ISSN 1971-680X
Vol. 8 N. 1
February 2013

International Review of Physics (IREPHY)

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International Review of Physics (IREPHY)

The ***International Review of Physics (IREPHY)*** is a publication of the **Praise Worthy Prize S.r.l..**
The Review is published bimonthly, appearing on the last day of February, April, June, August, October, December.

Published and Printed in Italy by **Praise Worthy Prize S.r.l.,** Naples, February 28, 2014.

Praise Worthy Prize

International Review of Physics (I.RE.PHY.), Vol. 8, N. 1
ISSN 1971-680X *February 2014*

Binder Cumulant for Bond Diluted Ising Model

I. Zergoug, R. Bouamrane

Abstract – *The fourth order Binder cumulant U and the critical Binder cumulant U^* of bond-diluted Ising model on a square lattice are studied using Monte Carlo techniques. The values of the transition temperature T_c obtained from U^* for different probabilities of bond dilution p are discussed. When p is no too large (p<0.35), T_c decreases when p increases and U^* also decreases. For p>0.35, things are not so clear and our results show that the determination of T_c from U is questionable.*

Keywords: *Diluted Ising Model, Binder Cumulant, Monte Carlo Simulation*

Nomenclature

U	Binder cumulant
U^*	Critical Binder cumulant
p	Concentration of dilution
T_c	Critical temperature of transition
L	Lattice size
H	Hamiltonian
J	Exchange coupling constant
S	Spin value
N	Total number of spins
k_B	Boltzmann constante
M	Magnetization
E	Energy
C_v	Specific heat

I. Introduction

The Binder cumulant U, the fourth order cumulant of the order parameter [1], plays an important role in the field of phase transition and critical phenomena. It is well known that the determination of the transition phase point is obtained by locating the intersection of the cumulant function of temperature at different sizes.

The cumulant may also be used to compute the critical exponent of the correlation length, and thence identify the universality class of the transition.

U^*, the value of the Binder cumulant at the transition temperature T_c, has received a lot of interest. The numerical value of critical binder cumulant has been determined very accurately in the case of two dimensional Ising model with ferromagnetic nearest neighbour, using Monte Carlo techniques [2], [15] and transfer matrix methods augmented by finite size extrapolations to the thermodynamic limit [3], [16]. In the case of square lattice with periodic boundary conditions, the resulting value is $U^* = 0.61069$ [3].

In fact, different values of U^* have been obtained when considering various boundary conditions, lattice shapes, and lattice structures (anisotropic interactions) [1], [3], [4], [5], [9]-[14]. For instance, with free boundary conditions, the critical cumulant of nearest neighbour Ising model on square and triangular lattice are respectively $U^* = 0.396 \pm 0.002$ and $U^* = 0.379 \pm 0.001$ [5]. In the present paper, we report the value of the critical Binder cumulant in the case of bond diluted Ising model on a square lattice with free boundary conditions.

The paper is organized as follows: in the next section, the model and the Monte Carlo method are introduced.

Then, simulation results are presented and finally, results are shown and discussed.

II. Model and Method

The Hamiltonian of the model considered here reads [6]:

$$\mathrm{H} = \sum_{<i,j>} J_{ij} S_i S_j \qquad (1)$$

where $S_i = \pm 1$ is the spin at the site i. The exchange coupling constant J_{ij} is 0 for non-nearest-neighbours and 1 or 0 with probabilities p or (1-p) respectively. Free boundary conditions are used, and the regular square lattice size is $L = \sqrt{N}$ (where N is the total number of spins in the system).

We have calculated the Binder cumulant at the phase transition T_c for different probability of bond dilution p (concentration of dilution). The exact critical temperature T_c for the regular square lattice is given by [7]

$$k_B T_c / J = 2 \Big/ ln\left(\sqrt{2}+1\right) = 2.26918...$$

The binder cumulant, the fourth-order cumulant of the magnetization, as usually defined, is [1]

$$U(T,L) = 1 - \frac{\left\langle M^4 \right\rangle}{3\left\langle M^2 \right\rangle^2} \qquad (2)$$

Manuscript received and revised January 2014, accepted February 2014

where $\langle M^2 \rangle$ and $\langle M^4 \rangle$ denote thermal averages of the second and fourth moments of the magnetization. In the Ising model case, the cumulant $U(T,L)$ approaches the value 2/3 at temperature $T < T_c$ and the value 0 at $T > T_c$, reflecting the Gaussian form of the magnetization distribution [1]. At T_c, the Binder cumulant U^* acquires a non-trivial value, which will be estimated in this paper for different p dilution value. To achieve this, we performed Monte Carlo simulation [8] using standard single spin flip algorithms. We divided the equilibration process into "timesteps", a Monte Carlo step per spin.

The measurement of the thermodynamic quantities is carried out after a certain number of timesteps which we name a "timeslice". To estimate accurately the fluctuations of thermodynamic quantities, measurements are taken at each timeslice and averaged over a larger number of samples. When the difference of the averaged energy between two successively timeslices is lower than a certain given value, the simulation is stopped and various thermodynamic quantities are obtained. This process is repeated for several temperature values T.

As usual, the energy E and the specific heat C_v are obtained by:

$$E = -\frac{1}{N} \sum_{<i,j>} J_{ij} S_i S_j \qquad (3)$$

$$C_v = N\beta^2 \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \qquad (4)$$

where N is the total number of spins in the system, $\beta = 1/k_B T$ (T is the temperature and k_B is the Boltzmann constant taken to unity here).

III. Results and Discussion

We consider nearest neighbour Ising model on the square lattice with free boundary conditions. The calculations were carried out for p = 0.0, 0.05, 0.10, 0.15 and 0.20 using lattice sizes L = 256, 1024 and 4096. 10000 samples are used for averaging.

First of all, thermodynamic quantities are plotted in Fig. 1 and Fig. 2 for L = 4096 and for various concentration of dilution.

A calculation is added in case of p = 0.5 for lattice size L = 512, 1024 and 4096 with 16384 averaging samples for the two first sizes, 590000 averaging samples for the last one. From Fig. 3, we can get the value of the critical temperature T_c for different concentration of dilution p from the intersection of the Binder cumulant for different lattice sizes. The critical temperature T_c are shown decrease linearly as the dilution p increases (see Fig. 4).

We focus now on the study of the critical binder cumulant U^*. In previous simulation [5], for isotropic nearest neighbour Ising model on square lattice and free boundary conditions the value of $U^* = 0.396 \pm 0.002$ has been found.

The author claimed that the critical cumulant depends only on the shape not on the lattice structure.

In our case, we study the critical binder cumulant U^* dependence as a function of the dilution p (see Fig. 5).

For $p = 0$ we get $U^* = 0.4022 \pm 0.0007$. The value of U^* decreases linearly the increase of the dilution p. An interesting results is shown for p = 0.5. On Fig. 6 and Fig. 7 is shown the variation of the Binder cumulant U and the specific heat C_v against the temperature respectively.

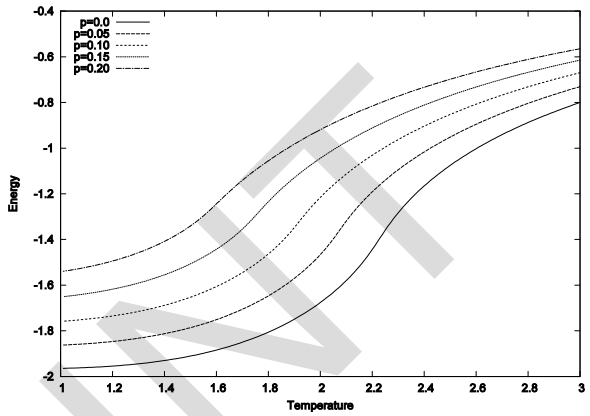

Fig. 1. The energy E as a function of the temperature for different concentration of dilution p

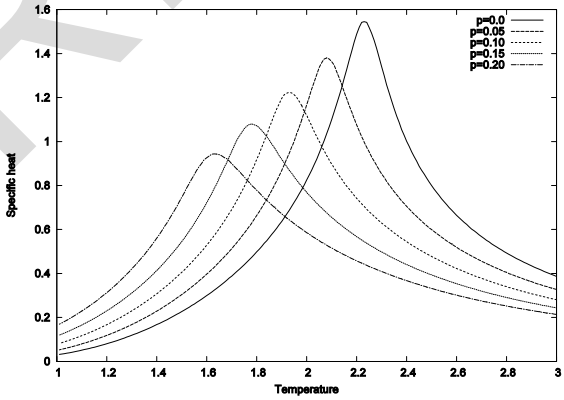

Fig. 2. The specific heat C_v as a function of the temperature for different dilution p

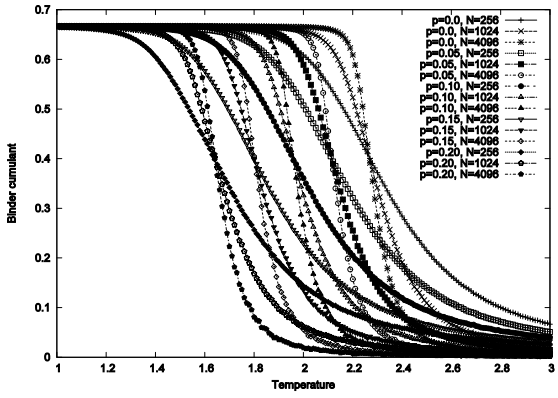

Fig. 3. The Binder cumulant U versus the temperature for different dilution p

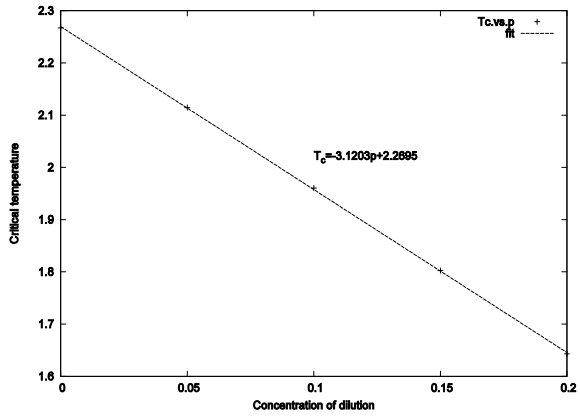

Fig. 4. Variation of the critical temperature T_c versus dilution p

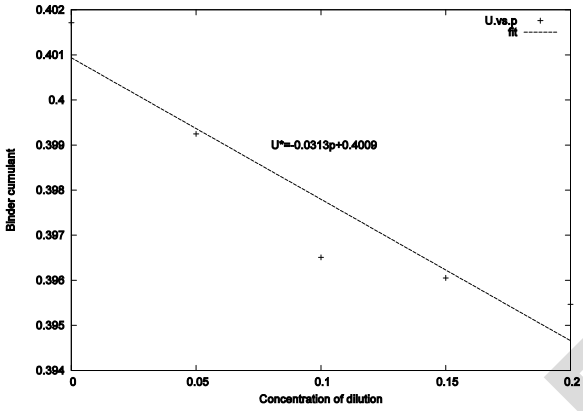

Fig. 5. Variation of the critical Binder cumulant U^* versus dilution p

It is comment practice that the value of the critical temperature T_c is obtained from intersecting critical Binder cumulant (U^*) curves for various system sizes. Also, T_c normally corresponds to the maximum value of the specific heat C_v(max). Using the first method, 590000 averaging samples are used for p=0.5 and the intersection of U(T) curves for different lattice sizes yields the value T_c = 0.39 (see Fig. 6). Moreover, if we seek T_c from locating the maximum of Cv(T), we get T_c = 1.03 (see Fig. 7).

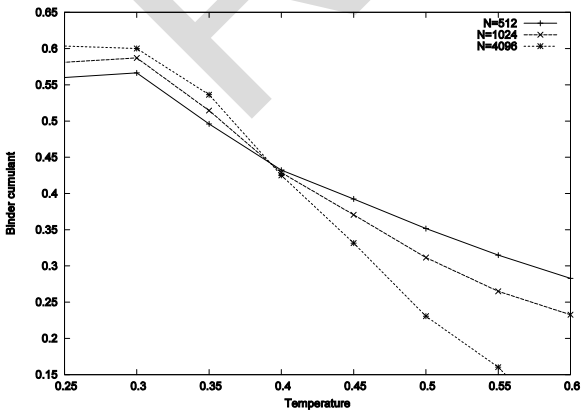

Fig. 6. Variation of the Binder cumulant U versus the temperature for p = 0.5

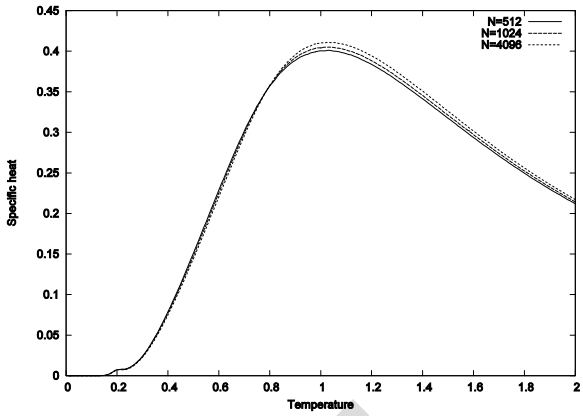

Fig. 7. Variation of the specific heat C_v versus the temperature for p = 0.5 for different lattice sizes

It appears that the Binder cumulant method of determining critical temperatures breaks down as the bond concentration p approaches the bond percolation threshold (p = 0.5).

The difference between the two methods in the determination of the value of T_c exceeds 1% for $p >$ 0.35. Table I shows values of T_c obtained by the two methods for various p.

For $p \leq 0.30$, T_c (from U) is slightly larger the T_c (from Cv) which can be explained from finite scaling law. But for $p \geq 0.35$, T_c (from U) is quite smaller than T_c (from Cv) which cannot be resolved by scaling laws.

TABLE I
THE VALUES OF T_C DETERMINED FROM THE TWO METHODS FOR DIFFERENT BOND CONCENTRATION P

p	T_c (From U)	T_c (From Cv max)
0.0	2.2670	2.2306
0.05	2.1145	2.0813
0.10	1.9605	1.9325
0.15	1.8024	1.7804
0.20	1.6430	1.6360
0.25	1.4817	1.4914
0.30	1.3163	1.2930
0.35	1.1342	1.2515
0.40	0.9252	1.1438
0.45	0.6733	1.1029
0.50	0.3924	1.0365

IV. Conclusion

The critical Binder cumulant U^* for two dimensional bond diluted Ising model on square lattice with free boundary conditions has been studied. The simulation findings show that the critical binder cumulant depends on the concentration of dilution p. The value of U^* for p = 0 was equal to 0.4022 ± 0.0007 with respect to [5] that was 0.396 ± 0.002.

The determination of the critical temperature T_c using the Binder cumulant must be use carefully for disordered systems. T_c obtained from C_v(max) is more likely reliable for strongly disordered systems. Further investigations are being done with larger system sizes and larger samples to get more precisely in order to settle this issue.

Acknowledgements

We would like to thank Matteo Marsili at the ICTP for very helpful discussions.

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Cambridge Scientific Abstracts (CSA/CIG)
Academic Search Complete (EBSCO Information Services)
Index Copernicus (Journal Master List): ***Impact Factor 6.39***

Autorizzazione del Tribunale di Napoli n. 26 del 27/03/2007

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1971-680X(201402)8:1;1-D