Phase Diagram of the BCC *S*=1/2 Heisenberg Antiferromagnet with First and Second Neighbour Exchange

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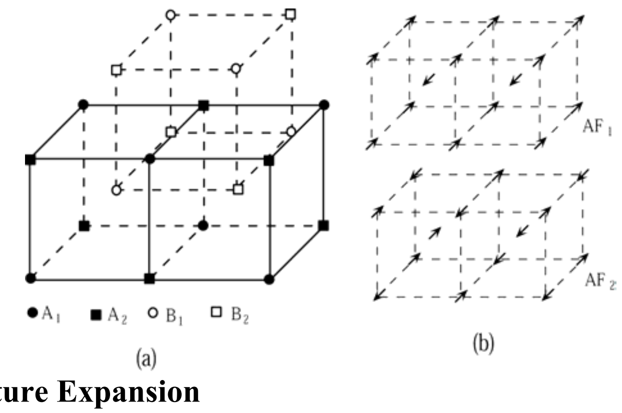
We analyse the phase structure of the spin-1/2 Heisenberg antiferromagnet with competing first and second neighbour interactions on the BCC lattice. A first-order quantum phase transition separates the AF_1 and AF_2 phases at *T=0*, and a finite *T* critical line bounds the AF_1 phase. The nature of the finite *T* transition for the AF_2 phase remains uncertain.

1. Introduction

The occurrence of competing exchange interactions in magnetic materials can give rise to a rich variety of magnetic ordered states, and of phase transitions between them. Studies of such phenomena, within the "molecular" or "mean-field" approximation go back half a century [1] or more. It is perhaps surprising that open questions remain, but, at least for quantum models, this is the case.

An example of such a system is the spin-1/2 Heisenberg antiferromagnet on the body-centred-cubic (BCC) lattice with nearest and next-nearest neighbour interactions of strength J_1, J_2. The limit J_2=0 is the pure nearest-neighbor BCC model, which has normal Néel anti-erromagnetic order (denoted AF_1) up to a finite critical temperature. On the other hand if J_2>>J_1 the ordered phase (denoted AF_2) has all second-neighbor spin ordered antiferromagnetically and the nearest neighbor spins locked to those in one of two degenerate configurations. Figure 1 shows the lattice and the ordered states.



2. Zero-Temperature Expansion

The Hamiltonian is written as

$$H = H_0 + \lambda V$$

where H_0 is the Ising Hamiltonian

$$H_0 = J_1 \sum_{<ij>} S_i^z S_j^z + J_2 \sum_{[ij]} S_i^z S_j^z$$

and the perturbation V is

$$H_0 = J_1 \sum_{<ij>} (S_i^x S_j^x + S_i^y S_j^y) + J_2 \sum_{[ij]} (S_i^x S_j^x + S_i^y S_j^y)$$

where the summations $<ij>$, $[ij]$ are over first and second neighbour pairs. Series are obtained in powers of λ, through λ^8, and extrapolated to $\lambda = 1$. Results are obtained for the ground state energy, the staggered magnetization and pair correlations for both AF_1 and AF_2 phases.

Figure 2 shows the ground state energy, and 3 the magnetization and the "discriminant"

$$\Delta C = \left| 3 < S_i^z S_j^z > - < \mathbf{S}_i \cdot \mathbf{S}_j > \right| \qquad [1]$$

which is a measure of the breaking of spin rotation symmetry.

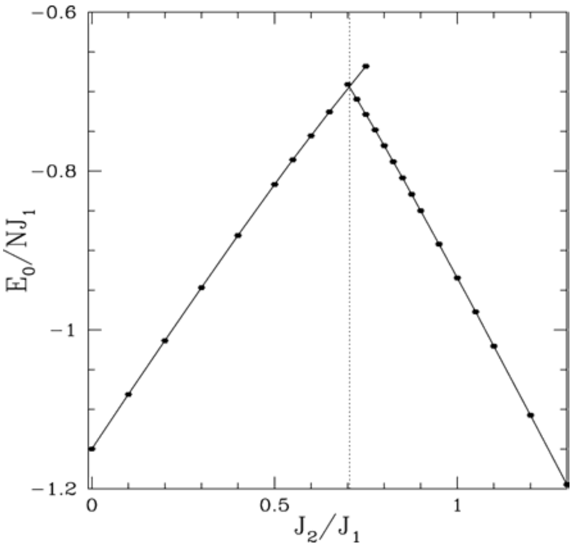


Fig.2 Ground state energy versus J_2/J_1 from Ising expansions for the AF_1 and AF_2 phases. The crossing point at 0.705±0.005 identifies the first-order quantum phase transition. Uncertainties in the series extrapolation are no larger than the symbols.

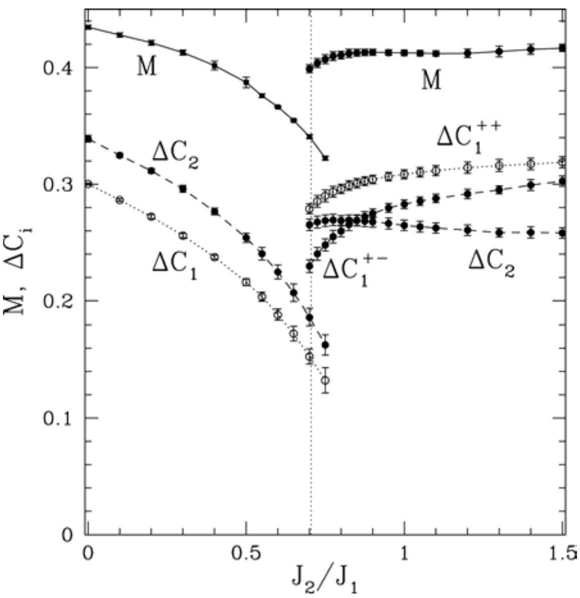


Fig.3 Staggered magnetizations (order-parameters) and correlator discriminants (Eq. 1) versus J_2/J_1, in both the AF_1 and AF_2 phases. ΔC_1, ΔC_2 refer to first and second neighbour correlators respectively. In the AF_2 phase the superscripts ++ and +− refer to first neighbour correlators for sites with like spins and unlike spins. The thin vertical line denotes the transition.

3. High-Temperature Expansion

The appropriate staggered susceptibility which diverges at the antiferromagnetic-paramagnetic phase boundary is obtained as a high-temperature expansion in the form

$$\chi = 1 + \sum_{r=1}^{\infty} a_r(\alpha) K^r$$

where $K = J_1 / k_B T$ and $\alpha = J_2 / J_1$. We have obtained the a_r polynomials through order 10 for the AF_1 phase and order 9 for the AF_2 phase, substantially extending previous series.

Analysis of the AF_1 series, using Padé approximants, finds a consistent singularity giving the locus of the AF_1-paramagnetic critical line. The critical exponent is $\gamma \approx 1.4$, as expected for the n=3 universality class. The AF_2 series is less regular. Analysis gives an apparent critical line but the exponent γ shows a steady decrease from large J_2, where the AF_2 phase is most stable, to smaller J_2 values. The resulting phase diagram is shown in Figure 4.

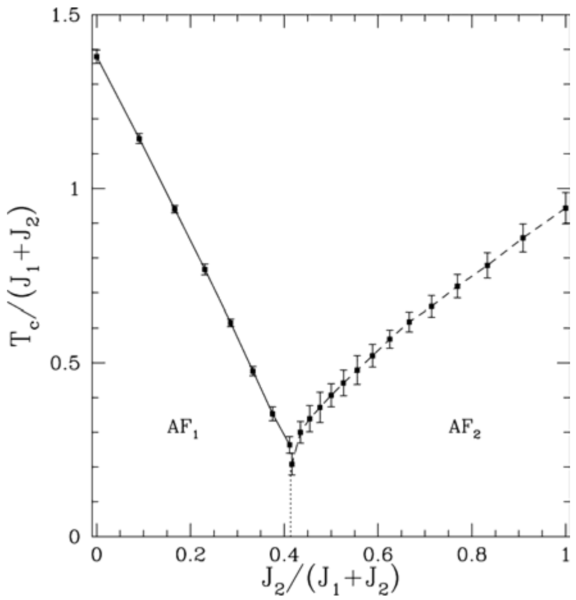


Fig.4 Phase diagram of the BCC $J_1 - J_2$ antiferromagnet. The solid line is the AF_1-paramagnetic critical line, with universal *n*=3 exponents. The dashed line is the AF_2-paramagnetic transition line, as determined from our series. The short vertical dotted line is the first-order AF_1-AF_2 transition line, extending from the bicritical point (or critical end-point) to the quantum phase transition point on the T=0 axis.

There are two possible scenarios for the AF2/paramagnetic transition

- The transition is second-order, in which case it meets with the AF_1/paramagnetic critical line at a bicritical point $J_2 / J_1 \approx 0.71$, $k_B T / J_1 \approx 0.34$. The transition lies in a different universality class, with an n=6 component order parameter. The apparent varying exponent can then be interpreted as due to crossover effects.
- The true transition is first-order, in which case our series is diverging on a "spinodal line" inside the ordered phase. This is suggested by a renormalization group calculation [4], and by the occurrence of a first-order transition in the corresponding Ising system [5].

On the basis of high-temperature series alone we cannot resolve this question.

Acknowledgments

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References

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