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Field-induced order and magnetization plateaux in frustrated antiferromagnets

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Abstract

We argue that collinearly ordered states which exist in strongly frustrated spin systems for special rational values of the magnetization are stabilized by thermal as well as quantum fluctuations. These general predictions are tested by Monte Carlo simulations for the classical and Lanczos diagonalization for the $S = \frac{1}{2}$ frustrated square-lattice antiferromagnet.

Keywords: Field-induced order; Magnetization plateaux

Frustrated 2D quantum spin systems can give rise to interesting behavior in high magnetic fields. For example, plateaux in the magnetization curve of $SrCu_2(BO_3)_2$ have been observed at[2] $\langle M \rangle = \frac{1}{8}, \frac{1}{4}$ and $\frac{1}{3}$ [1]. This has sparked theoretical interest in the magnetization process of the related 2D Shastry–Sutherland model (see e.g. Ref. [2]).

Owing to its simplicity, the frustrated square-lattice antiferromagnet (FSAFM) in a magnetic field is a useful model system [3,4]:

$$H = J \sum_{\langle \vec{x},\vec{y} \rangle} \vec{S}_{\vec{x}} \cdot \vec{S}_{\vec{y}} + J' \sum_{[\vec{x},\vec{y}]} \vec{S}_{\vec{x}} \cdot \vec{S}_{\vec{y}} - h \sum_{\vec{x}} S^z_{\vec{x}}. \tag{1}$$

Here the $\vec{S}_{\vec{x}}$ are spin-S operators at the sites $\vec{x}$ of a square lattice and the first and second sums are over nearest and diagonal neighbor pairs, respectively. This model is realized with $S = \frac{1}{2}$ in Li_2VOSiO_4 and Li_2VOGeO_4 [5].

For $J' = J/2$ the Hamiltonian (1) can be rewritten (up to a constant) as

$$H = \frac{1}{2^n} \sum_{\alpha} \{ J \vec{L}^2_{\alpha} - h L^z_{\alpha} \} \tag{2}$$

with $\vec{L}_{\alpha} = \sum_{\vec{x} \in \alpha} \vec{S}_{\vec{x}}$ the total spin of a (four-spin) plaquette α and $n = 2$. In 2D the Kagome and checkerboard lattice and in 3D the pyrochlore and garnet lattices share this special form of the Hamiltonian.

Consider first the classical variant of the model (2) with unit spins. Then, any state with $L^z_{\alpha} = h/2J$, $L^x_{\alpha} = L^y_{\alpha} = 0$ for all α is a ground state, resulting in huge degeneracies. Special collinear groundstates exist at special values of the magnetic field (an up-up-up-down 'uuud' state for $\langle M \rangle = \frac{1}{2}$ in the FSAFM, checkerboard and pyrochlore lattice and an up-up-down 'uud' state for $\langle M \rangle = \frac{1}{3}$ in the Kagome and garnet lattice). These collinear states have a particularly large number of zero modes leading to an excepationally large number of low-energy excitations above them. At finite temperature, the a probability function is therefore peaked close to the collinear states along the ground state manifold leading to a selection of this submanifold by thermal fluctuations. The subsequent lifting of degeneracy goes differently for the FSAFM and Kagome AFM. In the former case, a unique classical state is further selected [3], whereas in the latter case there is no such selection and a collinear spin-liquid state appears on the $\langle M \rangle = \frac{1}{3}$ plateau [6].

Semiclassical analysis [3] suggests that collinear states are also stabilized by quantum fluctuations, leading to a

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[2] We normalize the magnetization to $|\langle M \rangle| \leqslant 1$.

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plateau in the magnetization curve of the quantum spin model. In fact, plateaux with $\langle M \rangle = \frac{1}{2}$ are expected in the quantum FSAFM, checkerboard and pyrochlore lattice and with $\langle M \rangle = \frac{1}{3}$ in the Kagome and garnet lattice even if they may not correspond to collinearly ordered states. An $\langle M \rangle = \frac{1}{3}$ plateau is indeed observed in exact diagonalization studies of the $S = \frac{1}{2}$ Kagome lattice [7].

To test these general predictions, we have first performed Monte Carlo simulations of the classical FSAFM (see Fig. 3 of Ref. [3] for the magnetization curve at $J' = J/2$). Here, we present results for the static structure factor $S^{\alpha\beta}(\vec{q}) = (1/V^2)\sum_{\vec{x}} e^{i\vec{q}\cdot\vec{x}} \langle S_0^{\alpha} S_{\vec{x}}^{\beta} \rangle$ (V is the total number of spins) on a 24×24 cluster in Fig. 1. The top panel shows that at $h = 4J$ non-vanishing harmonics in the longitudinal structure factor both at $\vec{q} = (\pi, 0)$ and $\vec{q} = (\pi, \pi)$ exist only for $0.494 < J'/J < 0.508$. Neither, a lower field of $h = 2J$, nor a higher field of $h = 6J$ induces a nonzero value of $S^{zz}(\vec{q})$ at these points in the Brillouin zone. The lower panel of Fig. 1 presents the transverse structure factor. In the region of weak (strong) diagonal coupling J' one identifies Néel (striped) types of spin configuration. At $h = 4J$ the corresponding peaks jump to zero at exactly the same points where the peaks in the longitudinal structure factor appear, identifying the spin configuration in the intermediate region as the 'uuud' state. For $h = 2J$ and $h = 6J$, no significant peak is observed in any of the structure factors for $J' \approx J/2$, indicating disordered states above and below the uuud state.

Finally, we study the $S = \frac{1}{2}$ FSAFM using Lanczos diagonalization. A detailed discussion [3,4] of the magnetization curves and the static structure factors shows that an $\langle M \rangle = \frac{1}{2}$ plateau exists in the region $0.5 \lesssim J'/J \lesssim 0.65$ and that it corresponds to a state with uuud order. The finite-size analysis of states with $\langle M \rangle \neq \frac{1}{2}$ suffers from the problem that data for different system sizes is available only for very restricted values of $\langle M \rangle$. Here we propose to interpolate the data for a given cluster size. The contour-lines which one obtains in the J'/J-$\langle M \rangle$-plane are shown in Fig. 2 for 6×6 and 8×6 clusters. One indeed observes pronounced peaks on the 6×6 cluster at $\langle M \rangle = \frac{1}{2}$ which characterize the uuud state. The comparison with the data for the 8×6 cluster (which is available only for $\langle M \rangle \geqslant \frac{17}{24} \approx 0.70833$) suggests that the peak in $S^{zz}(\pi, 0)$ survives up to magnetizations as large as $\langle M \rangle \approx 0.75$ whereas $S^{zz}(\pi, \pi)$ presumably vanishes in this range. Although it remains to be clarified whether this (partial) order for $\langle M \rangle > \frac{1}{2}$ in the longitudinal components coexists with order in the transverse components (e.g. in $S^{xx}(\pi, \pi)$), this signals a supersolid phase above the uuud state. This scenario is in sharp contrast to the classical FSAFM, but similar to the 2D $S = \frac{1}{2}$

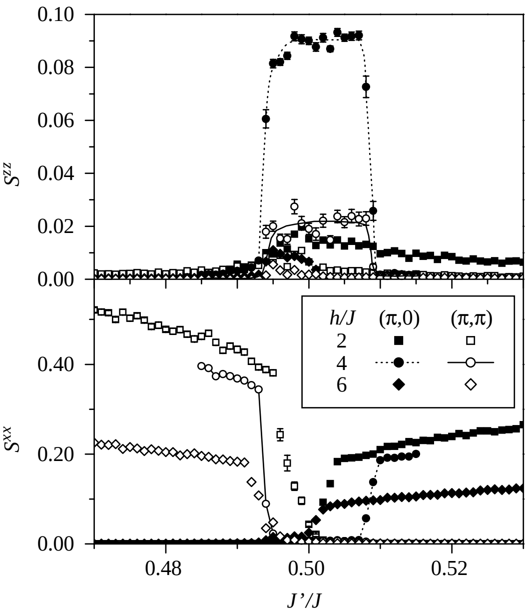

Fig. 1. Longitudinal (top panel) and transverse (bottom panel) components of the static structure factor $S^{\alpha\beta}(\vec{q})$ for the classical FSAFM at $T = 0.1J$.

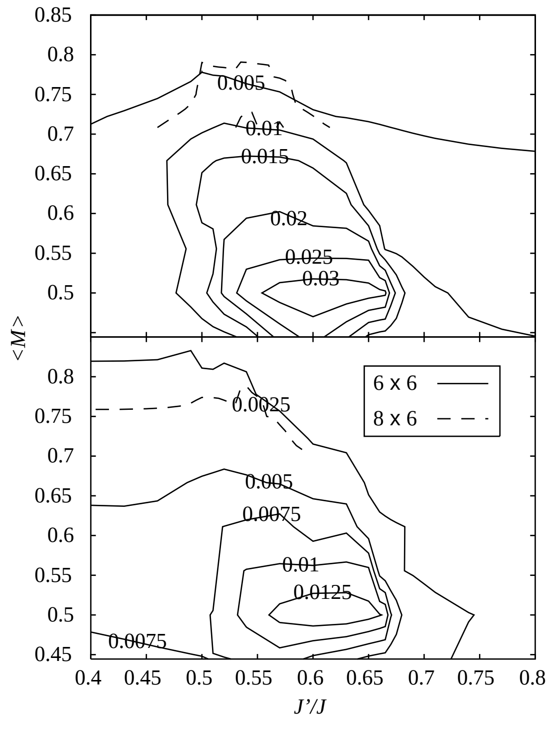

Fig. 2. Contour plot of $S^{zz}(\pi, 0)$ (top panel) and $S^{zz}(\pi, \pi)$ (bottom panel) for the $S = \frac{1}{2}$ FSAFM at $T = 0$.

Shastry–Sutherland model where supersolid states are presumably realized above the $\langle M \rangle = \frac{1}{3}$ and $\langle M \rangle = \frac{1}{2}$ plateaux [2].

To summarize, thermal as well as quantum fluctuations stabilize a collinear uuud state in the FSAFM for $J' \approx J/2$ at $\langle M \rangle = \frac{1}{2}$. For $S = \frac{1}{2}$, this leads to a pronounced plateau in the magnetization curve. In contrast to these similarities at $\langle M \rangle = \frac{1}{2}$, the classical and quantum model presumably differ for magnetic fields above this uuud state: Disorder in the classical system versus a partially ordered, supersolid state in the quantum system.

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