La 1ère Conférence Nationale sur la Transition Energétique en Algérie
CNTEA1-2020 Université Mohamed BOUDIAF
M'sila, le 8-9 Mars 2020

CLUSTER MONTE CARLO STUDY OF THE FERROMAGNETIC ISING-LIKE MODEL FOR SPIN CROSSOVER SYSTEMS

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Abstract

A comparison between some thermal quantities (magnetization and susceptibility) of a ferromagnetic Ising-like model obtained by Metropolis and Swendsen-Wang MC dynamics have been given.
The results shows that for a moderate ferromagnetic interactions these quantities are closely identically in the two MC dynamics, for strong ferromagnetic interactions the comparison study is done outside the hysteresis cycle only, this limitation was imposed by the method used in the study (ghost bonds method).

Introduction

Spin crossover materials offer promising opportunities for applications in information processing, sensors and/or displays devices, these materials are switchable by different external stimuli, such as temperature, radiation, magnetic field, pressure,…[1-3]. Beside the many experimental methods and techniques for preparing and studying spin transition compounds, there are some models for the theoretical investigations [2,3].
The percolation approach of Coniglio and Klein (C-K) for a ferromagnetic spin systems is an extension of Fortuin and Kasteleyn one's (F-K) [4], where they introduced a new set of variables [5]. The introduction of the cluster MC dynamics by Swendsen and Wang [6] get propel the percolation approach of Ising and Potts models, and the dynamics have been used by many authors to study phase transition phenomena under many other models [7, 8].
In this study, we simulate the ferromagnetic Ising-like model of spin transition systems via the Swendsen-Wang cluster MC dynamics and compared the results with those obtained by the Metropolis dynamics, and we essayed to justify the cases where the two dynamics don't agree.

Model and Method

We have extended (C-K) clusters formalism to ferromagnetic spin transition systems via the "ghost" spin method [9]. The considered ferromagnetic Ising-type Hamiltonian is:

$$H=\sum_i \frac{\Delta_i}{2}\sigma_i-\sum_{<i,j>} J_{ij}\sigma_i\sigma_j=\frac{\Delta}{2}\sum_i \sigma_i - J\sum_{<i,j>}\sigma_i\sigma_j$$

where $\Delta > 0$, $J > 0$, are the ligand field and the interaction constant respectively, $\sigma_{i} = \pm 1$ is a fictitious spin variable.
The canonical thermal partition function can be written as:

$$Z=\sum_{\{\sigma_i\}} exp\left(-\beta\left(-\sum_i h_{igh}(\sigma_{gh}\sigma_i-1)-J\sum_{<i,j>}(\sigma_i\sigma_j-1)\right)\right)$$
$$=\sum_{\{\sigma_i\}} exp(-\beta H')$$

Its corresponding percolation one is:

$$Z(G)=\frac{1}{2}\sum_{C_s} p^{|C_s|}(1-p)^{|A_s|}\,2^{N(C_s)}$$

With: $p=\begin{cases}1-exp(-2\beta J);\ \text{bond } \langle i,j\rangle\in C_s \text{ is real}\\ \left\{\begin{matrix}1-exp(-\beta\Delta_{eff}(T));\ T\le T_C;\ \text{bond } \langle i,j\rangle\in C_s \text{ is ghost}\\ 1-exp(+\beta\Delta_{eff}(T));\ T\ge T_C;\ \text{bond } \langle i,j\rangle\in C_s \text{ is ghost}\end{matrix}\right.\end{cases}$

$|C_s|$, $|A_s|$ and N(Cs) are the number of active bonds (reals and ghosts one's), the number of inactive bonds and the total number of clusters in the bonds configuration Cs (including the ghost cluster and individual spins).
From this partition function, we get [9]:

$$\langle\sigma_i\rangle=\begin{cases}-\langle\gamma_{igh}\rangle\ ;\ \sigma_{gh}=-1;\ for\ T\le T_C\\ \langle\gamma_{igh}\rangle\ ;\ \sigma_{gh}=+1;\ for\ T\ge T_C\end{cases}$$

It is the average thermal quantity "local magnetization" by the indicator γ_{igh}; $\gamma_{igh}=1$ if the spin i belongs to the ghost cluster (connected to the ghost spin directly or indirectly) and $\gamma_{igh}=0$ otherwise.
The "global magnetization" is given by: $\langle\sigma\rangle=\frac{1}{N_s}\sum_{i=1}^{N_s}\langle\sigma_i\rangle$
The fraction of sites in high spin state, n_{HS}, is given by: $n_{HS}=\frac{1}{2}(1+\langle\sigma\rangle)$

Results

Simulations for systems with weak cooperative interactions, where the systems spin transition is reversible (Fig. 1), show that results of measure on the thermal quantities (fraction of spins in HS and magnetic susceptibility) are practically identical in the two different MC dynamics whatever the systems size (Fig. 1).
In the case of highly cooperative systems, where the transition of the spin is with hysteresis (Fig. 2), the two MC dynamics give results of measures almost identical for wide size systems, but for small size one's the results show a disagreement between the two dynamics, this is due to the strong correlations between the constituents of the system, where the range of the interactions exceeds the system size, the cluster dynamics is less effective in these systems(Fig. 2).

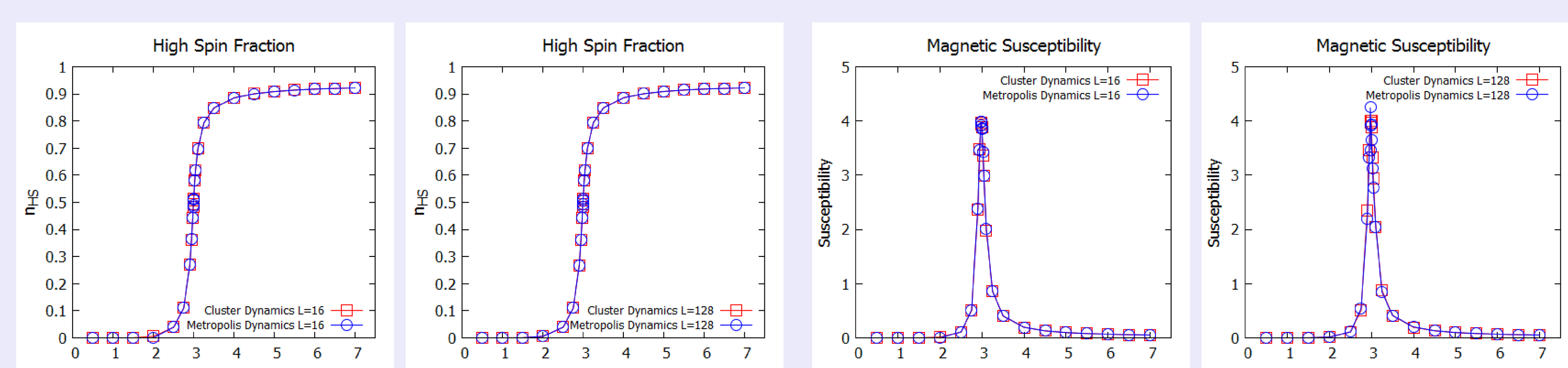

Fig. 1. *Fraction of spins in high spin state and Magnetic susceptibility for square lattices with sizes indicated in the figures, in the case of weak interactions (Δ=8.1, g_{HS}=15, g_{LS}=1), measured after (10^4) MCS according to Swendsen-Wang cluster dynamics and Metropolis dynamics.*

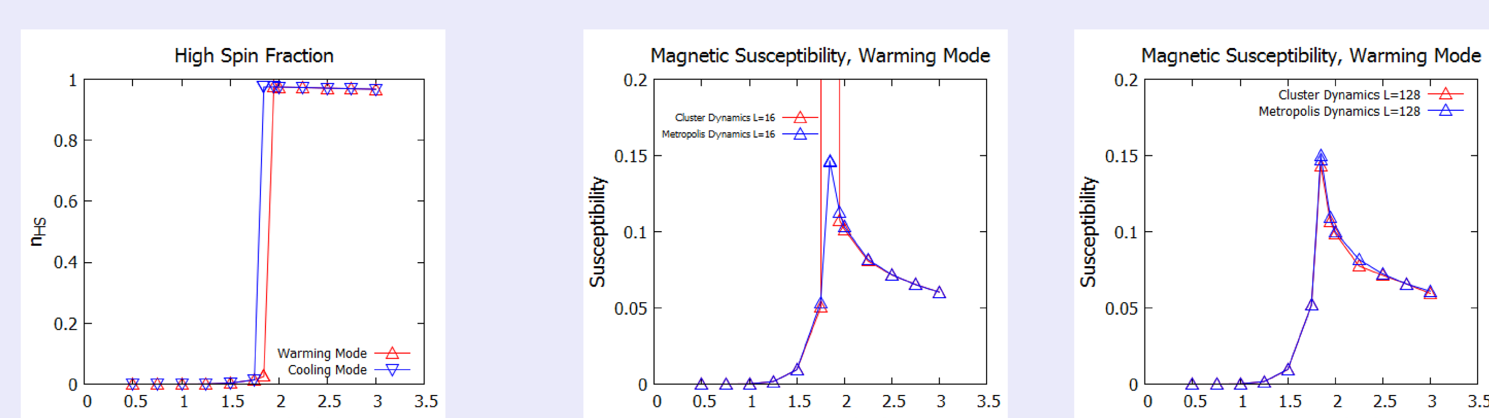

Fig. 2. *Fraction of spins in high spin state and Magnetic susceptibility for square lattices with sizes indicated in the figures, in the case of strong interactions(Δ=5.0, g_{HS}=15, g_{LS}=1), measured after (10^4) MCS according to Swendsen-Wang cluster dynamics and Metropolis dynamics.*

Conclusion

In this work we have simulated a clusters model for ferromagnetic Ising-like systems for spin transition by the Swendsen-Wang cluster MC dynamics, the cluster model have been obtained from its corresponding thermal's one by the ghost bonds method and the results for some thermal quantities of the system have been compared to those obtained by the Metropolis dynamics.
Simulations show that the two different MC dynamics gives results practically identical, in the case of weak and moderate cooperative interactions, regardless of the size of the system, this is not always the case for systems with high cooperative interactions and small sizes, where correlations are strong and the interactions range exceeds the size of the systems, the results show a disagreement between the two MC dynamics.

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