The Spin-1 Heisenberg Magnet with Uniaxial $(S^z)^2$ Anisotropy

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We revisit an old problem – the phase diagram of an S = 1 Heisenberg ferromagnet or antiferromagnet with an easy axis or easy plane crystal field anisotropy. Long series expansions at T = 0 and at high temperatures are used to compute the ground state energy, sublattice magnetization and critical temperature for the easy axis antiferromagnet on the square lattice.

1. Introduction

The physics of many magnetic materials depends not only on exchange but on single ion terms arising from crystal fields. The simplest generic Hamiltonian is

$$H = -J \sum_{<ij>} \mathbf{S_i} \cdot \mathbf{S_j} - D \sum_{i} (S_i^z)^2$$

which, depending on the signs of J,D describes ferromagnetic or antiferromagnetic exchange, with an **easy axis** or an **easy plane**. Figure 1 represents, schematically, the types of order expected.

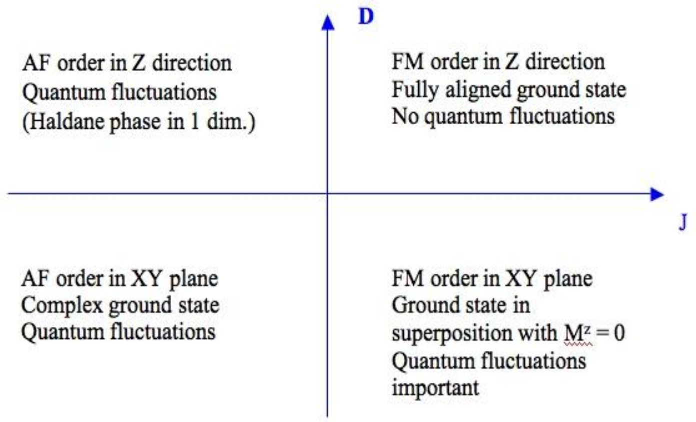

Fig. 1. Possible ground state scenarios for the J-D model.

Early studies of this kind of system were largely based on mean-field approximations [1] or Green's function decoupling schemes [2], which are of doubtful accuracy.

There has been renewed interest in such models, with S = 1, in connection with experiments on solid molecular oxygen (O_2) either in bulk or monolayers adsorbed on graphite [3]. In view of this, and in view of the availability now of accurate series expansion methods [4], we have decided to revisit this problem. In the initial study reported here, we consider the S = 1 easy axis antiferromagnet on the two-dimensional square (SQ) lattice.

2. Ground State Properties

It has been proven rigorously [5] that the S =1 antiferromagnet on the SQ lattice has long range Néel order, reduced by quantum fluctuations.

We compute 'Ising expansions' [4] to order λ^{10} by writing the Hamiltonian as $H = H_0+\lambda V$, with

$$H_0 = J \sum_{<ij>} S^z_i S^z_j - D \sum_{i} (S_i^z)^2,$$

$$V = J/2 \sum_{\langle ij \rangle} (S^+_i S^-_j + S^-_i S^+_j)$$

Series are computed for the ground state energy and sublattice magnetization, and evaluated at λ =1 by standard methods.

In Figures 2 and 3 we show these quantities versus the anisotropy parameter D. For comparison we also show the same quantities as obtained from linear spin wave theory (LSWT)

$$E_0 = -2(2J+D) + 1/N \sum_k \Omega_k$$

$$M = 3/2 - 2/N \sum_k (2J+D)/\Omega_k$$

where

$$\Omega_k = 4[(J+D/2)^2 - J^2 \gamma_k^2]$$
$$\gamma_k = 1/2(\cos k_x + \cos k_y)$$

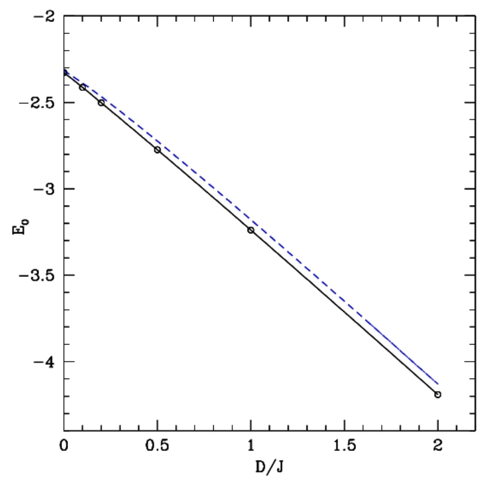

Fig.2. Ground state energy for the easy-axis antiferromagnet on the square lattice. The full line with points is the series result and the dashed line is LSWT.

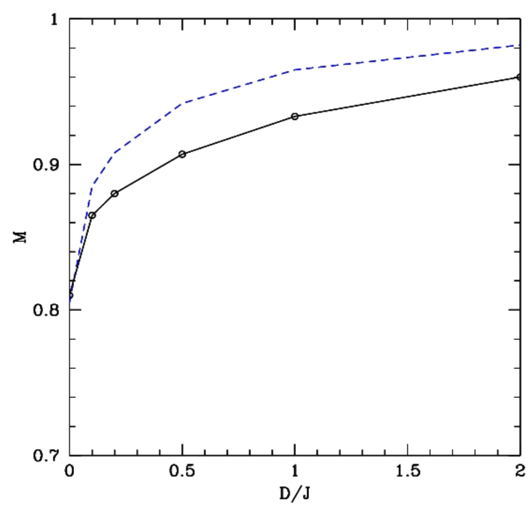

Fig. 3. Sublattice magnetization for the easy-axis antiferromagnet on the square lattice. The points and lines have the same meaning as in Fig. 2.

For D = 0 the quantum reduction in magnetization is about 20% and, as expected, this decreases with increasing D. As $D \rightarrow \infty$ the quantities approach the known Ising limits. It is evident that linear spin wave theory gives results in good agreement with these series data for the energy but overestimate the magnetization.

3. Finite Temperature Phase Transition

For D = 0 the isotropic antiferromagnet in 2 dimensions has no long range order at finite temperature (Mermin-Wagner theorem). However in the D > 0 easy-axis case the continuous symmetry of the order parameter is broken, and we expect a finite temperature transition lying in the Ising universality class.

To locate the transition line we have computed high-temperature expansions to order $(1/t)^{11}$ for the staggered susceptibility, for various values of D/J. The resulting critical line is shown in Figure 4. The critical exponent is consistent with the Ising value $\gamma = 7/4$. For comparison we show the mean-field result [1].

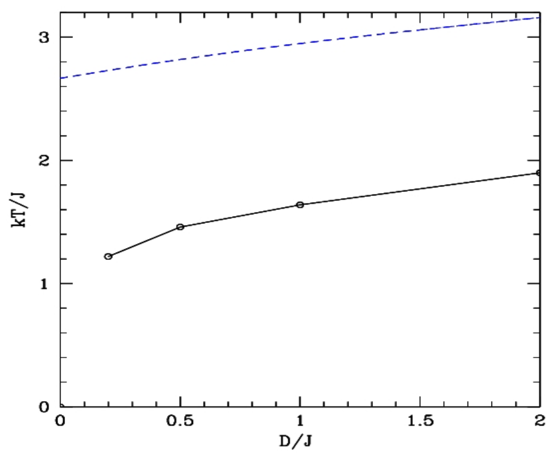

Fig. 4. Critical temperature versus anisotropy D, for the easy-axis S = 1 antiferromagnet on the square lattice. The dashed line is the mean-field result.

4. Further Work

This project is in its initial stages. We plan to continue in the following directions:

- compute the magnon excitation spectra
- consider other lattices including the frustrated triangular lattice
- investigate the more interesting (and more complex) easy-plane cases for both ferromagnetic and antiferromagnetic exchanges.

Acknowledgments

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