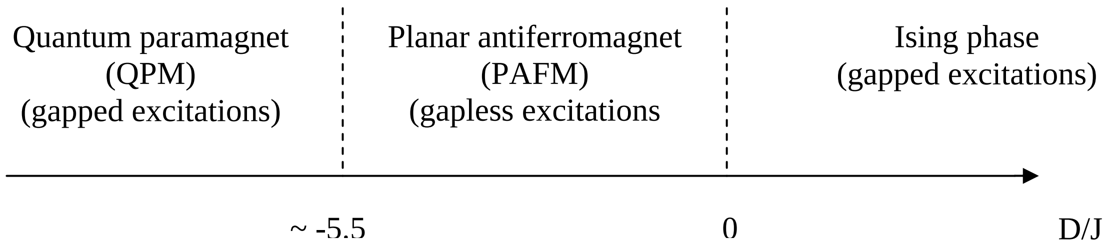

Fig.1. Phase diagram of the spin-1 D/J model on the square lattice.

The point D/J = 0 is a 1^{st}-order transition point. There is a *quantum phase transition* at D ~ -5.5 separating a small |D| planar antiferromagnetic phase (PAFM) from a large |D| paramagnetic phase (QPM).

The present paper reports new results, primarily in the D < 0 region. Preliminary results in the Ising phase were reported at Wagga2007, and a comprehensive paper will be submitted shortly [7].

2. Bulk Ground State Properties

The series expansion method at T = 0 relies on writing the Hamiltonian as $H = H_0 + \lambda V$ where H_0 is exactly solvable, with a simple ground state, and the remaining terms are treated perturbatively. Series are obtained in powers of λ, typically to order 11 or 12, and evaluated at $\lambda = 1$ using standard numerical methods. In the PAFM phase the planar symmetry will be spontaneously broken and we take $H_0 = J \Sigma S_i^x\ S_j^x$, where we denote the ordering direction as the x axis in spin space. In the large |D| QPM phase we take $H_0 = J \Sigma S_i^z\ S_j^z + |D| \Sigma (S_i^z)^2$. The ground state has all spins in the $S^z = 0$ Zeeman state.

Figures 2,3 show the ground state energy and magnetization per spin, as functions of D/J.

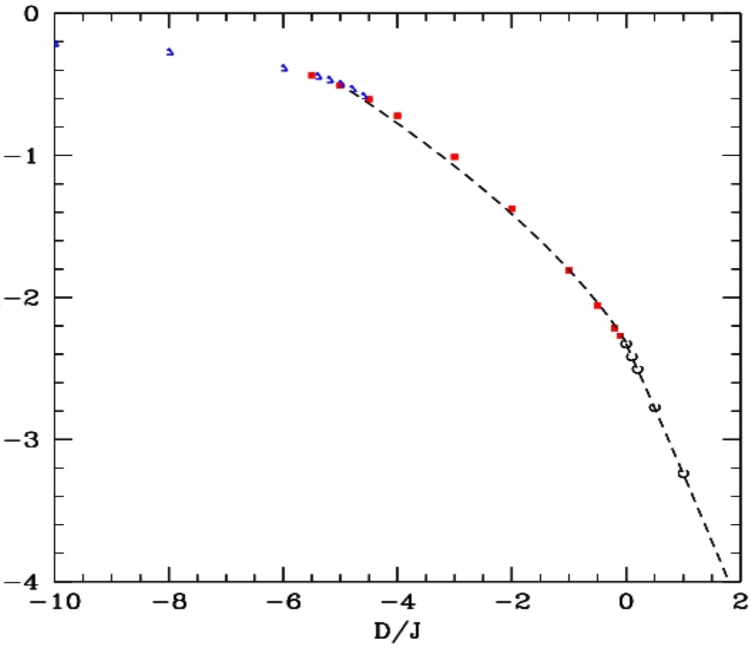

Fig. 2. Ground state energy per site versus D/J. The dashed lines are spin-wave estimates.

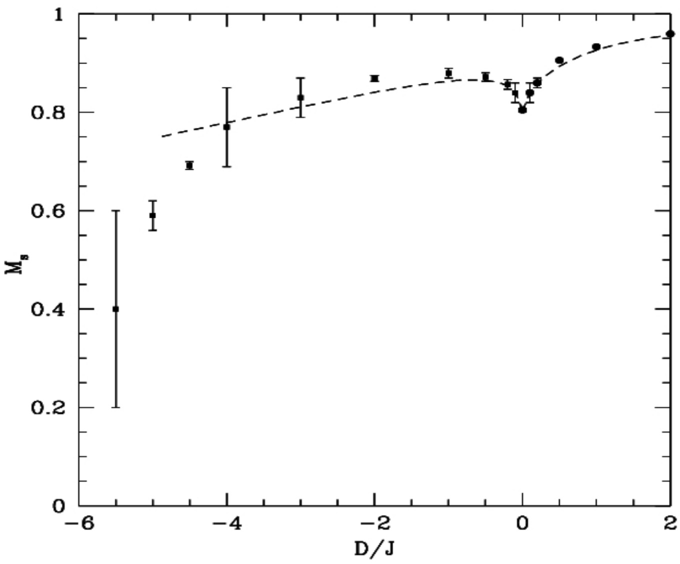

Fig. 3. Magnetization versus D/J. The dashed lines are spin-wave estimates.

We note the joining of the two energy curves (PAFM:squares and QPM: triangles) at D/J ~ -5.5. Any change of slope at the transition is small, suggesting a second order (or possibly weak 1st.

order) transition. The magnetization (Fig. 3) is falling sharply towards zero at the transition point, albeit with large error bars.

3. Elementary Excitations

The series expansion method is able to compute the energies of elementary excitations, and such calculations can often be compared directly with experimental neutron scattering results. In the PAFM phase the lowest excitations are magnons with S = 1. Figure 4 shows the dispersion curve along symmetry paths in the Brillouin zone. At D = 0 there are gapless excitations at both **k** = (0,0) and (π,π). Nonzero D leads to a gap opening at (0,0) but the gapless excitation at (π,π) persists throughout the phase.

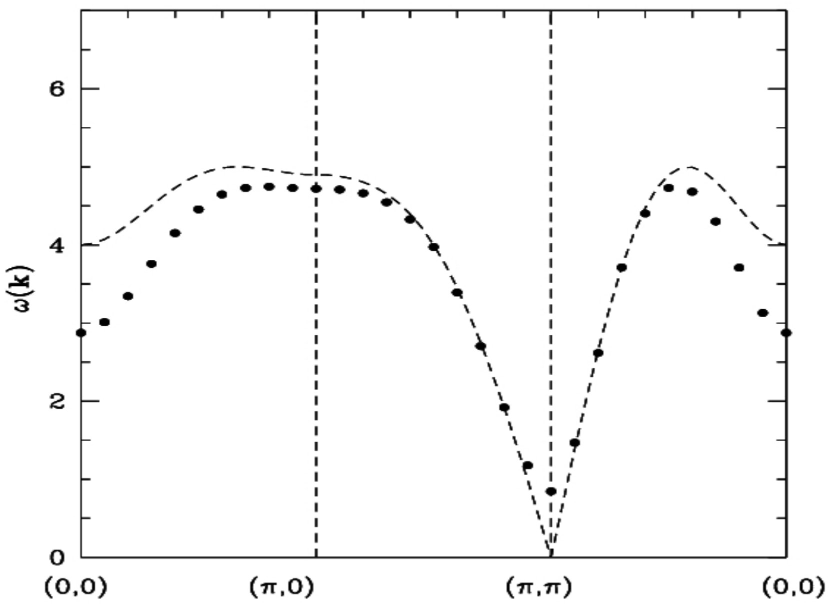

Fig. 4. Dispersion relation for a single magnon excitation at D/J = -1.0. The dashed curve is a spin-wave estimate.

In the QPM phase the elementary excitations arise from a transition at a single site from the S^z = 0 Zeeman state to either S^z = 1 or S^z = -1 (termed ‘excitons’ and ‘antiexcitons’ [8]). These spin deviations can then propagate as well-defined quasiparticles. Figure 5 shows the energy gap at (π,π) of these excitations as a function of D/J. The gap decreases and appears to vanish at D/J ≈ -5.5, heralding a quantum phase transition to the PAFM phase.

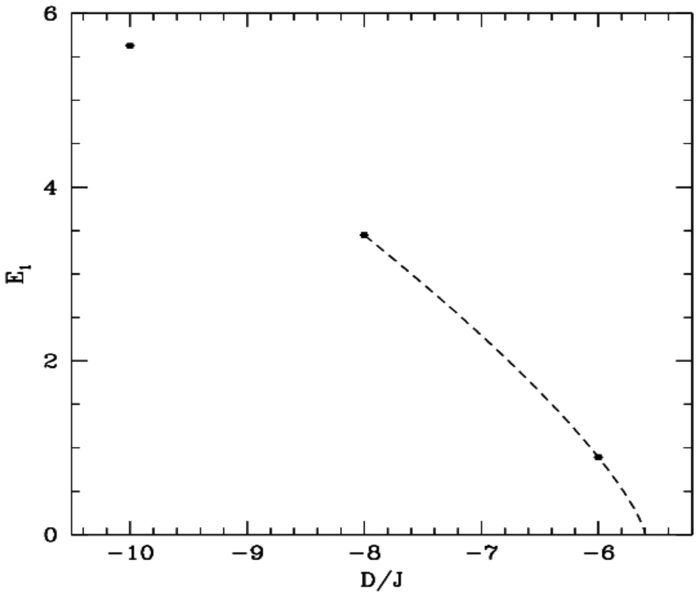

Fig. 5. Energy gap at **k** = (π,π) in the QPM region. The dashed line is a fit in the critical region.

4. Summary

We have calculated various properties of a quantum spin-1 model on the square lattice. Such models are relevant to a number of real systems of current interest. The series expansion method is systematic and reliable, and comparisons with analytic spin-wave approximations, presented elsewhere [7], demonstrate that spin-wave theory has a number of deficiencies. Details of the calculations and more comprehensive results will be presented elsewhere [7].

Acknowledgments

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