Heisenberg antiferromagnets with exchange and cubic anisotropies

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\textbf{Abstract.} We study classical Heisenberg antiferromagnets with uniaxial exchange anisotropy and a cubic anisotropy term on simple cubic lattices in an external magnetic field using ground state considerations and extensive Monte Carlo simulations. In addition to the antiferromagnetic phase field–induced spin–flop and non–collinear, biconical phases may occur. Phase diagrams and critical as well as multirrgical phenomena are discussed. Results are compared to previous findings.

1. Introduction

Recently, there has been a renewed interest in uniaxially anisotropic Heisenberg antiferromagnets in a field, for many years known to display antiferromagnetic and field–induced spin–flop phases. This interest is due to various reasons, among others, (i) to clarify the phase diagram of the prototypical XXZ model, especially for the square lattice [1, 2, 3], (ii) to study multicritical, like bi– and tetracritical, behavior [4, 5], and (iii) to elucidate ground states as well as thermal properties of low–dimensional quantum magnets exhibiting, possibly, ‘supersolid’ magnetic (i.e. non–collinear ’biconical’ [6]) structures [7, 8, 9]. Of course, rather recent pertinent experiments also should be mentioned [10, 11].

2. Results

As a starting point of theoretical studies on uniaxially anisotropic Heisenberg antiferromagnets, one often considers the XXZ model, with the Hamiltonian

\[ H_{\text{XXZ}} = J \sum_{i,j} \left[ \Delta (S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z \right] - H \sum_i S_i^z \]  \hspace{1cm} (1)

where \( J > 0 \) is the exchange coupling between spins being located on neighboring lattice sites \( i \) and \( j \). \( \Delta \) is the exchange anisotropy, \( 1 > \Delta > 0 \), and \( H \) is the applied magnetic field along the easy axis, the \( z \)-axis. The model has been found to display in the (temperature \( T \), field \( H \))-plane antiferromagnetic (AF) and spin–flop (SF) phases on square and simple cubic lattices. In two dimensions, the transition between the two phases had been argued to be of first order in case of the spin–1/2 quantum case [3, 12]. In contrast, in the classical case (with spin vectors of length one) there appears to be a narrow disordered phase in between the two ordered phases. The three phases seem to meet at zero temperature in a ‘hidden tetracritical point’ [2, 3] at
the critical field $H_c$. That point is a highly degenerate ground state, where also biconical (BC) spin configurations are stable [3]. The antiferromagnetic, biconical, and spin–flop classical spin configurations are shown in Fig. 1. For the XXZ model on the simple cubic lattice, the phase diagram has been believed to show the same topology as in the mean-field approximation, with a direct transition of first order between the AF and SF phases, ending in a bicritical point at which the two critical phase boundary lines between the paramagnetic (P) phase and the AF as well as the SF phases meet with the AF-SF transition line [13]. Recently, this scenario has been scrutinized using renormalization group methods [4, 5]. One of the aims of our study is to shed light upon this issue, applying extensive Monte Carlo simulations.

Figure 1. Spin orientations on neighboring sites showing antiferromagnetic (a), biconical (b), and spin–flop (c) ground state structures in the XXZ model.

The phase diagram obtained from our simulations, analyzing systems with up to $32^3$ spins in runs of, at least, $10^7$ Monte Carlo steps per spin, is shown in Fig. 2. Indeed, setting $\Delta = 0.8$, we can locate the triple point of the AF-P, SF-P, and AF-SP boundary lines accurately, at $k_B T_t/J = 1.025 \pm 0.015$ and $H_t/J = 3.90 \pm 0.03$, differing quite substantially from the old estimate based on appreciably shorter simulations [13].

Figure 2. Phase diagram of the XXZ antiferromagnet, with $\Delta = 0.8$. Inset: Vicinity of the triple point.

Moreover, studying the transitions in the vicinity of that triple point, we do not observe deviations from the previously anticipated bicritical scenario [13], with the AF-P boundary line belonging to the Ising, and the SF-P boundary line belonging to the XY universality class. We identify the universality classes from determining critical exponents, e.g., of the (staggered) longitudinal and tranverse susceptibilities, and from determining the critical Binder cumulants of the AF and SF order parameters [14]. Note that in a renormalization group calculation to high loop order, a different scenario had been put forward [4], favouring the existence of a tetracritical point or some kind of critical end point. In that scenario, one expects either a stable BC phase near $(T_t, H_t)$ or at least one of the AF-P and SF-P boundaries should become a line of transitions of first order near that point [4]. In our simulations, we observe that biconical spin configurations show up close to the AF-SF phase boundary at low temperatures, reflecting the, again, high degeneracy of the ground state at the critical field separating the AF and SF structures. However, these configurations do not destroy, in contrast to the situation in two dimensions, the direct AF-SF transition of first order [15]. Actually, applying also renormalization group arguments, it has been suggested very recently that the type of the triple point may depend on the strength...
of the anisotropy, allowing for a bicritical point [5]. Perhaps, Monte Carlo studies on different values of the anisotropy may provide further insights.

Adding, especially, single–ion terms due to crystal–field anisotropies to the XXZ model, eq. (1), BC spin configurations may be stabilized over a range of fields in the ground state. This behavior has been observed for quantum and classical spins on chains and square lattices for a quadratic single–ion term [7, 8, 9, 16]. Here we shall add to $\mathcal{H}_{XXZ}$ a cubic anisotropy term of the form [17]

$$\mathcal{H}_{CA} = F \sum_i \left[ (S_i^x)^4 + (S_i^y)^4 + (S_i^z)^4 \right]$$

where $F$ denotes the strength of the cubic anisotropy. The sign of $F$ determines whether the spins tend to align along the cubic axes, for $F < 0$, case 1, or, for $F > 0$, case 2, in the diagonal directions of the lattice. Because of these tendencies, the BC, (i.e. BC1 or BC2), structures, as well as the SF structures, show no full rotational invariance in the $xy$–plane, in contrast to the XXZ case discussed above. Now, obviously, the discretized spin projections in the $xy$–plane favour four directions [14, 15].

The resulting ground state phase diagram of the full Hamiltonian, $\mathcal{H}_{XXZ} + \mathcal{H}_{CA}$ with fixed exchange anisotropy, $\Delta = 0.8$, and varying cubic term, $F$, may be determined numerically without difficulty, as depicted in Fig. 3.

![Ground states of the full Hamiltonian with exchange anisotropy, $\Delta = 0.8$, and the cubic term.](image)

Note that, for $F < 0$, the transitions to the BC1 structures are typically of first order, with a jump in the tilt angles, $\Theta$, with respect to the $z$–axis, see Fig. 1, characterizing the BC configurations. However, in the reentrance region between the SF and BC1 structures at $F/J$ close to -1, the change in the tilt angles seems to be smooth at the transitions [14].

Obviously, at non-zero temperatures, several interesting scenarios leading, possibly, to multicritical behaviour, where AF, SF, BC, and P phases meet, may exist. So far, we focussed attention on two cases: (a) Positive cubic anisotropy $F > 0$, at constant field $H/J = 1.8$ [15], see Fig. 3. At small values of $F$, there is an AF ordering at low temperatures. Above a critical value, $F_c = 0.218...J$, the low–temperature phase is of BC2 type, followed by the AF and P phases, when increasing the temperature. The transition between the AF and P phases is found to belong to the Ising universality class, while the transition between the BC2 and AF phases seems to belong to the XY universality class, with the cubic term being then an irrelevant perturbation [15]. (b) Negative $F$, fixing the cubic term, $F/J = -2$, and varying the field, see Fig. 3. In accordance with the ground state analysis, we observe, at sufficiently low temperature, $k_B T/J = 0.2$, AF, SF, BC1, and P phases, when increasing the field, as depicted in Fig. 4. Interestingly, the BC1 phase seems to become unstable when raising the temperature, with the other phases being still present [14], see Fig. 5. This may suggest that the three boundary lines between the BC1–P, SF–BC1, and SF–P phases meet at a multicritical point. Of course, further
clarification and a search for other, possibly multicritical scenarios at different strengths of the cubic term, $F$, are desirable.

Figure 4. Staggered magnetizations versus field at $F/J = -2$ and $k_B T/J = 0.2$, indicating the AF, SF, BC1, and P phases, when increasing the field.

Figure 5. Staggered magnetizations versus field, at $F/J = -2$ and $k_B T/J = 0.4$, with the BC1 phase being squeezed out. Systems with 16³ spins are simulated.

In summary, we have studied antiferromagnets with fixed exchange and varying cubic anisotropies in a field on the simple cubic lattice. In the case of the XXZ model, the nature of the triple point and the thermal role of BC structures have been clarified. By adding the cubic anisotropy, discretized BC phases may be stabilized leading to interesting critical and multicritical phenomena.

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