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Wang-Landau algorithm in a two-dimensional spin−1 Blume-Capel Model

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Abstract

We study spin−1 Blume-Capel (BC) model in two-dimensions in terms of the Wang-Landau (WL) algorithm, which is one of typical entropic sampling methods with lots of applications in statistical physics and biophysics. The WL algorithm lets us estimate the joint density of states as a function of energy and the order parameter in the BC model.

Keywords: WL algorithm, spin−1 Blume-Capel model, joint density

1. Introduction

Monte Carlo simulations currently play a major role in statistical physics to study of phase transitions and critical phenomena. In order to reduce computing time and to obtain the accurate results, a number of simulation algorithms have been exploited.

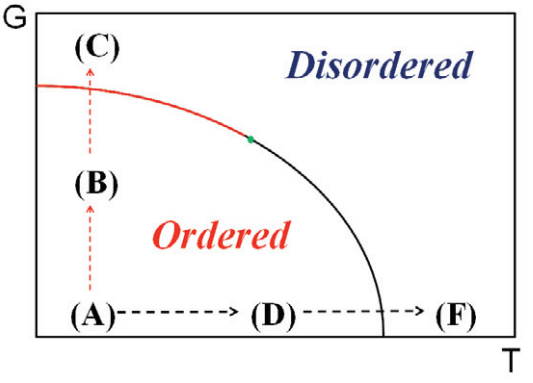

Figure 1: Schematic plot of phase diagram of spin−1 BC model as a function of crystal field G and temperature T.

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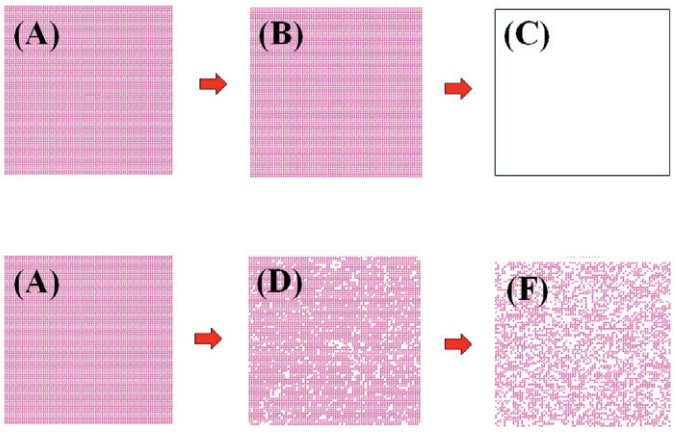

Figure 2: Equilibrium configurations of spin−1 BC model, where the path from (A) to (C) shows first-order phase transition and the path from (A) to (F) shows the second-order phase transition.

The Wang-Landau (WL) algorithm is widely used with equilibrium systems due to obtaining accurate results, reducing computing time, and easy parallelization [1, 2, 3, 5, 6, 7]. Using WL algorithm, it is possible to calculate the density of states for a system. Blume-Capel (BC) model is designed to study the first-order phase transition in spin systems [8, 9, 10, 11, 12]. The Hamiltonian of the spin−1 BC model is given by

$$\mathcal{H} = -J\sum_{\langle i,j\rangle} S_i S_j + G\sum_i {S_i}^2 + h\sum_i S_i, \tag{1}$$

where the first sum runs over all nearest-neighbor pairs with the ferromagnetic coupling constant J= +1 and the second and the third sums are carried out all sites in two dimensional $(2d)$ square lattice. In (1), G is anisotropy parameter and h is external magnetic field. The spin variable S_i assume values $-S, -S+1, ..., S-1, S$.

In this paper, we set the spin value $S = 1$ and $h = 0$. So, spin values are -1, 0, and 1. To check the properties of spin−1 BC model, we perform the Monte Carlo simulation with Metropolis rate $min\left(e^{-\beta\Delta\mathcal{H}}, 1\right)$, where β is inverse temperature and $\Delta\mathcal{H}$ is energy difference between the initial energy $\mathcal{H}_i$ and the trial final energy $\mathcal{H}_f$. Figure 1 shows the schematic plot of phase diagram of spin−1 BC model which exhibits a line of continuous phase transition, a line of first-order phase transition, and the tricritical point where two lines meet (see Figure 2).

2. Wang-Landau Algorithm

Using the WL algorithm, the $3d$ random walks are performed in $\left(E, M, M^2\right)$ space by randomly changing the states of spins $A\left(E, M, M^2\right)$, where the order parameter M is $\sum_i S_i$ and the square of order parameter M^2 is $\sum_i {S_i}^2$, but the state $A\left(E, M, M^2\right)$ associated with each spin configuration is only accepted with a probability proportional to the reciprocal of the joint density of states $g(A)$ [13, 14, 15, 16]. Therefore, the transition probability from state $A\left(E, M, M^2\right)$ to $A'\left(E', M', M'^2\right)$ is

$$p(A \to A') = min\left(\frac{g(A)}{g(A')}, 1\right), \tag{2}$$

which indicates that if $g(A') \le g(A)$, a state with spin configuration A' is always accepted, and that if $g(A') > g(A)$, it is accepted with a probability $g(A)/g(A')$.

During the simulation, we also accumulate the histogram $H\left(E, M, M^2\right)$, and the density of states $g(A)$ is modified in a systematic way using modification factor f. If a trial state A' is accepted, we update: $H(A') \to H(A') + 1$ and $g(A') \to g(A') \times f$. If the trial state is rejected, we also modify $g(A)$ and $H(A)$: $H(A) \to H(A) + 1$ and $g(A) \to g(A) \times f$.