Spin-wave Analysis of the Spin-1 Heisenberg Antiferromagnet with Uniaxial Anisotropy in a Field

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This spin-1 model belongs to a class which may show the spin analogue of 'supersolid' behaviour. We explore spin-wave approaches to the problem. These approaches are successful in some regions, but not near the transition to the quantum paramagnetic phase, where a more generalized approach is needed.

1. Introduction

Following the remarkable discovery of supersolid (SS) behaviour in solid ^{4}He [1], a search has begun for analogous behaviour in spin systems [2], namely a phase in which both 'diagonal' and 'off-diagonal' long-range order can coexist. In fact using a Matsubara-Matsuda transformation, one can transform directly from the relevant bosonic model to a lattice spin model. The spin-1/2 models are unrealistic, however, because they require too large an uniaxial exchange anisotropy [2]. Attention has therefore turned to spin-1 models, and in particular the spin-1 Heisenberg antiferromagnet with uniaxial anisotropy in a magnetic field, with Hamiltonian

$$H = J \sum_{<ij>} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z) + \sum_i (D(S_i^z)^2 + S h_z S_i^z)$$

where <ij> denotes nearest neighbour pairs of sites, D is the single-ion anisotropy term and Δ determines the uniaxial exchange anisotropy, while h_z is the external magnetic field, rescaled by a factor S equal to the total spin. A number of magnetic materials have already been discovered which belong in this class. None of these compounds appear to have the right parameters to give a supersolid phase however.

The spin-1 version of the model has been discussed in a number of theoretical papers. Holtschneider and Selke [3] considered the classical model on a square lattice, using Monte Carlo techniques, while Peters, McCulloch and Selke treated the linear chain model using density matrix renormalization group methods. Sengupta and Batista [2] discussed the square lattice case and the cubic lattice using the stochastic series expansion Monte Carlo method. They found that a `supersolid' or `biconical' phase should exist over a range of magnetic fields for $D>0$ and $\Delta>1$. The model also exhibits other interesting phenomena such as magnetization plateaus and a multicritical point.

Our aim here is to investigate spin-wave approaches to the problem. Spin-wave approaches to the uniform Heisenberg antiferromagnet ($D=0$, $\Delta=1$) in a field have been extensively discussed by Zhitomirsky nd Nikuni [4] and Zhitomirsky and Chernyshev [5], while the zero-field case ($h_z=0$, $\Delta=1$) has been treated by Oitmaa and Hamer [6] using perturbative series expansion methods on a square lattice.

Here we treat the general case for arbitrary D and h_z, but maintain $\Delta=1$, i. e. no exchange anisotropy. This restriction is expected to rule out the most interesting physical phenomena, unfortunately, such as the supersolid phase and multicritical points, but still allows for some very interesting phase transitions.

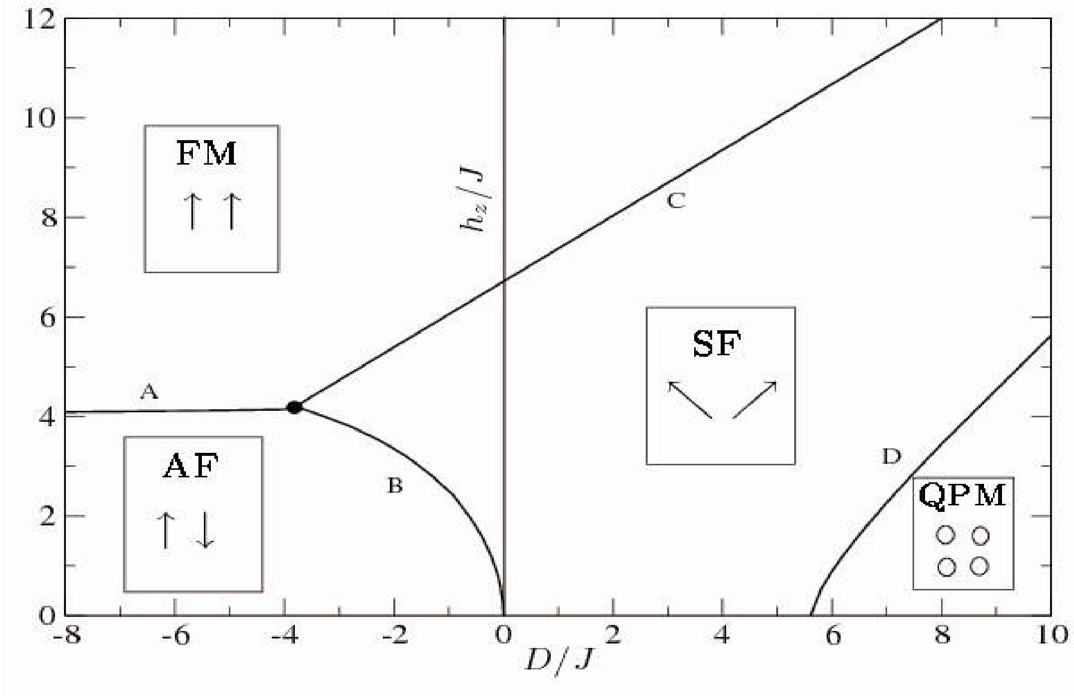

Fig. 1. Phase diagram for the square lattice.

The expected phase diagram for this case, derived from spin-wave and other theoretical approaches, is shown in Figure 1 for the case of the square lattice.

At large negative D and $h_z = 0$, the model is in a standard antiferromagnetic Néel phase (AF), with the spins aligned in the z direction ($S^z = +/-1$ on alternating sites).

At large positive D and $h_z = 0$, there is a quantum paramagnetic phase (QPM), with $S^z = 0$ at every site, so that all linear order parameters $<S^\alpha>$ vanish, and only a quadratic order parameter such as $Q_z = <2/3-(S^z_i)^2>$ is non-zero.

When h_z is very large, the system enters a simple ferromagnetic (FM) phase, with all spins aligned in the z direction.

Finally, in between these three regions is a fourth phase, the spin-flop (SF) phase with ferromagnetic order in the z direction M^z, and antiferromagnetic order in the xy plane ($M^x{}_S$, say), which spontaneously breaks the planar U(1) symmetry of the model. The Goldstone theorem then requires that the system should exhibit a gapless Goldstone mode in this region. One of the issues to be explored in this paper is whether spin-wave treatment confirms with the Goldstone theorem. The transitions between the AF phase and FM or SF phases are expected to be first order, while the transitions between the QPM and SF phases, and the SF and FM phases, are expected to be second order.

2. Spin-Flop Phase

In this phase, the spins are classically aligned at a canted angle to the x-y plane as shown in Figure 1, so we choose our quantization axes z on the A and B sublattices accordingly, canted at angle θ in the x-z plane, where θ is a variable to be determined. We then follow standard spin-wave procedure: a Holstein-Primakoff transformation from spin to boson variables, a Fourier transformation and then a Bogoliubov transformation to diagonalize the Hamiltonian through quadratic terms in the boson operators. It turns out that the angle θ is fixed by the requirement that linear terms vanish (i.e. the system is stable).

An important issue to be settled is whether the Goldstone theorem is respected by the spin-wave transformation. This is by no means obvious in the formulation; but we have been able to show that if the Hamiltonian is expanded strictly order-by-order in a 1/S expansion, the theorem is obeyed through second order - that is, a single Goldstone mode appears. In Figure 2a we see the linear Goldstone mode at (π,π), while in Figure 2b the mode becomes quadratic at the transition to the FM phase.

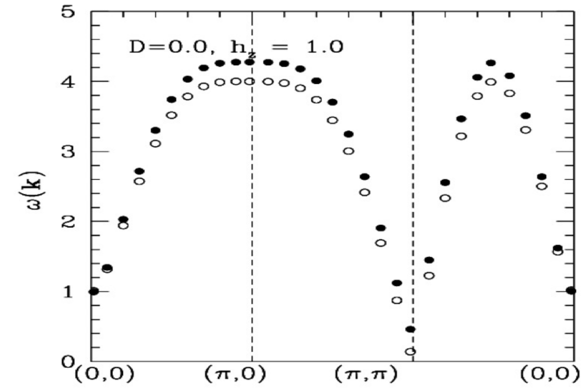

Fig. 2a. Dispersion relation at D=0, h_z = 1.
Open circles: first-order spin wave; filled circles: second-order spin wave estimates.

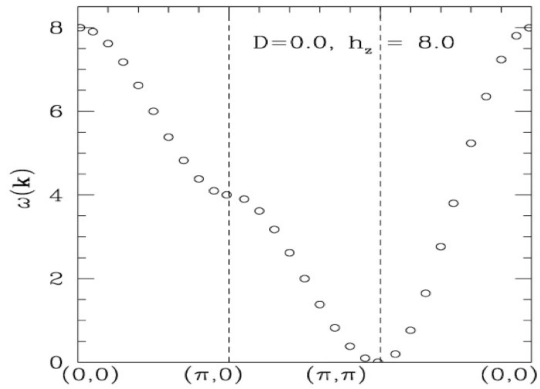

Fig. 2b. Dispersion relation at D=0, h_z=8 (first order only).

Numerically, we find that at D=0 the spin-wave expansion converges well, so that first and second order results are almost identical (Fig. 3a). At D=1, however, there is a substantial difference between first and second orders (Fig. 3b). Figure 4 shows the staggered magnetization M^x_S as a function of D at h_z=0. It can be seen that the spin-wave expansion does not reproduce the decrease towards zero at the transition to the QPM phase around D=5.6.

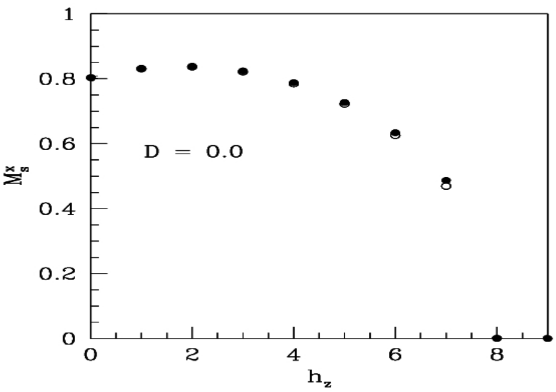

Fig. 3a. Staggered magnetization at D=0 versus h_z.

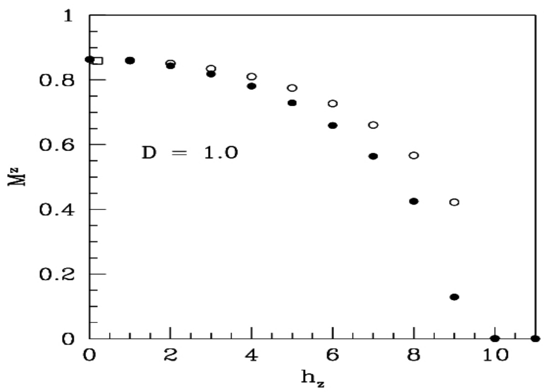

Fig. 3b. Staggered magnetization at D=1 versus h_z.

3. QPM Phase

This phase is not present in the classical (large S) limit. Here we adopt a 3-state formalism, where the vacuum is taken as the S^z=0 state at each site, and two boson fields are introduced to give excitations to the S^z = +/- 1 states respectively, using a Holstein-Primakoff formalism. The field h_z plays a trivial roe in this phase, producing a simple Zeeman splitting proportional to the total S^z. Figure 5 shows the energy gap at h_z=0 as a function of D, which vanishes at the transition point to the spin-flop phase. The second-order theory improves on the first order at large D, but higher-order terms become important near the critical point.

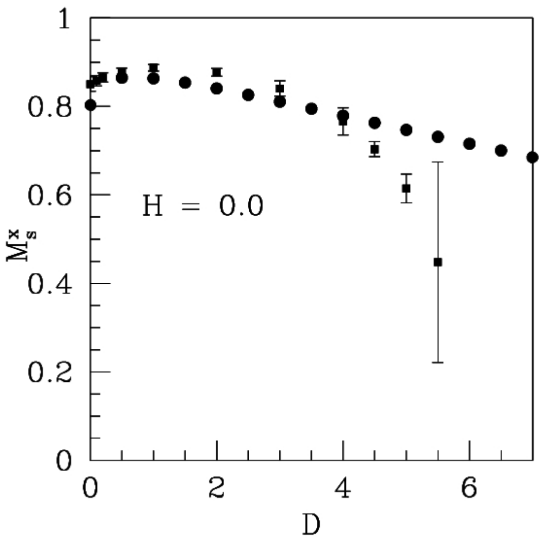

Fig. 4. Staggered magnetization as a function of D in the spin-flop phase at h_z=0. Points with error bars: series results. Filled dots: spin wave estimates.

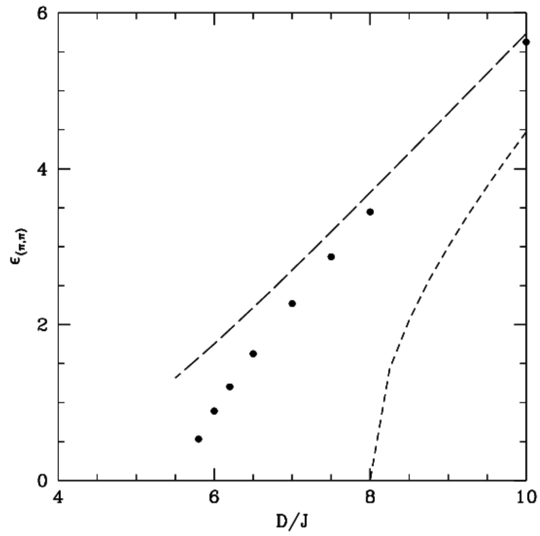

Fig. 5. Energy gap in the QPM phase as a function of D, at h_z=0. Points: series results. Short dashed line: first order, long-dashed second order spin-wave estimates.

4. Conclusions

We have studied spin-wave approaches to this spin-1 model in a magnetic field. The spin-flop phase has been treated using a standard 1/S expansion, with canted quantization axes, and we have shown that the Goldstone theorem is respected up to order 2 in 1/S. The method converges well at small D or near the FM phase boundary, but not near the transition to the QPM phase.

We have also discussed a two-boson spin wave approach within the QPM phase, where second order terms improve the results at large D, but higher-order terms become important near the critical line. Cristian Batista has commented that one needs to use a generalized expansion in this neighbourhood, choosing a more optimal basis among the three spin-1 states at each site before making the expansion.

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