



# Green's function approach of an anisotropic Heisenberg ferrimagnetic system

Gülistan Mert\*

Department of Physics, Selçuk University, 42075 Konya, Turkey



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## ABSTRACT

We have investigated the influence of the exchange anisotropy parameter on the magnetization, critical and compensation temperatures and susceptibility of the anisotropic Heisenberg ferrimagnetic system with the single-ion anisotropy under an external magnetic field using the double-time temperature-dependent Green's function theory. In order to decouple the higher order Green's functions, Anderson–Callen's decoupling and random phase approximations have been used. This model is useful for understanding the temperature dependence of total magnetization of Lithium–chromium ferrites  $\text{Li}_{0.5}\text{Fe}_{1.25}\text{Cr}_{1.25}\text{O}_4$  for which negative magnetization is characteristic. We observe that the critical temperature increases when the exchange anisotropy increases. When the system is under an external magnetic field, one obtains the first-order phase transition where the magnetization jumps for all the values of the exchange anisotropy parameters.

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## 1. Introduction

In recent years, the ferrimagnets have been studied both experimentally [1–9] and theoretically [10–20]. One of the most interesting properties of ferrimagnets is that they exhibit a compensation temperature. The different behaviors of temperature dependences of the sub-lattice magnetization are the main cause of the appearance of compensation temperature. At the temperatures below critical temperature  $T_c$ , if the magnetizations of two sub-lattices are equal but in opposite directions, then the total magnetization becomes zero. One calls the compensation temperature  $T_{comp}$  where total magnetization vanishes but sub-lattice magnetizations have equal and opposite non-zero values [1]. This property in ferrimagnets has various technological applications such as magneto-optical recording [21]. Compounds having spinel structure ( $\text{AB}_2\text{O}_4$ ) order ferrimagnetically at  $T_c$ .  $\text{FeCr}_2\text{S}_4$  with a cubic spinel structure is a typical example for these compounds. It has two different magnetic sublattices (Fe,  $S=2$ ; Cr,  $S=3/2$ ).  $\text{Fe}^{2+}$  ions occupy at A sites and  $\text{Cr}^{3+}$  ions at B sites. The magnetic interaction between  $\text{Cr}^{3+}$  ions is ferromagnetic and  $\text{Fe}^{2+}$  ions are coupled with the  $\text{Cr}^{3+}$  ions with antiferromagnetic interaction.  $\text{FeCr}_2\text{S}_4$  displays an orbital order phase transition [22]. Lithium–chromium ferrites  $\text{Li}_{0.5}\text{Fe}_{1.25}\text{Cr}_{1.25}\text{O}_4$  exhibiting the compensation point  $T_{comp}=310$  K and the critical temperature  $T_c=500$  K have shown the magnetic reversal behavior [23,24].

Experiments have demonstrated that there exists an anisotropy field in magnetic materials. The anisotropy plays an important part in the magnetic properties of these substances [25–30]. The spontaneous

magnetization for a ferromagnetic film and a bulk crystal will occur only when there is certain anisotropy [31,32]. Anisotropic Heisenberg model with and without the single-ion anisotropy have been investigated by using the various theoretical methods for the ferromagnetic, antiferromagnetic and ferrimagnetic systems [33–46]. Magnetization of an anisotropic Heisenberg model in these systems can be described also by the double-time temperature-dependent Green's function technique [47–56]. In this method, in reducing the higher-order Green's functions into the lower ones, one obtains an infinite hierarch of coupled nonlinear differential equations. The coupled equations derived from the equation of motion transformed to uncoupled equations using appropriate decoupling approximations and then solve the uncoupled equations. Decoupling is not a systematic method, but provides a fundamental manner in a wide range of temperature with reasonable accuracy. We use Anderson–Callen's decoupling [57] and random phase approximations [58–60].

In this work, we apply the formalism of the double-time temperature-dependent Green's function to study the magnetic properties of a mixed spin-3/2 and spin-2 anisotropic Heisenberg ferrimagnetic model with the single-ion anisotropy in the presence of an external magnetic field. The outline of this paper is arranged as follows. A formulation of the problem is presented in Section 2. In Section 3, the results and discussions are given. Finally, Section 4 contains conclusions.

## 2. Model

We consider the mixed spin-3/2 and spin-2 anisotropic Heisenberg ferrimagnetic model on a square lattice divided into two equivalent

\* Tel.: +90 05556578777; fax: +90 332 2376195.  
E-mail address: [gmert@selcuk.edu.tr](mailto:gmert@selcuk.edu.tr)

sub-lattices A and B. Both sub-lattices are also again a square lattice. We assume the Hamiltonian as follows:

$$\begin{aligned}
 H = & -\sum_{\langle ij \rangle} J_{ij} [\eta(S_{ai}^x S_{bj}^x + S_{ai}^y S_{bj}^y) + S_{ai}^z S_{bj}^z] \\
 & -\sum_{\langle i\bar{i} \rangle} J_{i\bar{i}} [\eta(S_{ai}^x S_{\bar{a}i}^x + S_{ai}^y S_{\bar{a}i}^y) + S_{ai}^z S_{\bar{a}i}^z] \\
 & -\sum_{\langle j\bar{j} \rangle} J_{j\bar{j}} [\eta(S_{bj}^x S_{\bar{b}j}^x + S_{bj}^y S_{\bar{b}j}^y) + S_{bj}^z S_{\bar{b}j}^z] \\
 & -D_a \sum_i (S_{ai}^z)^2 - D_b \sum_j (S_{bj}^z)^2 - h (\sum_i S_{ai}^z + \sum_j S_{bj}^z), \quad (1)
 \end{aligned}$$

where the subscripts  $i$  and  $j$  label lattice sites.  $ai$  refers to the lattice site  $i$  in the sub-lattice A (spin-3/2) and  $bj$  refers to the sub-lattice site  $j$  in the sub-lattice B (spin-2).  $S_{ai}^x$ ,  $S_{ai}^y$ ,  $S_{ai}^z$  represent the three components of the Heisenberg spin operators for a spin at  $i$  site in sub-lattice A and  $S_{bj}^x$ ,  $S_{bj}^y$ ,  $S_{bj}^z$  for a spin at  $j$  site in sub-lattice B.  $J$  is the exchange interaction between the nearest-neighbor spins  $S_{ai}$  and  $S_{bj}$  and in the case of antiferromagnetic interaction,  $J < 0$ .  $J_1$  is the exchange interaction between the next-nearest-neighbor spins  $S_{ai}$  and  $S_{\bar{a}i}$  and in the case of ferromagnetic,  $J_1 > 0$ .  $J_2$  is the exchange interaction between the next-nearest-neighbor spins  $S_{bj}$  and  $S_{\bar{b}j}$  in the case of ferromagnetic,  $J_2 > 0$ .  $\eta$  denotes the degree of the exchange anisotropy varying from 0 to 1.  $D_a$  is the single-ion anisotropy parameter of the sub-lattice A and  $D_b$  is that of the sub-lattice B. Finally,  $h$  is an external magnetic field applied along the z-axis.

It is convenient to introduce the spin raising and lowering operators:  $S_i^\pm = S_i^x \pm iS_i^y$  which satisfy the commutation relations  $[S_{ai}^+, S_{bj}^-] = 2S_{ai}^z \delta_{ij} \delta_{ab}$  and  $[S_{ai}^\pm, S_{bj}^\pm] = \mp S_{ai}^\pm \delta_{ij} \delta_{ab}$ . Then, Hamiltonian given in the Eq. (1) can be rewritten as

$$\begin{aligned}
 H = & -J \sum_{\langle ij \rangle} \left[ \frac{\eta}{2} (S_{ai}^+ S_{bj}^- + S_{ai}^- S_{bj}^+) + S_{ai}^z S_{bj}^z \right] \\
 & -J_1 \sum_{\langle i\bar{i} \rangle} \left[ \frac{\eta}{2} (S_{ai}^+ S_{\bar{a}i}^- + S_{ai}^- S_{\bar{a}i}^+) + S_{ai}^z S_{\bar{a}i}^z \right] \\
 & -J_2 \sum_{\langle j\bar{j} \rangle} \left[ \frac{\eta}{2} (S_{bj}^+ S_{\bar{b}j}^- + S_{bj}^- S_{\bar{b}j}^+) + S_{bj}^z S_{\bar{b}j}^z \right] \\
 & -D_a \sum_i (S_{ai}^z)^2 - D_b \sum_j (S_{bj}^z)^2 - h (\sum_i S_{ai}^z + \sum_j S_{bj}^z). \quad (2)
 \end{aligned}$$

In order to study the magnetic properties of the model, we use the many-body Green's function theory. Green's functions should be chosen as follows:

$$G_{aa}(t) = \langle \langle S_{ai}^+(t); B_{al}(0) \rangle \rangle \quad \text{and} \quad G_{ba}(t) = \langle \langle S_{bj}^+(t); B_{al}(0) \rangle \rangle \quad (3)$$

$$G_{bb}(t) = \langle \langle S_{bj}^+(t); B_{bl}(0) \rangle \rangle \quad \text{and} \quad G_{ab}(t) = \langle \langle S_{ai}^+(t); B_{bl}(0) \rangle \rangle \quad (4)$$

where  $B_l = e^{aS_l^z} S_l^-$ ,  $\alpha$  is a Callen's parameter [61].

Time evaluation of the Green's functions follows from their equations of motion. The equations of motion for the four Green's functions are obtained as

$$\begin{aligned}
 \omega \langle \langle S_{ai}^+, B_{al} \rangle \rangle = & \frac{\delta_{il}}{2\pi} \langle [S_{ai}^+, e^{aS_{ai}^z} S_{ai}^-] \rangle - J\eta \sum_{\langle ij \rangle} \langle \langle S_{ai}^z S_{bj}^+, B_{al} \rangle \rangle \\
 & + J \sum_{\langle ij \rangle} \langle \langle S_{ai}^+ S_{bj}^z, B_{al} \rangle \rangle \\
 & - J_1 \eta \sum_{\langle i\bar{i} \rangle} \langle \langle S_{ai}^z S_{\bar{a}i}^+, B_{al} \rangle \rangle + J_1 \sum_{\langle i\bar{i} \rangle} \langle \langle S_{ai}^+ S_{\bar{a}i}^z, B_{al} \rangle \rangle \\
 & + D_a \langle \langle (S_{ai}^+ S_{ai}^z + S_{ai}^z S_{ai}^+); B_{al} \rangle \rangle + h \langle \langle S_{ai}^+, B_{al} \rangle \rangle, \quad (5)
 \end{aligned}$$

$$\begin{aligned}
 \omega \langle \langle S_{bj}^+, B_{al} \rangle \rangle = & -J\eta \sum_{\langle ij \rangle} \langle \langle S_{bj}^z S_{ai}^+, B_{al} \rangle \rangle + J \sum_{\langle ij \rangle} \langle \langle S_{bj}^+ S_{ai}^z, B_{al} \rangle \rangle \\
 & - J_2 \eta \sum_{\langle j\bar{j} \rangle} \langle \langle S_{bj}^z S_{\bar{b}j}^+, B_{al} \rangle \rangle + J_2 \sum_{\langle j\bar{j} \rangle} \langle \langle S_{bj}^+ S_{\bar{b}j}^z, B_{al} \rangle \rangle \\
 & + D_b \langle \langle (S_{bj}^+ S_{bj}^z + S_{bj}^z S_{bj}^+); B_{al} \rangle \rangle + h \langle \langle S_{bj}^+, B_{al} \rangle \rangle, \quad (6)
 \end{aligned}$$

$$\begin{aligned}
 \omega \langle \langle S_{bj}^+, B_{bl} \rangle \rangle = & \frac{\delta_{jl}}{2\pi} \langle [S_{bj}^+, e^{aS_{bj}^z} S_{bj}^-] \rangle - J\eta \sum_{\langle ij \rangle} \langle \langle S_{bj}^z S_{ai}^+, B_{bl} \rangle \rangle \\
 & + J \sum_{\langle ij \rangle} \langle \langle S_{bj}^+ S_{ai}^z, B_{bl} \rangle \rangle \\
 & - J_2 \eta \sum_{\langle j\bar{j} \rangle} \langle \langle S_{bj}^z S_{\bar{b}j}^+, B_{bl} \rangle \rangle + J_2 \sum_{\langle j\bar{j} \rangle} \langle \langle S_{bj}^+ S_{\bar{b}j}^z, B_{bl} \rangle \rangle \\
 & + D_b \langle \langle (S_{bj}^+ S_{bj}^z + S_{bj}^z S_{bj}^+); B_{bl} \rangle \rangle + h \langle \langle S_{bj}^+, B_{bl} \rangle \rangle, \quad (7)
 \end{aligned}$$

$$\begin{aligned}
 \omega \langle \langle S_{ai}^+, B_{bl} \rangle \rangle = & -J\eta \sum_{\langle ij \rangle} \langle \langle S_{ai}^z S_{bj}^+, B_{bl} \rangle \rangle + J \sum_{\langle ij \rangle} \langle \langle S_{ai}^+ S_{bj}^z, B_{bl} \rangle \rangle \\
 & - J_1 \eta \sum_{\langle i\bar{i} \rangle} \langle \langle S_{ai}^z S_{\bar{a}i}^+, B_{bl} \rangle \rangle + J_1 \sum_{\langle i\bar{i} \rangle} \langle \langle S_{ai}^+ S_{\bar{a}i}^z, B_{bl} \rangle \rangle \\
 & + D_a \langle \langle (S_{ai}^+ S_{ai}^z + S_{ai}^z S_{ai}^+); B_{bl} \rangle \rangle + h \langle \langle S_{ai}^+, B_{bl} \rangle \rangle, \quad (8)
 \end{aligned}$$

where  $\delta$  is Dirac's delta function and  $\langle \dots \rangle$  denotes the canonical thermal average. We have taken the value of  $\hbar$  as unit.

In the equations of motion, the higher-order Green's functions will appear. The Green's functions coming from the exchange terms can be decoupled by using random phase approximation [58–60]

$$\langle \langle S_{ai}^z S_{bj}^+, B_l \rangle \rangle \cong \langle S_{ai}^z \rangle \langle \langle S_{bj}^+, B_l \rangle \rangle, \quad (9)$$

Random phase approximation is not an appropriate decoupling for the Green's functions coming from the single-ion anisotropy. For these kinds of decoupling, we perform a generalization of the Anderson and Callen's decoupling schema [57]

$$\begin{aligned}
 \langle \langle (S_{ai}^+ S_{ai}^z + S_{ai}^z S_{ai}^+); B_l \rangle \rangle & \cong \tau_a \langle \langle S_{ai}^+, B_l \rangle \rangle \quad \text{and} \\
 \langle \langle (S_{bj}^+ S_{bj}^z + S_{bj}^z S_{bj}^+); B_l \rangle \rangle & \cong \tau_b \langle \langle S_{bj}^+, B_l \rangle \rangle, \quad (10)
 \end{aligned}$$

where

$$\begin{aligned}
 \tau_a = 2m_a \left\{ 1 - \frac{1}{2S_a^2} [S_a(S_a + 1) - Q_a] \right\} \quad \text{and} \quad \tau_b = 2m_b \left\{ 1 - \frac{1}{2S_b^2} [S_b(S_b + 1) - Q_b] \right\}, \quad (11)
 \end{aligned}$$

where  $m_a$ ,  $m_b$  stand for the spontaneous magnetization of the sub-lattices A and B, respectively.  $Q_a$  and  $Q_b$  stand for the averages of square of the magnetizations called the quadrupolar moments of the sub-lattices A and B, respectively.

After Fourier transforming these equations with respect to the space and time variables, we obtain the following Green's functions

$$G_{aa}(\omega, K) = \frac{\Theta_{aa}(a)}{2\pi(E^+ - E^-)} \left[ \frac{E^+ - C - h}{\omega - E^+} - \frac{E^- - C - h}{\omega - E^-} \right], \quad (12)$$

$$G_{bb}(\omega, K) = \frac{\Theta_{bb}(a)}{2\pi(E^+ - E^-)} \left[ \frac{E^+ - A - h}{\omega - E^+} - \frac{E^- - A - h}{\omega - E^-} \right], \quad (13)$$

where

$$\begin{aligned}
 \Theta_{aa}(a) = & \langle [S_{ai}^+, e^{aS_{ai}^z} S_{ai}^-] \rangle \quad \text{and} \quad \Theta_{bb}(a) = \langle [S_{bj}^+, e^{aS_{bj}^z} S_{bj}^-] \rangle, \\
 E^\pm = & \frac{1}{2} \left\{ (A + C + 2h) \pm [(A - C)^2 + 4BD]^{1/2} \right\}, \\
 A = & D_a \tau_a + J \sum_{\langle ij \rangle} m_b + J_1 \sum_{\langle i\bar{i} \rangle} m_a [1 - \eta \exp(ik \cdot (i - i))], \\
 B = & -J\eta \sum_{\langle ij \rangle} m_a \exp(ik \cdot (j - i)), \\
 C = & D_b \tau_b + J \sum_{\langle ij \rangle} m_a + J_2 \sum_{\langle j\bar{j} \rangle} m_b [1 - \eta \exp(ik \cdot (j - j))], \\
 D = & -J\eta \sum_{\langle ij \rangle} m_b \exp(ik \cdot (j - i)). \quad (14)
 \end{aligned}$$

One obtains the magnetizations and quadrupolar moments of the sub-lattices A and B by means of the spectral theorem and Callen's technique [61] as follows:

$$m_\nu = \frac{(S_\nu - \Phi_\nu)(1 + \Phi_\nu)^{2S_\nu + 1} + (S_\nu + 1 + \Phi_\nu)\Phi_\nu^{2S_\nu + 1}}{(1 + \Phi_\nu)^{2S_\nu + 1} - \Phi_\nu^{2S_\nu + 1}}, \quad (15)$$

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