Quantum Heisenberg antiferromagnetic chains with exchange and single-ion anisotropies

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Abstract. Using density matrix renormalization group calculations, ground state properties of the spin–1 Heisenberg chain with exchange and quadratic single-ion anisotropies in an external field are studied, for special choices of the two kinds of anisotropies. In particular, the phase diagram includes antiferromagnetic, spin-liquid (or spin-flop), IS2, and supersolid (or biconical) phases. Especially, new features of the spin-liquid and supersolid phases are discussed. Properties of the quantum chains are compared to those of corresponding classical spin chains.

1. Introduction
Recently, low dimensional quantum anisotropic Heisenberg antiferromagnets in a field have been shown to display the analog of the supersolid phase [1, 2, 3, 4, 5]. In the language of classical magnetism, the phase is usually denoted as the biconical phase [6], in which the order parameters of both the antiferromagnetic and the spin-flop phase do not vanish. For instance, the supersolid phase has been found to occur in the ground state of a spin–1 antiferromagnetic chain with exchange and single-ion anisotropies, applying Monte Carlo simulations and perturbation theory [2]. The ratio between the uniaxial exchange anisotropy $\Delta$ and the competing quadratic single–ion anisotropy $D$ had been fixed, $D/J = \Delta/2$ [1, 2]. In our subsequent study on the same model, using density matrix renormalization group (DMRG) techniques, we provided evidence, for spin chains of finite length, for having two types of supersolid as well as two types of spin–liquid, known in classical magnetism as spin–flop, structures [5]. In this contribution, we shall elaborate on our previous study. Moreover, we shall also investigate another part of the ground state phase diagram by fixing $\Delta$, $\Delta = 5$, and varying $D$, as had been done before for a limited range of $D$ [7]. Again, the supersolid phase is stable. In addition, we identify commensurate and incommensurate spin-liquid structures. We compare results on the quantum chains to ones on corresponding classical spin chains, discussing similarities and striking differences.

2. Results
In the following, we shall consider the spin–1 anisotropic antiferromagnetic Heisenberg chain in a field described by the Hamiltonian

$$\mathcal{H} = \sum_i (J(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z) + D(S_i^z)^2 - BS_i^z)$$ (1)

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where \( i \) denotes the lattice sites. For \( \Delta > 1 \), there is an uniaxial exchange anisotropy, along the direction of the field, \( B > 0 \), the \( z \) axis. Depending on the sign of \( D \), the single-ion term leads to a competing planar, \( D > 0 \), or to an enhancing uniaxial anisotropy. We shall analyse ground state properties using DMRG techniques \([8, 9]\) for chains with open boundary conditions and up to \( L = 128 \) sites. In addition, we shall determine the ground states of corresponding infinite chains with classical spin vectors of length one \([10, 11]\).

We first briefly deal with the case \( D/J = \Delta/2 \) \([2, 5]\). The ground state phase diagram in the \((\Delta, B/J)\) plane has been found \([2, 5]\) to comprise antiferromagnetic (AF), spin-liquid (SL), supersolid (SS), ferromagnetic (F), and (IS2), with a magnetization plateau at half saturation, phases. At small values of \( \Delta \) and small fields, the Haldane phase is observed \([12]\). In comparison, the corresponding classical spin chain shows a much broader biconical (BC) phase, being effectively replaced not only by the supersolid phase but also, largely, by the spin-liquid and IS2 phases. Note that the IS2 phase is similar to the \((1,0)\) phase in the corresponding classical Ising model, the antiferromagnetic Blume Capel model.

Interesting information is given by the magnetization profiles, \( m_i = \langle S_z^i \rangle \), with brackets, \( \langle ... \rangle \), denoting quantum mechanical expectation values. In particular, we observed distinct profiles in the SS phase in between the AF and IS2 and in between the AF and SL phases, respectively. For odd \( L \), in the SS phase on approach to the IS2 phase, the local magnetizations \( m_i \) at odd sites stay close to one, while at even sites they tend roughly to zero. In contrast, in the SS phase on approach to the SL phase, the magnetizations on odd and even sites tend to take on the same values \([5]\). In the SL phase we found also (studying situations with \( \Delta \) exceeding \( \approx 2.5 \)) two distinct types of profiles, for finite chains, when varying \( M/L \), where \( M \) is the total magnetization \([5]\): For \( M < L/2 \), the profiles exhibit a broad plateau in the center of the chain, as expected for a classical spin-flop (SF) structure, while pronounced modulations in \( m_i \) occur at \( M > L/2 \), see Fig. 1. This may signal a change from commensurate (C) to incommensurate (IC) structures \([5]\). The suggestion is now confirmed and quantified by analysing the Fourier transform of the profiles, especially at \( \Delta = 3.5 \). The modulation in the IC region of the SL phase is described nicely by the wavenumber (setting the lattice spacing equal to one) \( q = 2\pi(1 - m) \), \( m = M/L \). Such an IC modulation, with algebraic decay, is expected to hold in the entire SL phase of the spin–1/2 anisotropic Heisenberg chain in a field \([13]\). In the classical variant, we find no IC structures in the spin-flop phase, for finite and infinite chains.

![Figure 1](image)

Figure 1. Magnetization profiles in the spin-liquid phase for \( \Delta = 2D/J = 3.5 \) at various total magnetizations for a chain with \( L = 63 \) sites.

Let us now turn to the case of fixed exchange anisotropy, \( \Delta = 5.0 \), varying the single-ion term, \( D \). The ground state phase diagrams for the spin–1 and the classical chains are depicted in Figs. 2 and 3. For the classical model the calculation of the phase borders can be carried out exactly, see e.g. \([10, 11]\) for comparison with Monte Carlo data. In the quantum case we determined the ground-state energies, magnetization profiles, spin-spin correlation functions for each possible magnetization of chains with up to 63 sites and from these properties obtained the phase borders. We considered positive and negative single-ion anisotropies, \( D \).
For $D > 0$, the supersolid or biconical phase is stable at zero temperature. As in the case of $D/J = \Delta/2$, the broad BC phase of the classical chain is effectively replaced, in the quantum chain, by the corresponding, rather narrow SS phase as well as SL and IS2 phases.

**Figure 2.** Ground state phase diagram of the classical infinite anisotropic Heisenberg chain with $\Delta = 5.0$.

In contrast to the case $D/J = \Delta/2$, the supersolid phase is always bordered by the AF and SL phases. Accordingly, we observe only one type of magnetization profile. Illustrative examples are depicted in Fig. 4, at $D/J = 3.0$ and various fields. In the SS phase, at given single-ion anisotropy, $D$, and field, $B$, the magnetization takes on different values at odd and even sites in the center of the chain. The local magnetization $m_i$ tends to acquire the same value at odd and even sites on approach to the SL phase in the quantum chain. Actually, the classical BC phase is usually described by two tilt angles, with respect to the $z$ axis for the two sublattices formed by neighboring sites, with the tilt angles approaching each other when getting closer to the SF phase [10, 11]. Obviously, this behavior is completely analogous to the one depicted in Fig. 4.

**Figure 3.** Ground state phase diagram of the spin–1 anisotropic Heisenberg chain with $\Delta = 5.0$.

Increasing $D$, the ‘large D’ phase [14, 15, 16, 17] may eventually be stable. It corresponds to the planar phase in the classical model with vanishing field, with the spin vectors pointing perpendicular to the $z$ axis, being the ground state for $D/J \geq 4$. The new phase may be expected to give rise to a SL phase at non zero fields. A discussion of this interesting aspect is, however, beyond the scope of the present contribution.

**Figure 4.** Magnetization profiles in the supersolid phase at $\Delta = 5.0$, $D/J = 3.0$, and fields $B/J$ varying between 6.5 and 6.8. Spin chains with $L = 63$ sites are considered. The lower symbols denote the even sites, the upper ones the odd sites.

For $D < 0$, the biconical or supersolid phase is no longer stable. In fact, only AF, SL (or SF), and F structures are encountered. The SL phase can be either commensurate, with a wide plateau in the magnetization profile away from the boundaries, or incommensurate, with
modulations superimposed on the average magnetization. Obviously, there are two IC phases, see Fig. 3. The one, denoted by ‘IC’ in Fig. 3, occurring essentially in between the AF and F phases, has been found before, having exponentially decaying transversal spin-spin correlations \[7\], in contrast to the usual spin-liquids with algebraic decay. It has no analog in the classical model, see Fig. 2. The related transition between the IC and SL\(_C\) phases has been obtained before, being either of first order or, at large average magnetization, continuous \[7\]. Our results agree with that description. We find another C-IC transition line between the SL\(_C\) and SL\(_{IC}\) phases at somewhat larger fields for given \(D/J\), see Fig. 3 (full circles). Note that this transition seems to take place at \(M/L\) significantly larger than 1/2 for \(D < 0\). Increasing \(D\), \(D > 0\), in the vicinity of the IS2 phase, the line goes over to the above discussed scenario with commensurate, \(M/L < 1/2\), and incommensurate, \(M/L > 1/2\), structures. By further increasing the planar single-ion anisotropy, \(D/J\) being larger than roughly 3.6, we observe in the ‘SL\(_C\)’ phase close to the IS2 phase modulated structures for rather short chains, \(L \leq 31\). The possible, additional C-IC border is not displayed in Fig. 3. Indeed, a more detailed analysis, taking into account finite size effects, is desirable.

In summary, we have studied ground state properties of spin–1 antiferromagnetic anisotropic Heisenberg chains with exchange and single-ion anisotropies in a field, for given ratio of the two kinds of anisotropies, \(D/J = \Delta/2\), and for fixed exchange anisotropy, \(\Delta = 5\), with varying single-ion anisotropy. In both cases, supersolid phases are observed, in accordance with the behavior of the corresponding classical spin chain, displaying biconical phases. The extent of the supersolid phases is, however, substantially reduced as compared to that of the biconical phases. Furthermore, the spin-liquid phases show distinct commensurate and incommensurate regions, presumably, separated by sharp transitions. A detailed analysis of the character of those novel transitions is beyond the scope of the present paper. The corresponding spin-flop phases in the classical model are always of commensurate type. In the quantum model, a IS2 phase appears as a ground state, being present in the classical variant only in the Ising limit, the Blume-Capel model.

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