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# The magnetic properties of the spin-1 Heisenberg antiferromagnetic chain with single-ion anisotropy

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ABSTRACT

The magnetic properties of the spin-1 Heisenberg antiferromagnetic chain with exchange anisotropy and single-ion anisotropy are studied by the double-time Green's function method. The determinative equations for the critical temperature, the magnetization, and the zero-field susceptibility are derived analytically. The effects of the anisotropies on the magnetic properties are presented.

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## 1. Introduction

Since the early semiquantitative analytical predictions by Haldane [1] that properties for integer spin must differ qualitatively from those for half-integer spin, the interest in studying the integer spin systems has been triggered. So far, various Heisenberg models with spin magnitude $S=1$ have been theoretically investigated [2–16]. Already in the earlier stage of vigorous studies on the Haldane problem, Botet et al. [2] have indicated that the single-ion anisotropy generated by crystal fields plays an essential role in larger spin systems, so the effects of the single-ion anisotropy on the magnetic behavior of the magnetic systems have become an important content of research. It has been shown that the single-ion anisotropy suppresses the quantum and thermal spin fluctuations, and can have a fundamental influence on the ground state phases [2,8,11,15] and thermodynamic properties [5–7,12,16] of the spin systems with spin greater than one-half.

Because of the complexities caused by the single-ion anisotropy term, various theoretical methods have been devoted, such as quantum Monte Carlo simulation [3], coupled-cluster approximation [4], exact diagonalization [8], series expansion [11,12], double-time Green's funciton [6,9,13,14], density and transfer renormalization group [7,15], and modified spin wave theory [16]. Among the above methods, the double-time Green's function approach [17,18], which is applicable for all temperature regions and all dimensions, has got a great success in the research area of quantum magnetism. When the single-ion anisotropy parameter is small, the Anderson–Callen decoupling approximation (ACA) [19] can be used to decouple the hierarchy of Green's function equation, and obtain reliable results. By using Green's function approach and the Anderson–Callen decoupling approximation, the magnetic properties of the one, two, and three dimensional (1D, 2D and 3D) ferromagnetic (FM) spin-1 Heisenberg models with single-ion anisotropy have been studied [9,13,20–22], as well as the 2D and 3D antiferromagnetic (AFM) models [14,23]. It is worth noting that in Ref. [6], a theoretical formulation of the second-order double-time Green's function method for the 1D AFM model with single-ion anisotropy in a phase without long-range order was presented.

In this paper, we will use Green's function approach and the ACA approximation to study the 1D spin-1 antiferromagnetic Heisenberg model with the easy-axis single-ion anisotropy in the antiferromagnetic phase, presenting the effects of the single-ion anisotropy on the magnetic properties. As mentioned above, the second-order Green's function method has been applied in Ref. [6], however, where only the isotropic case without long-range order was numerically calculated and discussed. Furthermore, the effects of the single-ion anisotropy which are important for the 1D spin-1 AFM model were not discussed in Ref. [6]. The importance of the effects is based on the following two points: firstly, it is known that the role of single-ion anisotropy in phase transitions is of particular importance when it has an opposite sign with respect to exchange interactions, while the AFM model with the easy-axis single-ion anisotropy just belongs to this case; secondly, in low dimensional spin systems, the intensity of the thermal and the

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quantum fluctuations is relatively stronger than that in high dimensional systems, so studying the 1D systems will better reveal the suppression of the fluctuations from single-ion anisotropy.

This paper is organized as follows: In Section 2, we present our 1D Heisenberg model and the formalism of Green's function approach. The basic self-consistent equations are obtained. In Section 3, we present our numerical results, investigating the effects of the single-ion anisotropy and exchange anisotropy on the critical temperature, staggered magnetization and zero-field susceptibility. In Section 4, a brief conclusion is given.

## 2. The model and Green's function approach

The Hamiltonian of the 1D spin-1 antiferromagnetic Heisenberg model with the exchange anisotropy and single-ion anisotropy under the staggered magnetic field can be described as

$$H = J\sum_{\langle ij\rangle}[a(S_{Ai}^{x}S_{Bj}^{x}+S_{Ai}^{y}S_{Bj}^{y})+S_{Ai}^{z}S_{Bj}^{z}]-D\left[\sum_{i}(S_{Ai}^{z})^{2}+\sum_{j}(S_{Bj}^{z})^{2}\right]$$
$$-h\sum_{i}S_{Ai}^{z}+h\sum_{j}S_{Bj}^{z}. \tag{1}$$

where $\langle i,j\rangle$ denotes that the summation is over the nearest-neighbor spins $i$ and $j$. The parameters $a$ and $D$ denote the exchange anisotropy and the single-ion anisotropy respectively. Increasing $D$ and decreasing $a$ both lead to stronger anisotropy. Here we only consider the easy-axis case with $0<a<1$ and $D>0$. In this parameter region, the ground-state phase is antiferromagnetic [2], so that we write the Hamiltonian (1) in the two-sublattice formulation as usually done in Green's function approach. $A$ and $B$ denote the two sublattices. This two-sublattice treatment was also used in linked-cluster series expansion approach in Ref. [12]. $J$ is the exchange coupling constant between neighboring spins. $h$ is the staggered magnetic field, which makes the system to be in the antiferromagnetic phase even in the isotropic case with $a=1$ and $D=0$.

In the following, we apply the spin raising and lowering operators $S_j^{\pm}=S_j^{x}\pm iS_j^{y}$ to simplify the above Hamiltonian, which can be rewritten as

$$H = J\sum_{\langle ij\rangle}\left[\frac{a}{2}(S_{Ai}^{+}S_{Bj}^{-}+S_{Ai}^{-}S_{Bj}^{+})+S_{Ai}^{z}S_{Bj}^{z}\right]-D\left[\sum_{i}(S_{Ai}^{z})^{2}+\sum_{j}(S_{Bj}^{z})^{2}\right]$$
$$-h\sum_{i}S_{Ai}^{z}+h\sum_{j}S_{Bj}^{z}. \tag{2}$$

In order to calculate the magnetic properties of this model, we introduce the retarded Green's functions, which are defined as

$$\langle\langle S_{Ai}^{+}(t);S_{Ai'}^{-}\rangle\rangle=-i\theta(t)\langle[S_{Ai}^{+}(t),S_{Ai'}^{-}]\rangle, \tag{3}$$
$$\langle\langle S_{Ai}^{+}(t);S_{Bj}^{-}\rangle\rangle=-i\theta(t)\langle[S_{Ai}^{+}(t),S_{Bj}^{-}]\rangle, \tag{4}$$
$$\langle\langle S_{Bj}^{+}(t);S_{Ai}^{+}\rangle\rangle=-i\theta(t)\langle[S_{Bj}^{+}(t),S_{Ai}^{+}]\rangle, \tag{5}$$
$$\langle\langle S_{Bj}^{+}(t);S_{Bj'}^{-}\rangle\rangle=-i\theta(t)\langle[S_{Bj}^{+}(t),S_{Bj'}^{-}]\rangle, \tag{6}$$
$$\langle\langle S_{Ai}^{+}(t);(S_{Ai'}^{-})^{2}S_{Ai'}^{+}\rangle\rangle=-i\theta(t)\langle[S_{Ai}^{+}(t),(S_{Ai'}^{-})^{2}S_{Ai'}^{+}]\rangle. \tag{7}$$

The equations of motion for $S_{Ai}^{+}(t)$ and $S_{Bj}^{+}(t)$ can be written as

$$i\frac{d}{dt}S_{Ai}^{+}=[S_{Ai}^{+},H]=J\sum_{j}(aS_{Ai}^{z}S_{Bj}^{+}-S_{Ai}^{+}S_{Bj}^{z})$$
$$+D(S_{Ai}^{+}S_{Ai}^{z}+S_{Ai}^{z}S_{Ai}^{+})+hS_{Ai}^{+}, \tag{8}$$

$$i\frac{d}{dt}S_{Bj}^{+}=[S_{Bj}^{+},H]$$
$$=J\sum_{i}(aS_{Bj}^{z}S_{Ai}^{+}-S_{Bj}^{+}S_{Ai}^{z})+D(S_{Bj}^{+}S_{Bj}^{z}+S_{Bj}^{z}S_{Bj}^{+})-hS_{Bj}^{+}. \tag{9}$$

Using Eqs. (8) and (9) we can obtain the equations of motion for Green's functions:

$$i\frac{d}{dt}\langle\langle S_{Ai}^{+}(t);S_{Ai'}^{-}\rangle\rangle=2\delta_{t}\delta_{ii'}\langle S_{Ai}^{z}\rangle+\langle\langle[S_{Ai}^{+},H];S_{Ai'}^{-}\rangle\rangle$$
$$=2\delta_{t}\delta_{ii'}\langle S_{Ai}^{z}\rangle+J\sum_{j}\langle\langle aS_{Ai}^{z}S_{Bj}^{+}-S_{Ai}^{+}S_{Bj}^{z};S_{Ai'}^{-}\rangle\rangle$$
$$+D\langle\langle S_{Ai}^{+}S_{Ai}^{z}+S_{Ai}^{z}S_{Ai}^{+};S_{Ai'}^{-}\rangle\rangle+h\langle\langle S_{Ai}^{+};S_{Ai'}^{-}\rangle\rangle, \tag{10}$$

$$i\frac{d}{dt}\langle\langle S_{Ai}^{+}(t);S_{Bj}^{-}\rangle\rangle=\langle\langle[S_{Ai}^{+},H];S_{Bj}^{-}\rangle\rangle$$
$$=J\sum_{j'}\langle\langle aS_{Ai}^{z}S_{Bj'}^{+}-S_{Ai}^{+}S_{Bj'}^{z};S_{Bj}^{-}\rangle\rangle$$
$$+D\langle\langle S_{Ai}^{+}S_{Ai}^{z}+S_{Ai}^{z}S_{Ai}^{+};S_{Bj}^{-}\rangle\rangle+h\langle\langle S_{Ai}^{+};S_{Bj}^{-}\rangle\rangle, \tag{11}$$

$$i\frac{d}{dt}\langle\langle S_{Bj}^{+}(t);S_{Ai}^{-}\rangle\rangle=\langle\langle[S_{Bj}^{+},H];S_{Ai}^{-}\rangle\rangle$$
$$=J\sum_{i'}\langle\langle aS_{Bj}^{z}S_{Ai'}^{+}-S_{Bj}^{+}S_{Ai'}^{z};S_{Ai}^{-}\rangle\rangle$$
$$+D\langle\langle S_{Bj}^{+}S_{Bj}^{z}+S_{Bj}^{z}S_{Bj}^{+};S_{Ai}^{-}\rangle\rangle-h\langle\langle S_{Bj}^{+};S_{Ai}^{-}\rangle\rangle, \tag{12}$$

$$i\frac{d}{dt}\langle\langle S_{Bj}^{+}(t);S_{Bj'}^{-}\rangle\rangle=2\delta_{t}\delta_{jj'}\langle S_{Bj}^{z}\rangle+\langle\langle[S_{Bj}^{+},H];S_{Bj'}^{-}\rangle\rangle$$
$$=2\delta_{t}\delta_{jj'}\langle S_{Bj}^{z}\rangle+J\sum_{i}\langle\langle aS_{Bj}^{z}S_{Ai}^{+}-S_{Bj}^{+}S_{Ai}^{z};S_{Bj'}^{-}\rangle\rangle$$
$$+D\langle\langle S_{Bj}^{+}S_{Bj}^{z}+S_{Bj}^{z}S_{Bj}^{+};S_{Bj'}^{-}\rangle\rangle-h\langle\langle S_{Bj}^{+};S_{Bj'}^{-}\rangle\rangle, \tag{13}$$

$$i\frac{d}{dt}\langle\langle S_{Ai}^{+}(t);(S_{Ai'}^{-})^{2}S_{Ai'}^{+}\rangle\rangle$$
$$=\delta_{t}\delta_{ii'}\langle[S_{Ai}^{+}(t),(S_{Ai'}^{-})^{2}S_{Ai'}^{+}]\rangle+\langle\langle[S_{Ai}^{+},H];(S_{Ai'}^{-})^{2}S_{Ai'}^{+}\rangle\rangle$$
$$=\delta_{t}\delta_{ii'}\langle[S_{Ai}^{+}(t),(S_{Ai'}^{-})^{2}S_{Ai'}^{+}]\rangle$$
$$+J\sum_{j}\langle\langle aS_{Ai}^{z}S_{Bj}^{+}-S_{Ai}^{+}S_{Bj}^{z};(S_{Ai'}^{-})^{2}S_{Ai'}^{+}\rangle\rangle$$
$$+D\langle\langle S_{Ai}^{+}S_{Ai}^{z}+S_{Ai}^{z}S_{Ai}^{+};(S_{Ai'}^{-})^{2}S_{Ai'}^{+}\rangle\rangle$$
$$+h\langle\langle S_{Ai}^{+};(S_{Ai'}^{-})^{2}S_{Ai'}^{+}\rangle\rangle. \tag{14}$$

In order to solve the system of the equations generated by Eqs. (10)–(14), we need to break the higher-order Green's functions. We apply the random phase approximation (RPA) [17] for the exchange coupling terms:

$$\langle S_{Ai}^{+}S_{l}^{z};S_{Bj}^{-}\rangle=\langle S_{l}^{z}\rangle\langle\langle S_{Ai}^{+};S_{Bj}^{-}\rangle\rangle, \tag{15}$$

and apply the Anderson–Callen approximation (ACA) [19] for the single-ion anisotropy term:

$$\langle\langle S_{i}^{+}S_{i}^{z}+S_{i}^{z}S_{i}^{+};S_{j}^{-}\rangle\rangle$$
$$=\left[2\langle S_{i}^{z}\rangle-\frac{1}{2S^{2}}\langle S_{i}^{z}\rangle\left(\langle S_{i}^{+}S_{i}^{-}\rangle+\langle S_{i}^{-}S_{i}^{+}\rangle\right)\right]\langle\langle S_{i}^{+};S_{j}^{-}\rangle\rangle. \tag{16}$$

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