Lanczos study of the $S = 1/2$ frustrated square-lattice antiferromagnet in a magnetic field

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We study the zero-temperature phase diagram of the frustrated square-lattice $S = 1/2$ antiferromagnet in an external magnetic field numerically with the Lanczos algorithm. For strong frustration, we find disordered phases at high (and low) magnetic fields. Between these two disordered phases we find a plateau in the magnetization curve at half of the saturation magnetization which corresponds to a state with up-up-up-down (usual) spin order. This and other considerations [1] suggest an unusual ordering scenario: There are an ordered phase with a spin gap (the plateau) and disordered magnetically gapless phases above and below.

The transition to saturation is studied in further detail and problematic conclusions in earlier investigations of this region are pointed out.

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I. INTRODUCTION

Frustrated magnets are known to exhibit rich physics and diverse properties in zero external field (compare this volume and [1]). Exciting behavior in an external magnetic field was also observed recently in several cases: For instance, the $S = 7/2$ three-dimensional antiferromagnet $\text{Gd}_2\text{Ga}_2\text{O}_{12}$ is disordered (but gapless) in zero external field and orders only in finite magnetic fields [2]. Another example is the recently discovered two-dimensional $S = 1/2$ spin-gap material $\text{SrCu}_2(\text{BO}_3)_2$ which exhibits several plateaux in the magnetization curve [3]. The origin of these plateaux and the nature of the corresponding spin states are under intense debate [4] and it is suggested that some of the plateaux in $\text{SrCu}_2(\text{BO}_3)_2$ might be described by certain types of ordered states.

A plateau in the magnetization curve of the triangular lattice at one third of the saturation magnetization is theoretically well known (see, e.g., [5]). However, general magnetization plateaus in two dimensions (including those of $\text{SrCu}_2(\text{BO}_3)_2$) are still not well understood despite recent progress on the subject [1].

II. THE MODEL

In [1] we have studied the aforementioned issues in one of the simplest two-dimensional frustrated magnets, the frustrated square lattice antiferromagnet whose Hamiltonian is given by

$$ H = J \sum_{\langle \vec{x}, \vec{y} \rangle} \vec{S}_{\vec{x}} \cdot \vec{S}_{\vec{y}} + J' \sum_{[\vec{x}, \vec{y}]} \vec{S}_{\vec{x}} \cdot \vec{S}_{\vec{y}} - h \sum_{\vec{x}} S_{\vec{x}}^z \quad (1) $$

where the first sum is over nearest neighbor pairs $\langle \vec{x}, \vec{y} \rangle$ and the second one over diagonal neighbor pairs $[\vec{x}, \vec{y}]$.

Here we will present details of [1] and further results obtained from a numerical diagonalization of the $S = 1/2$ version of the Hamiltonian [1] with the Lanczos method.

At zero field, the frustrated square lattice $S = 1/2$ Heisenberg model has been studied extensively using also exact diagonalization [6,7]. One reason for the popularity of this model is that it exhibits melting of long-range magnetic order by quantum fluctuations: For small frustration $J' \ll J$, one finds antiferromagnetic Néel order while for $J' \gg J$ a certain type of collinear order described by a wave vector $(\pi,0)$ or $(0,\pi)$. Finally, in an intermediate region around $J' = J/2$, a spin-liquid groundstate with a gap to magnetic excitations is found.

In the presence of an external field, an important quantity is the magnetization

$$ \langle M \rangle = \frac{1}{SV} \left\langle \sum_{\vec{x}} S_{\vec{x}}^z \right\rangle \quad (2) $$

which we normalize to saturation values $|\langle M \rangle| = 1$. Magnetization curves for the model [1] have already been computed by exact diagonalization [11,12]. However, the study of [11] was restricted to a special lattice of $4 \times 4$ sites which can also be interpreted in terms of several other geometries. For instance, a strip of width 4 is equivalent to a frustrated four-leg ladder and then plateaux are expected in the magnetization curve at $\langle M \rangle = 0, 1/4, 1/2$ and 3/4 (see, e.g., [13]). Precisely these values were also observed in [11], but it remains to be clarified whether they are an artifact of the special geometry. The other study [12] excluded the region $J' > J/2$ which we find to be the most interesting one and boundary conditions were used in [12] which frustrate the order which wants to develop.

III. SINGLE MAGNON DISPERSION

It is instructive to look first at the dispersion of a single magnon above the ferromagnetic state with $\langle M \rangle = 1$ (all spins aligned along the field). When we formally set
\(h = 0\), the one-magnon dispersion for the \(S = 1/2\) model is given by

\[
E_{1\alpha}(k_x, k_y) = -2(J + J') + J \left( \cos k_x + \cos k_y \right) + 2J' \cos k_x \cos k_y. \tag{3}
\]

For \(J' < J/2\), this dispersion has a single minimum at \(k_x = k_y = \pi\) corresponding to Néel order. On the other hand, for \(J' > J/2\) two equivalent minima are found at \(k_x = 0, k_y = \pi\) or \(k_x = \pi, k_y = 0\) which signal collinear order. The case \(J' = J/2\) is special: Here lines of minima are found for either \(k_x = \pi\) or \(k_y = \pi\).

### IV. Magnetization Curves

![Graph](image)

**FIG. 1.** Zero-temperature magnetization curves of the \(S = 1/2\) model at \(J'/J = 0.6\). The lines are for clusters of size \(4 \times 4\) (dashed), \(6 \times 4\) (dotted), \(6 \times 6\) (full) and \(8 \times 6\) (dashed-dotted) (Inset: \(8 \times 8\) (dotted) and \(10 \times 10\) (dashed)). The bold line is an extrapolation (compare the text for details).

We now discuss the behavior in the entire field range using exact diagonalization. Guided by the dispersion (3), we have considered only rectangular clusters with an even number of sites in both directions. Finite-size magnetization curves are shown in Fig. 1 for \(J'/J = 0.6\). As we have pointed out in section IV, finite-size effects must be examined carefully. Even if the \(\langle M \rangle = 3/4\) and \(1/4\) plateaux are quite pronounced on the \(4 \times 4\) and \(6 \times 4\) clusters, we believe that they are artifacts of the special system sizes. Indeed, the data for wider strips indicates a vanishing plateau at \(\langle M \rangle = 3/4\) in the thermodynamic limit. In contrast, the plateau at \(\langle M \rangle = 1/2\) is only a little narrower on the \(6 \times 6\) cluster than for the smaller clusters. In the extrapolation (bold line in Fig. 1), we have therefore drawn a plateau with \(\langle M \rangle = 1/2\) but none at \(\langle M \rangle = 1/4\) and \(3/4\). The value of the spin gap (i.e. the boundary of the \(\langle M \rangle = 0\) plateau) has been taken from [4]. Otherwise the extrapolation was obtained by the standard procedure of connecting the mid-points of the steps of the magnetization curves at the largest available system size.

Fig. 2 shows the projection of the magnetization curves onto the horizontal axis, i.e. the locations of the finite-size jumps in the magnetization curves. From this one can then first read off how the width of the \(\langle M \rangle = 1/2\) plateau varies with \(J'/J\). An analysis of its finite-size behavior [1] indicates that the \(\langle M \rangle = 1/2\) plateau exists in the region \(0.5 \lesssim J'/J \lesssim 0.65\).

![Graph](image)

**FIG. 2.** Transition lines for the \(S = 1/2\) model. The lines are for clusters of size \(4 \times 4\) (dotted), \(6 \times 4\) (dashed) and \(6 \times 6\) (full).

Fig. 2 further shows that the transition to saturation is special at \(J' = J/2\), as is expected from (3). A jump of size \(\delta\langle M \rangle = 1/L\) occurs just below saturation where \(L\) is the length of the shorter edge of the cluster. This implies a smooth transition to saturation in the thermodynamic limit. The particularity of the transition to saturation for \(J' \approx J/2\) was already noted in [12] where, however, the jump was obscured by the choice of cluster geometries. We therefore believe the asymptotic form proposed in [12] just to be a manifestation of these boundary effects in combination with the questionable assumption that \(h(\langle M \rangle)\) has a power series expansion. It should be possible to obtain the correct asymptotic form from Bose condensation of magnons [13] into the lines of minima of the single magnon dispersion (3), but this computation has not yet been carried out.

For \(J' \approx J/2\), the magnetization curves further show a pronounced finite-size plateau at \(\langle M \rangle = 1 - 1/L\), i.e. just below the jump. It was actually proposed in [14] that a plateau just below saturation should exist for \(J' \gtrsim J/2\), but our candidate disappears as \(L \to \infty\) and we suspect an error in the treatment [14] of the single-magnon dispersion (3).

### V. Static Structure Factors

To gain further insight into the phase diagram and in particular in order to understand the nature of the
\[ \langle M \rangle = 1/2 \text{ plateau state better, we use the static structure factors which are defined as} \]
\[ S^{\alpha\beta}(k_x, k_y) = \frac{1}{V^2} \sum_{x, y, r, s} e^{i(k_x x + k_y y)} \left( S^\alpha_{r,s} S^\beta_{r+x, s+y} \right). \] (4)

The finite magnetization leads to a trivial peak in \( S^{zz}(0, 0) \). We observe additional peaks in \( S^{\alpha\beta}(k_x, k_y) \) at \((0, \pi)\) or \((\pi, 0)\) and \((\pi, \pi)\). The evolution of these peaks with \( J'/J \) is shown in Figs. 3 and 4 for two values of \( \langle M \rangle \).

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{fig3.png}
\caption{Peaks of the static structure factors of the \( S = 1/2 \) model as a function of \( J'/J \) at \( \langle M \rangle = 2/3 \) on the 6 \times 6 cluster. The longitudinal structure factor \( S^{zz}(0, \pi) \) is shown by triangles pointing up, \( S^{zz}(\pi, \pi) \) by triangles pointing down and the transverse structure factor \( S^{xx}(0, \pi) \) by circles and \( S^{xx}(\pi, \pi) \) by squares.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{fig4.png}
\caption{Same as Fig. 3 but for \( \langle M \rangle = 1/2 \) and on the 6 \times 6 cluster (filled symbols) as well as on the 4 \times 4 cluster (open symbols).}
\end{figure}

Néel and collinear order develops in the transverse components for small and large \( J' \), respectively. Just at \( \langle M \rangle = 1/2 \) and for \( 0.5 \lesssim J'/J \lesssim 0.65 \), the longitudinal components develop uuud order with three spins pointing up and one down on a four-spin plaquette. While it may be possible that some order exists in \( S^{zz}(0, \pi) \) at \( \langle M \rangle = 2/3 \) for intermediate \( J' \) (see Fig. 3), the structure factors at other magnetizations and Monte Carlo simulations of the classical model indicate disordered states for magnetizations sufficiently far above or below the uuud state at \( \langle M \rangle = 1/2 \).

VI. GROUNDSTATE QUANTUM NUMBERS

For an odd number of magnons \( V/2 - S^z \), one expects the groundstate to carry \( k_x = k_y = \pi \) (corresponding to Néel order) for \( J' \ll J \) while for \( J' \gg J \) one expects collinear order and thus \( k_x = 0, k_y = \pi \) or \( k_x = \pi, k_y = 0 \) – compare the discussion of the one-magnon sector in section [1]. When \( V/2 - S^z \) is even, the groundstate carries momentum \( k_x = k_y = 0 \). However, as was pointed out in [1], groundstate level crossings are still expected in the sectors with \( V/2 - S^z = 2n \) and \( n \) odd. Then the groundstate is even under diagonal reflections for \( J' \ll J \) and odd for \( J' \gg J \).

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{fig5.png}
\caption{Positions of unique groundstate level crossings. Triangles are for the 4 \times 4 cluster, squares for the 6 \times 6 cluster and circles for the 8 \times 8 cluster.}
\end{figure}

The \textit{unique} groundstate level crossings are shown in Fig. 4 (in some sectors more than one groundstate level crossing is observed). The crossing at \( \langle M \rangle = 0 \) on the 6 \times 6 cluster was taken from [10]. Note that according to [3], the crossing point must move to \( J' = J/2 \) for \( \langle M \rangle \rightarrow 1 \) where a first-order transition between Néel order and collinear order occurs. The position of the crossing at \( \langle M \rangle = 1/2 \) agrees with our earlier estimates for the transition between the uuud plateau state and collinear order. Also the crossing at \( \langle M \rangle = 0 \) is close to recent estimates (see, e.g., [4]) for the location of the zero-field transition between the disordered spin-liquid state and the collinear state.

\* The symmetrized variant \( \left( S^{\alpha\beta}(k_x, k_y) + S^{\alpha\beta}(k_y, k_x) \right)/2 \) is used when the cluster is not square or the groundstate not symmetric under reflection across the diagonal of the cluster \((x \leftrightarrow y)\).
VII. SUMMARY

We have studied the frustrated square lattice $S = 1/2$ Heisenberg model in the presence of a strong magnetic field using the Lanczos method. A plateau with $\langle M \rangle = 1/2$ exists in the region $0.5 \lesssim J'/J \lesssim 0.65$ and corresponds to an up-up-up-down ordered state. The transverse spin components show Néel and collinear order for small and large $J'$, respectively. The intermediate region contains the ordered $\langle M \rangle = 1/2$ state and disordered regions at higher and lower fields \[1\]. Finally, we have found that the transition to saturation is special at $J' = J/2$.

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