Microcanonical entropy as a function of energies for the Triangular-Lattice Blume-Capel magnetic system

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Abstract. The triangular-lattice Blume-Capel magnetic system is investigated using efficient Wang-Landau Monte Carlo algorithm. From extensive Wang-Landau Monte Carlo simulations with massive large-scale computing, the microcanonical entropy as a function of energy variables, the most fundamental quantity in statistical thermodynamics, for the triangular-lattice Blume-Capel ferromagnet and antiferromagnet at the same time is evaluated for the first time. The important properties of the microcanonical entropy as a function of energy variables are discussed for the triangular-lattice Blume-Capel magnetic system.

1. Introduction

Magnetic materials have been widely known since ancient times. The English word Magnet originated from Magnesia, ancient civilization in western Turkey. East Asian have used a loadstone compass more than two thousand years ago. Magnetic materials are usually ferromagnetic ones. In ferromagnet, microscopic magnetic spins interact strongly each other, and most spins align to the same direction even at a room temperature, resulting in macroscopic strong magnetic field [1]. Above Curie temperature (named after Pierre Curie, Nobel prize winner in 1903), because microscopic magnetic spins align randomly due to large thermal fluctuations, ferromagnet becomes paramagnet.

In addition to paramagnet and ferromagnet, antiferromagnet is also an important magnetic material, first introduced by Neel (Nobel prize winner in 1970) [1]. In antiferromagnet, neighboring magnetic spins align antiparallel each other, not resulting in macroscopic magnetic field. Therefore, it is very difficult to detect an antiferromagnetic material and to distinguish it from a paramagnetic material. Above Neel temperature, antiferromagnet changes its phase into paramagnet. Antiferromagnet plays an important role in giant magnetoresistance [2] and high-temperature superconductivity [3]. Antiferromagnetic materials are important in various industrial applications including hard disk drives.

Modern theory of magnetic materials, phase transitions, and critical phenomena began with the simplest magnetic system, the spin-1/2 Ising system [4], to understand paramagnetism-ferromagnetism phase transition. In the spin-1/2 Ising magnetic system, a microscopic magnetic spin can take 1 (upward) or −1 (downward). Simple and easy theory for understanding the spin-1/2 Ising system is the Weiss molecular field theory [1], well explained in textbooks on magnetic materials or phase transitions. The results of the Weiss molecular field theory are reasonable but not accurate. The

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exact solution for the square-lattice spin-1/2 Ising system [5] was first obtained by Onsager (Nobel prize winner in 1968) with transfer-matrix method. It is now called the Onsager revolution [6] because modern theory of phase transitions and critical phenomena is based on the Onsager solution for the square-lattice spin-1/2 Ising system.

2. Blume-Capel magnetic system

More complex magnetic system is the spin-1 Ising system whose exact solution even on simple square lattice has not been known. In the spin-1 Ising magnetic system, a microscopic magnetic spin can take 1 (upward), 0 (vacancy), or −1 (downward). The Blume-Capel magnetic system [7, 8] is an extension of the spin-1 Ising system with a vacancy-favoring term. The Blume-Capel system has been extensively studied to understand the behaviors of He^3-He^4 mixtures. Also, it has been studied to understand various systems such as multicomponent fluids, metamagnets, molecule-based chain magnets, and ternary alloys. For example, the square-lattice Blume-Capel system [9] shows second-order phase transitions, first-order phase transitions, and a tricritical point separating these different transitions.

The physical origin of the vacancy-favoring term (the so-called crystal field $D$) for the Blume-Capel magnetic system arises from non-central potentials for metal atoms coordinated with various ligands in the crystal. The Blume-Capel system with $D > 0$ prefers the spin vacancy and shows second-order phase transitions, first-order phase transitions, and a tricritical point. The Blume-Capel system with $D < 0$ is similar to the spin-1/2 Ising system. In this work, we investigate the triangular-lattice Blume-Capel magnetic system whose properties are not known, using efficient Wang-Landau Monte Carlo algorithm [10]. From extensive Wang-Landau Monte Carlo simulations with massive large-scale computing, we obtain the microcanonical entropy as a function of energy variables of the triangular-lattice Blume-Capel ferromagnet and antiferromagnet at the same time for the first time.

The triangular-lattice Blume-Capel magnetic system is defined by the Hamiltonian

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j + D \sum_i \sigma_i^2,$$

where $J$ is the coupling constant, $D$ is the crystal field (also called the single-spin anisotropy parameter or the spin impurity chemical potential), $\langle i, j \rangle$ represents a sum over all nearest-neighbor pairs, and $\sigma_i (= -1, 0, 1)$ is the microscopic magnetic spin at the lattice site $i$. Positive coupling constant ($J > 0$) defines the Blume-Capel ferromagnet, whereas negative coupling constant ($J < 0$) indicates the Blume-Capel antiferromagnet.

3. Microcanonical entropy of the triangular-lattice Blume-Capel magnetic system

If we define the density of states, $g(E, S)$, with two energy variables $E = \sum_{\langle i, j \rangle} \sigma_i \sigma_j$ and $S = \sum_i \sigma_i^2$, the partition function of the Blume-Capel system, $Z = \sum_{\{\sigma_i\}} e^{-\beta H}$, can be written as

$$Z(T; J, D) = \sum_E \sum_S g(E, S) e^{\beta J(E \frac{D}{T} S)},$$

where $\beta = 1/k_BT$ ($k_B$ is the Boltzmann constant and $T$ is temperature). Then, we obtain the microcanonical entropy, the most fundamental quantity in statistical thermodynamics, according to the Boltzmann formula $M(E, S) = k_B \ln g(E, S)$. In this work, we evaluate the microcanonical entropy as a function of $E$ and $S$ for the Blume-Capel magnetic system on a $12 \times 12$ triangular lattice with

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j + D \sum_i \sigma_i^2,$$
Wang-Landau Monte Carlo simulations, as shown in Figure 1. It should be noted that this kind of figure for the triangular-lattice Blume-Capel magnetic system is obtained for the first time.

![Figure 1. Top view of the microcanonical entropy $M(E,S)$ (in units of $k_b$) for the Blume-Capel magnetic system on a $12 \times 12$ triangular lattice, where two energy variables $E$ and $S$ are defined as $E = \sum_{\alpha, \beta} \sigma_i \sigma_j$ and $S = \sum_i \sigma_i^2$ with $\sigma_i = -1, 0, 1$.

As shown in the figure, the microcanonical entropy has four vertices in the $E-S$ plane. The microcanonical entropy is not allowed outside the polygon defined by four vertices. The vertex $(E, S) = (0, 0)$ is the spin vacancy state $\sigma_i = 0$ for all $i$. The density of states is $g(0, 0) = 1$ for the spin vacancy state. The density of states on the straight line from the vertex $(E, S) = (-144, 144)$ to $(-144, 96)$ corresponds to the antiferromagnetic ground states, whereas the vertex $(E, S) = (432, 144)$ to the ferromagnetic ground states. The density of states is $g(N_s, N_s) = 2$ for the ferromagnetic ground states, but the density of states is highly degenerate for the antiferromagnetic ground states.

Furthermore, the partition function can be written as

$$Z(T; J, D) = \sum_{E} \sum_{S} \exp \left[ \frac{M(E, S)}{k_B} + \frac{J}{k_B T} \left( E - \frac{D S}{J} \right) \right]. \quad (3)$$

If we define the combined energy $\tilde{E} = E - \frac{D}{J} S$, the partition function can be simply written as

$$Z(T) = \sum_{E} \exp \left[ \frac{M(\tilde{E})}{k_B} + \frac{J \tilde{E}}{k_B T} \right]. \quad (4)$$
for a fixed value of $D/J$. Now the microcanonical entropy $M(\tilde{E})$ is dependent on the only one energy variable $\tilde{E}$.

Figure 2. Microcanonical entropy $M(\tilde{E})$ (in units of $k_B$) of the Blume-Capel magnetic system on a $12 \times 12$ triangular lattice for $D/J = 1$, where the combined energy $\tilde{E} = E - \frac{D}{J}$. Figure 2 shows the microcanonical entropy $M(\tilde{E})$ of the Blume-Capel magnetic system on a $12 \times 12$ triangular lattice for $D/J = 1$. As shown in the figure, the maximum entropy is located at $\tilde{E} = -96$. The antiferromagnetic ground states is located at $\tilde{E} = -288$, and the ferromagnetic ground states at $\tilde{E} = 288$. The energy interval $\tilde{E} = [-288, -96]$ corresponds to the Blume-Capel antiferromagnet. Similarly, the energy interval $\tilde{E} = [-96, 288]$ corresponds to the Blume-Capel ferromagnet.

4. Conclusion
We have studied the triangular-lattice Blume-Capel magnetic system using Wang-Landau Monte Carlo method to calculate its microcanonical entropy. From extensive Wang-Landau Monte Carlo simulations with massive large-scale computing, we have evaluated the microcanonical entropy as a function of energy variables (exchange energy and vacancy-favoring energy), the most fundamental quantity in statistical thermodynamics, for the triangular-lattice Blume-Capel ferromagnet and antiferromagnet at the same time for the first time.

Given the microcanonical entropy, we can investigate the important properties of the triangular-lattice Blume-Capel magnetic system through various methods such as canonical analysis [11, 12, 13, 14], microcanonical analysis [15, 16, 17], and partition function zeros [18, 19, 20]. In canonical analysis, we can obtain the canonical thermodynamic functions (such as specific heat and other response functions) as a continuous function of temperature. In microcanonical analysis, we can use the whole information on the microcanonical entropy, directly analyzing its topological and geometric
properties. If we have the microcanonical entropy of a given system, we can calculate its partition function zeros from which we can understand its phase transitions and critical phenomena accurately.

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