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# Ground-state properties of the triangular-lattice Heisenberg antiferromagnet with arbitrary spin quantum number $s$

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ABSTRACT

We apply the coupled cluster method to high orders of approximation and exact diagonalizations to study the ground-state properties of the triangular-lattice spin-$s$ Heisenberg antiferromagnet. We calculate the fundamental ground-state quantities, namely, the energy $e_0$, the sublattice magnetization $M_{\rm sub}$, the in-plane spin stiffness $\rho_s$ and the in-plane magnetic susceptibility $\chi$ for spin quantum numbers $s = 1/2, 1, \ldots, s_{\rm max}$, where $s_{\rm max} = 9/2$ for $e_0$ and $M_{\rm sub}$, $s_{\rm max} = 4$ for $\rho_s$ and $s_{\rm max} = 3$ for $\chi$. We use the data for $s \geq 3/2$ to estimate the leading quantum corrections to the classical values of $e_0$, $M_{\rm sub}$, $\rho_s$, and $\chi$. In addition, we study the magnetization process, the width of the 1/3 plateau as well as the sublattice magnetizations in the plateau state as a function of the spin quantum number $s$.

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## 1. Introduction

In the 1970s Anderson and Fazekas [1,2] first considered the quantum spin-1/2 Heisenberg antiferromagnet (HAFM) for the geometrically frustrated triangular lattice and they proposed a liquid-like ground state (GS) without magnetic long-range order (LRO). Later on it was found that the spin-1/2 HAFM on the triangular lattice possesses semi-classical three-sublattice Néel order, see, e.g., Refs. [3–19]. However, the sublattice magnetization $M_{\rm sub}$ is drastically diminished in the $s = 1/2$ model [11,14–18] because of the interplay between quantum fluctuations and strong frustration. The small magnetic order parameter indicates that the semi-classical magnetic LRO is fragile and that small additional terms in the Hamiltonian may destroy the magnetic LRO, see, e.g., Refs. [20–28].

Although very precise data for the relevant GS quantities are available for unfrustrated HAFM's on bipartite two-dimensional lattices, see, e.g., Refs. [29–32] related to the square lattice, the corresponding data for the triangular lattice are less precise. This lack of precision is related to the strong frustration in the system that, e.g., does not allow one to apply the quantum Monte Carlo method. Moreover, the spin-wave approach is less efficient for frustrated lattices than it is for non-frustrated lattices. Nevertheless, spin-wave theories are considered as appropriate, in particular, if the spin quantum number $s$ is not $s = 1/2$ or $s = 1$. Perhaps the most accurate result for the GS order parameter (i.e., the sublattice magnetization $M_{\rm sub}$) for $s = 1/2$ has been obtained by a recent density matrix renormalization group study [16], where a result of $M_{\rm sub} = 0.205$ has been found.

The continuous interest in the triangular-lattice HAFM is (last but not least) also related to a fluctuation-induced magnetization plateau at 1/3 of the saturation magnetization [33–53]. In particular, two model compounds, namely $Ba_3CoSb_2O_9$ with $s = 1/2$ and $Ba_3NiSb_2O_9$ with $s = 1$, have been shown very recently to demonstrate an excellent agreement between the experimentally measured magnetization curves and those curves from theoretical predictions, see Refs. [39,45,46] for $s = 1/2$ and Refs. [44,48] for $s = 1$.

In the present paper we consider the Hamiltonian

$$H = \sum_{\langle ij \rangle} \mathbf{s}_i \mathbf{s}_j - h \sum_i s_i^z, \tag{1}$$

where the sum runs over nearest-neighbor bonds $\langle ij \rangle$ on the triangular lattice, $(\mathbf{s}_i)^2 = s(s+1)$, and $h$ is an external magnetic field. We consider arbitrary spin quantum number $s$. We use the coupled cluster method (CCM) to high orders of approximation to determine the GS properties in zero magnetic field, i.e., the GS energy per spin $e_0$, the sublattice magnetization $M_{\rm sub}$ (order parameter), the spin stiffness $\rho_s$, and the uniform susceptibility $\chi$. These quantities constitute the fundamental parameters determining the low-energy physics of the triangular Heisenberg antiferromagnet. Moreover, the stiffness and the susceptibility are

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used as input parameters in scaling functions for various observables [54].

In addition to the zero-field quantities we also consider the magnetization process $M(h)$ and determine the 1/3 plateau in the $M(h)$-curve. We complement the CCM calculations by carrying out Lanczos exact diagonalization of finite lattices.

## 2. Methods

### 2.1. Lanczos exact diagonalization

The Lanczos exact diagonalization (ED) is one of the most useful methods that can be used to investigate frustrated quantum spin systems, see, e.g., Refs. [55–62]. Although lattices of size $N=36$ are common for ED calculations for spin $s = 1/2$, the system size $N$ accessible for ED shrinks significantly, see, e.g., Refs. [48,57,60,63–65]. Hence, we use the ED here in order to complement the results of the CCM (that yields results in the limit $N \to \infty$). We use Schulenburg's *spinpack* code [66] to calculate the magnetization curves for $s = 1/2, 1, \ldots, 5/2$. The maximum lattice size for $s=2$ and 5/2 is $N=12$, whereas for $s = 3/2$ we have results for $N = 12, 18, 21$. For $s=1$ the largest lattice we can consider is $N=27$. We use these data to analyze the $s$-dependence of the 1/3 plateau.

### 2.2. Coupled cluster method

The coupled cluster method (CCM) is a universal many-body method widely used in various fields of quantum many-body physics, see, e.g., Refs. [67,68]. Meanwhile, the CCM has been established as an effective tool in the theory of frustrated quantum spin systems, see, e.g., the recent papers [14,27,39,48,69–80]. Here we illustrate only some features of the CCM relevant for the present paper. For more general information on the methodology of the CCM, see, e.g., Refs. [68,81–85].

The CCM calculation starts with the choice of a normalized reference state $|\Phi\rangle$. We choose the classical GS of the model as reference state, which is well known for the triangular HAFM for arbitrary fields, see, e.g., Refs. [35,39,40] and Fig. 1. For zero field it is the three-sublattice Néel state, i.e., state I with $\alpha=60^\circ$ in Fig. 1. For finite magnetic fields non-collinear planar states with field dependent pitch angles $\alpha$ and $\beta$ are classical GS's, see Fig. 1. The reference state is a collinear state (so-called up–up–down state, see state II in Fig. 1) only at the 1/3 plateau. With respect to the corresponding reference state, we then define a set of mutually commuting multispin creation operators $C_I^+$, which are themselves defined over a complete set of many-body configurations $I$. We perform a rotation of the local axis of the spins such that all spins in the reference state align along the negative $z$-axis. The specific form of the spin-operator transformation depends on the pitch angles of the reference state. In this new set of local spin coordinates the reference state and the corresponding multispin creation operators $C_I^+$ are given by

$$|\Phi\rangle = |\downarrow\downarrow\downarrow\cdots\rangle; \quad C_I^+ = \hat{s}_n^+,\ \hat{s}_n^+\hat{s}_m^+,\ \hat{s}_n^+\hat{s}_m^+\hat{s}_k^+, \ldots, \tag{2}$$

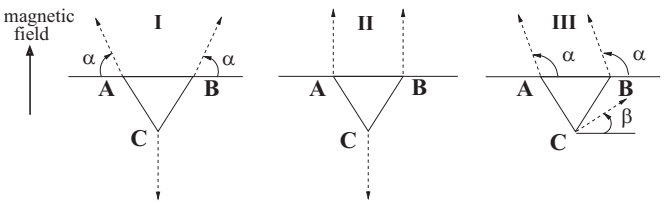


**Fig. 1.** Reference states used for the CCM calculations.

where the indices $n, m, k, \ldots$ denote arbitrary lattice sites. In the rotated coordinate frame the Hamiltonian becomes dependent on the pitch angles. With the set $\{|\Phi\rangle, C_I^+\}$ the CCM parametrization of the exact ket and bra GS eigenvectors $|\Psi\rangle$ and $\langle\tilde{\Psi}|$ of the many-body system is given by

$$|\Psi\rangle = e^S|\Phi\rangle, \quad S = \sum_{I\neq 0} a_I C_I^+ \tag{3}$$

$$\langle\tilde{\Psi}| = \langle\Phi|\tilde{S}e^{-S}, \quad \tilde{S} = 1 + \sum_{I\neq 0} \tilde{a}_I C_I^-, \tag{4}$$

where $C_I^- = (C_I^+)^\dagger$. The CCM correlation operators, $S$ and $\tilde{S}$, contain the correlation coefficients, $a_I$ and $\tilde{a}_I$, which can be determined by the CCM ket-state and bra-state equations

$$\langle\Phi|C_I^- e^{-S}He^S|\Phi\rangle = 0; \quad \forall\, I \neq 0 \tag{5}$$

$$\langle\Phi|\tilde{S}e^{-S}[H, C_I^+]e^S|\Phi\rangle = 0; \quad \forall\, I \neq 0. \tag{6}$$

Note that each ket-state equation belongs to a specific creation operator $C_I^+ = s_n^+,\ s_n^+s_m^+,\ s_n^+s_m^+s_k^+, \ldots$, i.e., it corresponds to a specific set (configuration) of lattice sites $n, m, k, \ldots$. By using the Schrödinger equation, $H|\Psi\rangle = E|\Psi\rangle$, we can write the GS energy as $E = \langle\Phi|e^{-S}He^S|\Phi\rangle$. The sublattice magnetization is given by $M_{\rm sub} = -(1/N)\sum_i^N \langle\tilde{\Psi}|s_i^z|\Psi\rangle$, where $s_i^z$ is expressed in the transformed coordinate system. The total magnetization $M$ aligned in the direction of the applied magnetic field $h$ in terms of the global axes prior to rotation of the local spin axes is given by $M = (M_A + M_B + M_C)/3$, where $M_A$, $M_B$, and $M_C$ are the magnetizations of the three individual sublattices, cf. Fig. 1, given by

$$M_{A,B,C} = \frac{1}{N_{A,B,C}} \sum_{i_{A,B,C}} \langle\tilde{\Psi}|s_{i_{A,B,C}}^z|\Psi\rangle, \tag{7}$$

where the index $i_A$ runs over all $N_A$ sites on sublattice $A$, the index $i_B$ runs over all $N_B$ sites on sublattice $B$, and the index $i_C$ runs over all $N_C$ sites on sublattice $C$, and $N = N_A + N_B + N_C$. The CCM results for the ground state energy and the total magnetization as a function of the magnetic field can be used to calculate the uniform magnetic susceptibility, given by

$$\chi \equiv \frac{dM}{dh} = -\frac{1}{N}\frac{d^2E}{dh^2}. \tag{8}$$

Note that we consider here $\chi$ as susceptibility per site [86].

The GS energy depends (in a certain CCM approximation, see below) on the pitch angles. In the quantum model the pitch angles may be different from the corresponding classical values. Therefore, we do not choose the classical result for the pitch angles in the quantum model. Indeed, we consider them as a free parameter in the CCM calculation, which has to be determined by minimization of the CCM GS energy with respect to the pitch angles. An exception is the zero-field case, where the pitch angle is fixed to $\alpha=60^\circ$ (the three-sublattice Néel state).

The spin stiffness $\rho_s$ measures the increase of energy rotating the order parameter of a magnetically long-range ordered system along a given direction by a small twist (pitch) angle $\theta$ per unit length, i.e.,

$$\frac{E(\theta)}{N} = \frac{E(\theta=0)}{N} + \frac{1}{2}\rho_s\theta^2 + O(\theta^4), \tag{9}$$

where $E(\theta)$ is the ground-state energy as a function of the twist angle. For the triangular lattice the twist is imposed along a lattice basis vector and it is within the plane defined by the order parameter, see Refs. [8,10], where the twist along both directions leads

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