The phase diagram of the antiferromagnetic XXZ model on the triangular lattice

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We determine the quantum phase diagram of the antiferromagnetic spin-1/2 XXZ model on the triangular lattice as a function of magnetic field and anisotropic coupling $J_z$. Using the density matrix renormalization group (DMRG) algorithm in two dimensions we establish the locations of the phase boundaries between a plateau phase with 1/3 Neel order and two distinct coplanar phases. The two coplanar phases are characterized by a simultaneous breaking of both translational and $U(1)$ symmetries, which is reminiscent of supersolidity. A translationally invariant umbrella phase is entered via a first order phase transition at relatively small values of $J_z$ compared to the corresponding case of ferromagnetic hopping and the classical model. The phase transition lines meet at two tricritical points on the tip of the lobe of the plateau state, so that the two coplanar states are completely disconnected. Interestingly, the phase transition between the plateau state and the upper coplanar state changes from second order to first order for large values of $J_z \gtrsim 2.5J$.

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Competing interactions between quantum spins can prevent conventional magnetic order at low temperatures. In the search of interesting and exotic quantum phases frustrated systems are therefore at the center of theoretical and experimental research in different areas of physics \textsuperscript{1}. One of the most straight-forward frustrated system is the spin-1/2 antiferromagnet (AF) on the triangular lattice, which was also the first model to be discussed as a potential candidate for spin-liquid behavior without conventional order by Anderson \textsuperscript{2}. It is now known that the isotropic Heisenberg model on the triangular lattice is not a spin liquid and does show order at zero temperature \textsuperscript{3}. Nonetheless, the phase diagram as a function of magnetic field is still actively discussed with recent theoretical calculations \textsuperscript{4, 5} as well as experimental results \textsuperscript{6-9} on Ba$_2$CoSi$_2$O$_9$, which appears to be very well described by a triangular AF. Interesting phases have also been found for anisotropic triangular lattices \textsuperscript{10, 12} and for the triangular extended Hubbard model \textsuperscript{13}. However, surprisingly little attention has been paid to the role of an isotropic exchange interaction away from half-filling \textsuperscript{14, 15}, even though the XXZ model on the triangular lattice

\begin{equation}
\label{eq:1}
H = J \sum_{\langle ij \rangle} (\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y) + J_z \sum_{\langle ij \rangle} \hat{S}_i^z \hat{S}_j^z - B \sum_i \hat{S}_i^z, \quad (1)
\end{equation}

is arguable one of the most fundamental examples of frustrated antiferromagnetism. Moreover, due to the rapid advances in experimental techniques with ultracold bosons, this model can potentially be realized experimentally with tunable parameters on a triangular optical lattice \textsuperscript{14, 17}. In particular, using the Holstein-Primakoff transformation the model in Eq. \textsuperscript{1} is exactly equivalent to hard-core bosons with a finite nearest neighbor interaction $V$

\begin{equation}
\label{eq:2}
H = -t \sum_{\langle ij \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i) + V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j - \mu \sum_i \hat{n}_i, \quad (2)
\end{equation}

with $J_z = V$, $J = -2t$ and $B = \mu - 3V$. For ordinary hopping $t > 0$ the boson model therefore corresponds to a ferromagnetic (FM) $xy$-coupling $J < 0$, which can be simulated efficiently using quantum Monte Carlo (QMC) methods \textsuperscript{18}. In this case a so-called supersolid phase near half-filling has been established for large interactions \textsuperscript{18, 19}, which is characterized by two order parameters, namely a superfluid density and a $\sqrt{3} \times \sqrt{3}$ charge density order. Impurity effects show that the two order parameters are competing \textsuperscript{20}. The transition to the superfluid state is first order \textsuperscript{21, 22}.

The theoretically more interesting and more challenging case occurs for antiferromagnetic $xy$-coupling $J > 0$ or $t < 0$, which leads to an additional frustration in the $xy$-plane. In the boson systems negative hopping $t < 0$ can be achieved by dressing the optical lattice with fast oscillations \textsuperscript{17}. Unfortunately, however, QMC simula-
tions are not efficient in this case due to the infamous minus-sign problem \cite{22}, so that we now present density matrix renormalization group (DMRG) \cite{23} calculations in two dimensions on order parameters and entanglement measures in order to establish the quantitative phase diagram as a function of field \( B \) and anisotropic coupling \( J_z \).

Our findings are summarized by the phase diagram in Fig. 1. At large values of \( J/J_z \) (i.e. large hopping) the bosons condense in a state with wavevector \( \mathbf{Q} = (4\pi/3, 0) \) (modulo reciprocal wavevectors) with a finite superfluid density. In contrast to an ordinary \( \mathbf{Q} = 0 \) superfluid for positive hopping this superfluid state has an additional \( Z_2 \) symmetry \( \mathbf{Q} \rightarrow -\mathbf{Q} \). In terms of the spins this corresponds to an umbrella state, with broken \( U(1) \) symmetry but no broken sublattice symmetry. With increasing \( J_z \) and at small magnetic fields a first order transition occurs to a state where the spins on one sublattice align against the field, while the other two sublattices form a honeycomb structure with spins still partially pointing in the xy-plane, so that all spins lie in a plane. This coplanar state is analogous to the bosonic supersolid for \( t > 0 \) \cite{18} with a finite bosonic superfluid density, but instead of a single wavevector \( \mathbf{Q} = (4\pi/3, 0) \) the state is described by an antisymmetric superposition \( \langle |\mathbf{Q}\rangle - |\mathbf{Q}^\perp\rangle \) due to the broken translational invariance. The transition shifts from \( J/J_z = 1 \) for \( B = 0 \) \cite{27} to \( J/J_z > 1 \) for finite fields, i.e. at smaller values of \( J_z \) than for ferromagnetic anisotropy \cite{18}. At larger fields a second coplanar (supersolid) phase is found with parallel canting spins on two sublattices and one sublattice pointing in a different direction. This upper coplanar phase corresponds to a different type of bosonic supersolid with a symmetric condensate \( \langle |\mathbf{Q}\rangle + |\mathbf{Q}^\perp\rangle \), which does not exist for ferromagnetic xy-coupling and extends to much larger values of \( J/J_z \). The two coplanar phases do not touch, since the \( 1/3 \) Néel phase has a direct phase transition to the umbrella phase, resulting in two tri-critical points where the phase transition lines meet. Interestingly we find that the second order phase transition between the \( 1/3 \) Néel phase and the upper coplanar phase curiously turns first order for strong interactions \( J/J_z \lesssim 0.4 \).

For comparison we also show the mean field solution in Fig. 1 corresponding to the classical triangular antiferromagnet \cite{14, 24, 30}. After parametrizing the direction of the spins on each of the three sublattices by two angles, it is straight-forward to obtain the classical solution by minimizing the energy in respect to the six angles. In this case the phase transition to the umbrella phase always occurs at \( J_z = J \) and all four phases touch at \( B = 1.5 J_z = 1.5 J \).

We now discuss the detailed numerical DMRG data at selected points in the phase diagram. The DMRG simulations were done with periodic boundary conditions in both directions in order to avoid edge states, which can lead to boundary dominated phases in frustrated systems \cite{61}. Note, that the DMRG operates in the canonical ensemble, i.e. the data is given as a function of magnetization and the corresponding fields can be obtained as the derivative of the ground state energy \( E(M) \) with respect to \( M \), i.e. \( B(M) = [E(M + 1/N) - E(M)]/\partial M \) \cite{32, 33}. The Heisenberg system \( J = J_z \) in a field has previously been considered using exact diagonalization \cite{3, 4, 27}, spin waves \cite{38, 39} and coupled cluster methods (CCM) \cite{3}. It is well known that the uniform magnetization has a plateau at \( M = 1/6 \) which is characteristic of the \( 1/3 \) Néel phase as shown in the inset of Fig. 2. For a system size of \( 6 \times 9 \) we estimate the range of the plateau phase to be \( -2.1776 < B/J_z < -1.3011 \) which is consistent with experiments on Ba\(_3\)CoSb\(_2\)O\(_9\) \cite{6} and theoretical studies \cite{4, 5, 12}.

The structure factors in the z-direction \( S^z(Q) = \langle |\sum_{k=1}^{N} S^z_k e^{iQ \cdot r_k} |^2 \rangle/N \) and in the xy-direction \( S^\perp(Q) = \langle |\sum_{k=1}^{N} S^\perp_k e^{iQ \cdot r_k} |^2 \rangle/N \) at \( Q = (4\pi/3, 0) \) are useful order parameters to measure the diagonal and the off-diagonal order, respectively. If \( S^z/N \) is finite the system has a broken sublattice symmetry (charge order), while a finite \( S^\perp/N \) indicates a broken \( U(1) \) rotational symmetry (superfluidity). As shown in Fig. 1 both order parameters are finite in the upper and lower coplanar (supersolid) phases. At zero magnetization \( S^\perp/N \) is larger than \( S^z/N \), but then decreases with \( M \) and scales to zero with \( 1/N \) at \( M = 1/6 \), which is exactly the point where \( S^z \) becomes largest. In the experiments on Ba\(_3\)CoSb\(_2\)O\(_9\) an additional cusp in the susceptibility was observed at higher magnetization \( M \approx 1/3 \) \cite{4}, which could indicate another phase transition. However, our data does not show any
However, the coplanar spin state has only a limited susceptibility for $M \approx 1/3$, which is due to the fact that the spins on one of the sublattices is able to align along the $xy$-plane at approximately this magnetization as shown in Fig. 2. Spins that are aligned within the $xy$-plane have in turn the largest susceptibility in the $z$-direction, so this could in part explain the observed maximum in Ref. [3].

We now turn to larger values of $J_z = 2.5J$, where the magnetization plateau is larger as shown in the inset of Fig. 3. The behavior of the order parameters $S_\pm$ and $S^z$ is qualitatively similar to the isotropic case as a function of magnetization. The second order phase transition between the lower supersolid phase and the plateau phase is well understood from a strong coupling expansion [22] in terms of holes which start to occupy the honeycomb sublattice at a critical value of $B \approx 3J/2 + 5J^2/8J_z - 71J^3/32J_z^2$, which is consistent with our numerical data. For the phase transition between the $1/3$ Néel phase and the upper supersolid state such a simple argument does not exist, however, and indeed there is a subtle, but important difference in the magnetization curve at strong interactions. Cays inspection reveals that the susceptibility is negative near the upper phase boundary as shown in the inset of Fig. 3 which indicates an instability that leads to a jump in the magnetization according to the Maxwell construction. This jump vanishes somewhere between $J_z = 2.5J$ and $J_z = 2J$, so that we predict a bicritical point where the second order phase transition turns first order in the strong coupling limit as shown in Fig. 1. This surprising behavior can in part be explained from the fact that the end of the $M = 1/6$ plateau approaches the saturation field, so that there is only a small field region where the magnetization changes from $M = 1/2$ down to $M = 1/6$. However, the coplanar spin state has only a limited susceptibility close to saturation, so that a jump in magnetization may be the only way to resolve this contradiction. In other words, starting from the $1/3$ Néel state the configuration must make a finite jump to reach the coplanar state if the upper critical field is too large, since the coplanar state is already canted significantly towards the field in this case. In any case, the quantum mechanical mechanism for this behavior is an interesting aspect for future studies.

In order to determine the phase boundaries to the umbrella (superfluid) phase in the weak coupling limit $J > J_z$ it is useful to also consider the reduced density matrix $\rho_{ij}$ of two neighboring spins in the center of the lattice, which can be determined from the correlation functions [40]. The trace over spin $j$ gives the reduced density matrix of a single spin $\rho_i = \Tr_j\rho_{ij}$. The von-Neumann entropy of a general density matrix $S_A = -\Tr_A\log\rho_A$ can be used to define the entanglement entropy $S_i$. The concurrence [40, 41]

$$C_{ij} = 2\max(0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}),$$

is given in terms of the eigenvalues $\lambda_i$ of the matrix $\rho_{ij}^\dagger\rho_{ij}$, where $\rho_{ij}^\dagger$ characterizes the spin-flipped state. The quantum discord [40, 42] has been proposed as a good indicator for quantum phase transitions

$$D_{ij} = \min_{(\Pi_\nu^\dagger)} (S_i - S_{ij} + S_{ij}^\dagger),$$

which is calculated in terms of the conditional quantum entropy

$$S_{ij} = \sum_{\nu=1}^{2} p_\nu S(\rho_{ij}^{(\Pi_\nu^\dagger)}),$$

where $\rho_{ij}^{(\Pi_\nu^\dagger)} = \Pi_\nu^\dagger\rho_{ij}\Pi_\nu$ and $p_\nu = \Tr\Pi_\nu\rho_{ij}$. The projectors $\Pi_\nu = |\psi_\nu\rangle\langle\psi_\nu|$ are defined in terms of the variational wavefunctions

$$|\psi_1\rangle = \cos \theta |\downarrow\rangle_j + e^{-i\phi} \sin \theta |\uparrow\rangle_j$$

$$|\psi_2\rangle = e^{+i\phi} \sin \theta |\downarrow\rangle_j - \cos \theta |\uparrow\rangle_j.$$  

The minimization over the projectors in [41] then corresponds to a minimization over angles $\theta$ and $\phi$ in the wavefunctions.

In Fig. 4 we show the two order parameters, the concurrence, the entanglement entropy, and the quantum discord at two selected points in the phase diagram, which are indicated by red circles in Fig. 1. All measures give the same locations of the phase transition (in this case $B = 1.398J_z$, $J = 1.31J_z$ and $B = 2.161J_z$, $J = 1.55J_z$, respectively), but with different accuracy. The structure factor $S^z/N$ drops sharply and scales to zero in the umbrella phase, while $S^\pm/N$ is enhanced. From all indicators for the phase transition the quantum discord $D_{ij}$ [40, 42] has the sharpest change. Even more interesting, the variational angle $\theta$ which is used to minimize the quantum discord takes on different values...
FIG. 4: The structure factor \( S^z(Q)/N, S^\pm(Q)/N \), concurrence, entanglement entropy, quantum discord and the variational angle \( \theta \) in the 6 \( \times \) 9 lattice in the regions shown by red circles in Fig. 1 indicate a phase transition to the superfluid (umbrella) state from the lower (a) and the upper (b) coplanar (supersolid) state.

on the two sides of the phase transition. It is so far unclear if this jump in a variational parameter is a generic feature, but it may be useful in future studies as well. We find that the phase transition between the ordered states (solid and supersolids) to the umbrella (superfluid) phase is always first order, except at the isotropic point \( B = 0 \), where it is known to be second order. At two tri-critical points \( B = 1.586J_z, J = 1.38J_z \) and \( B = 1.958J_z, J = 1.47J_z \) for a 6 \( \times \) 9 system the second order phase transitions between solid and supersolids meet the first order transition. During the preparation of this manuscript a preprint appeared that obtained a phase diagram using a cluster mean-field method [15], which agrees well with our findings.

In conclusion, we have analyzed the spin-1/2 XXZ model on the triangular lattice using a two dimensional DMRG method with periodic boundary conditions. The phase diagram shows two supersolid (coplanar) phases with different symmetries of the superfluid condensate, which is separated by an ordered plateau 1/3 Néel phase, with fixed magnetization \( M = 1/6 \). The transition to the superfluid (umbrella) state is always first order for finite fields and the line \( J_z(B) \) is monotonically increasing, so that a larger field always leads to an extended ordered state. The transition between the supersolids and the 1/3 Néel phase is generically second order but curiously the upper phase transition line turns first order for \( J_z \gtrsim 2.5J \), which is yet not fully understood.

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