Multicritical points in the three-dimensional XXZ antiferromagnet with single-ion anisotropy

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The classical Heisenberg antiferromagnet with uniaxial exchange anisotropy, the XXZ model, and competing planar single-ion anisotropy in a magnetic field on a simple cubic lattice is studied with the help of extensive Monte Carlo simulations. The biconical (supersolid) phase, bordering the antiferromagnetic and spin-flop phases, is found to become thermally unstable well below the onset of the disordered, paramagnetic phase, leading to interesting multicritical points.

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Uniaxially anisotropic Heisenberg antiferromagnets in a magnetic field have been studied quite extensively in the past, both experimentally and theoretically [1, 2]. Usually, they display, at low temperatures and fields, the antiferromagnetic (AF) phase and, when increasing the field, the spin–flop (SF) phase. A prototypical model describing these phases as well as multicritical points, is the Heisenberg model with a uniaxial exchange anisotropy, \( H_{\text{xxz}} \):

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

(1)

where \( J > 0 \) is the antiferromagnetic exchange coupling between classical spins, \((S_i^x, S_i^y, S_i^z)\), of length one at neighboring sites, \(i\) and \(j\), on a simple cubic lattice, \( \Delta \) is the uniaxial exchange anisotropy, \(1 > \Delta > 0\), and \(H\) is the applied magnetic field along the easy axis, the \(z\) axis.- Recently, we presented numerical evidence for the existence of a bicritical point in the Heisenberg universality class [3], at which the AF, SF and paramagnetic (P) phases meet. Especially, there the value of the critical isotropic Binder cumulant agrees closely with the one of the perfect Heisenberg model. The scenario is in accordance with early renormalization group (RG) analyzes in one–loop–order [4, 5], as well as a subsequent RG calculation in two–loop–order [6] showing that such a bicritical point may exist. Note that a conflicting characterization of the multicritical AF-SF-P point as a 'biconical fixed point' [7, 8] has been suggested, mainly based on high-order RG arguments, augmented by Monte Carlo simulations.

In this contribution, we shall consider the XXZ model, Eq. (1), with an additional planar single-ion anisotropy, competing with the uniaxial exchange anisotropy. This term reads

\[
H_{\text{si}} = D \sum_i (S_i^z)^2
\]

(2)

The full model, \( H_{\text{xxz}} + H_{\text{si}} \), has been investigated, in the last few years, carefully, especially, for \(S = 1\) quantum antiferromagnetic spin chains, displaying a supersolid phase [9–11], being the analog of the mixed or biconical (BC) phase [5, 12, 13] in standard notation for magnets. One may also mention a study for the classical full model on square lattices [14]. Again, the BC phase arises from the competition between the uniaxial exchange and planar single-ion anisotropies.

In the BC phase, see Fig. 1, spins on the bipartite sublattices form cones with different opening angles so that one gets coexisting orders of the staggered transverse, \(xy\), spin components, like in the SF phase, as well as longitudinal, \(z\), components, like in the AF phase.

The resulting ground state phase diagram for the classical model on a simple cubic lattice may be determined analytically [12, 14]. Possible ground states are depicted in Fig. 1, showing AF, SF, and BC spin configurations. A concrete example of the ground state phase diagram in the \((H/J, D/J)\) plane, setting \(\Delta = 0.8\), is displayed in Fig. 2. The BC structure is seen to intervene between the AF and SF structures for non-zero planar single-ion anisotropy \(D/J < 0.6\). The opening angles \(\Theta_A\) and \(\Theta_B\) are uniquely related, depending on the field, continuously approaching the limiting values of the AF and SF orientations. The BC structure reaches its maximal extent close to \(D/J = 0.4\). The lower critical field between the AF and BC ground states, \(H_{ab}\), is given by

\[
H_{ab} = \sqrt{(6J - 2D)^2 - (6J\Delta)^2}
\]

(3)

and the upper critical field, separating the BC and SF ground states, \(H_{bs}\), is given by

\[
H_{bs} = \frac{[36J^2 - (6J\Delta + 2D)^2]}{H_{ab}}.
\]

(4)
The transition from the SF to the ferromagnetic (F) ground state occurs at the field $H_{sf}$ with

$$H_{sf} = 6J(1 + \Delta) + 2D.$$  \hspace{1cm} (5)

At non-vanishing temperatures, the BC phase may be expected to lead to a tetracritical point \cite{17, 18, 19}, at which the AF, SF, BC, and P phases meet. One of the aims of the present study has been to clarify this expectation by using extensively Monte Carlo (MC) techniques \cite{16}.

Following previous MC studies on the XXZ model and variants \cite{3, 14, 17, 18}, we fixed the exchange anisotropy at $\Delta = 0.8$. The single-ion anisotropy has been chosen to be, mostly, $D/J \approx 0.2$. At the end of this paper, results for $D/J = 0.4$ will be briefly discussed as well. To take into account systematically finite-size effects \cite{19}, we simulated cubic lattices with $L^3$ spins, with $L$ ranging from 4 to 32, employing full periodic boundary conditions. To obtain data of the desired accuracy, runs with, at least, $5 \times 10^7$ Monte Carlo steps per spin were performed, applying the standard Metropolis MC algorithm. Error bars result from averaging over a few of such runs. When error bars are not depicted in the figures, then they are smaller than symbol sizes.

To determine the phase diagram, we record, especially, quantities related to the Ising, XY, Heisenberg, and biconical order parameters. In particular, we monitor the absolute values of the staggered longitudinal, $m_{st}^z$, transverse, $m_{st}^{xy}$, and isotropic, $m_{st}^{yz}$, magnetizations as well as of the product of the staggered longitudinal and transverse magnetization components. Furthermore, related staggered susceptibilities, namely, $\chi_{st}^z$, $\chi_{st}^{xy}$, and $\chi_{st}^{yz}$, are computed. In addition, we calculate corresponding longitudinal, transverse, and isotropic Binder cumulants \cite{20}, $U^z$, $U^{xy}$, and $U^{yz}$.

The interesting part of the resulting phase diagram is depicted in Fig. 3: Two distinct multicritical points occur, the AF-SP-P and the AF-BC-SF points.

As before \cite{3}, to obtain the AF–P boundary, with the transition being in the Ising universality class, the size dependence of the height and position of the maximum in the longitudinal staggered susceptibility, $\chi_{st}^z$, allows for reliable estimates. $U^{xy}$ turns out to be very useful in estimating the SF–P transition line. There one observes rather small finite–size correction terms to the critical Binder cumulant for cubic lattices in the XY universality class \cite{21}, $(U^{xy})^c = 0.586..$, with the critical Binder cumulant being the cumulant at the transition in the thermodynamic limit, $L \to \infty$. It turned out to be less straightforward to identify the transition between the AF and SF phases, with, possibly, an intervening BC phase.

Indeed, the extent of the BC phase follows from the behavior of the staggered longitudinal and transverse susceptibilities, $\chi_{st}^z$ and $\chi_{st}^{xy}$, with the AF-SF transition being signalled by the peak in $\chi_{st}^{xy}$, and the BC-SF transition being indicated by the location of the maxima in the longitudinal susceptibility. Obviously, the BC phase shrinks with increasing temperature, becoming, eventually, very narrow. Accordingly, further analyzes are needed to check the possible vanishing of the BC phase, which would then imply the existence of an AF-BC-SF multicritical point.

A convenient way for identifying the AF-BC-SF point is demonstrated in Fig. 4. There, the size dependence of the height of the maxima in the staggered longitudinal and transverse susceptibilities is shown, both in the case of an intervening BC phase, at the lower temperature, $k_BT/J = 0.6$, and in case of a direct AF-SF transition of first order, at the higher temperature, $k_BT/J = 0.9$.

In fact, at the higher temperature, the maxima of both susceptibilities grow to a good approximation like $L^3$, for $L$ exceeding about 8, see Fig. 4. This behavior is in accordance with a transition of first order. In marked contrast, at the lower temperature, $k_BT/J = 0.6$, both maxima occur at distinct fields, reflecting the separate AF-BC and BC-SF transitions. Moreover, the heights of

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**FIG. 2.** Ground states in the $(H/J, D/J)$ plane of the full model on a cubic lattice with uniaxial exchange anisotropy $\Delta = 0.8$ and planar single-ion anisotropy, $D/J > 0$.

**FIG. 3.** Phase diagram in the temperature-field plane of the three-dimensional full model with $\Delta = 0.8$ and planar single-ion anisotropy $D/J = 0.2$. The broken line indicates transitions of first order.
the peaks grow much weaker with system size: The effective exponents, described by the local slopes between successive points in the doubly logarithmic plot, are clearly smaller than 3, as illustrated in Fig. 4. Actually, for both susceptibilities we find similar results for the effective exponents, dropping down, for the largest sizes we studied, to values even well below 2, to about 1.6.

Actually, one may expect the AF-BC transition to belong to the XY, and the BC-SF transition to the Ising universality class. A detailed description of these transitions is, however, beyond the scope of the present study. We also refrained from attempting to locate the AF-BC-SF point very accurately, and to elucidate its (critical) properties. Its position is roughly at $k_B T_{ \text{abs}}/J = 0.85 \pm 0.05$.

In any event, the AF-BC-SF point occurs well below the AF-SF-P multicritical point, $k_B T_{\text{abs}}/J = 1.075 \pm 0.01$, $H_{\text{abs}}/J = 3.490 \pm 0.002$, at which the continuous AF-P and SF-P phase transition lines meet the AF-SF transition line of first order. Obviously, the upper multicritical point reminds of the multicritical point in the XXZ model on the cubic lattice. Accordingly, the planar single-ion anisotropy leads to a BC phase, but it does not lead to a tetracritical AF-BC-SF-P point, at least, in the case we considered so far, $D/J = 0.2$.

To elucidate the nature of the AF-SF-P multicritical point, we studied in its vicinity, especially, the isotropic Binder cumulant $U^{xyz}(T, H, L)$. In case of a bicritical point with Heisenberg symmetry, the critical Binder cumulant $(U^{xyz})^*$ may be expected to acquire the characteristic value 0.620 $(\pm 0.003)$, using periodic boundary conditions for lattices of cubic shape.

Similarly to the findings for the perfect XXZ model, $D = 0$, we may distinguish three different scenarios, when varying the temperature and monitoring the size dependence of $U^{xyz}$ as a function of the field $H$.

Below the AF-SF-P point, e. g., at $k_B T/J = 1.05$, $U^{xyz}$ increases with larger lattice size $L$, so that there are no intersection points of the isotropic cumulants near the direct AF-SF transition.

At $k_B T/J = 1.075$, see Fig. 5, all intersection points of the isotropic cumulants, for lattices of sizes $L$ ranging from 8 to 32, occur closely to the characteristic Heisenberg value, $(U^{xyz})^* \approx 0.620$. This fact may be interpreted as evidence for being in the immediate vicinity of a bicritical point of Heisenberg symmetry. Actually, moving to higher temperatures, another scenario shows up. For example, at $k_B T/J = 1.1$, there are still intersection points of the cumulants for different lattice sizes, but they shift systematically for larger lattices to lower and lower values below that of the critical cumulant in the Heisenberg case. For instance, the intersection point of the cumulants for the two largest sizes, $L = 24$ and 32, is even below 0.58.

As for the perfect XXZ model, these observations on the isotropic Binder cumulant are consistent with the AF-SF-P point, at $D/J = 0.2$, being a bicritical point in the Heisenberg universality class.

Note that the staggered isotropic susceptibility seems to be the less sensitive quantity to identify the nature of the AF-SF-P point, with the values of the critical exponent for bicritical and biconical multicritical points being very close to each other.

Finally, we mention briefly results of our (preliminary) simulations for an enhanced planar single-ion anisotropy, $D/J = 0.4$. Again, there is no evidence for a tetracritical AF-BC-SF-P point. Instead, we find an AF-BC-SF point. It is followed, at higher temperatures, by a direct transition of first order between the AF and SF phases, with the BC phase being squeezed out. Upon further increase of the temperature, an AF-SF-P multicritical point occurs.

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