Probing critical behavior of 2D Ising ferromagnet with diluted bonds using Wang-Landau algorithm

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Abstract. Randomness is an important subject in the study of phase transition as defect and impurity may present in any real material. The pre-existing ordered phase of a pure system can be affected or even ruined by the presence of randomness. Here we study ferromagnetic Ising model on a square lattice with a presence of randomness in the form of bond dilution. The pure system of this model is known to experience second order phase transition, separating between the high temperature paramagnetic and low-temperature ferromagnetic phase. We used Wang-Landau algorithm of Monte Carlo method to obtain the density of states from which we extract the ensemble average of energy and the specific heat. We observed the signature of phase transition indicated by the diverging peak of the specific heat as system sizes increase. These peaks shift to the lower temperature side as the dilution increases. The lower temperature ordered phase preserves up to certain concentration of dilution and is totally ruined when the bonds no longer percolates.

1. Introduction
Phase transitions are very common natural phenomena. Although they may appear in various realizations, they can be grouped into two main categories, namely the first and the second order phase transitions (SOPT) [1]. A first order transition is characterized by discontinuous changes in free energy at critical temperature, firmly exemplified by transition of the PVT systems such as water. In this type of transition, we can always find latent heat in the course of transition as there is co-existence phases. The SOPT which is also called a continues phase transition is characterized by the continuous change of the free energy during the transition. The famous example of these is the spontaneous magnetization of ferromagnetic material, which change from disorder spin configuration at higher temperature to ordered phase below Curie ($T_c$) temperature, commonly referred to as critical point, and the phenomena nearby this point is called critical phenomena. Spontaneous magnetization is a typical type critical phenomena of systems consisting of many microscopic interacting components. The interesting aspect of studying critical phenomena is that the behavior of system (the critical properties) usually indicates universality, in the sense that totally different systems may exhibit similar behavior, which is characterized by similar set of exponents called critical exponents.

In the study of critical phenomena, the exponent values or essentially the critical properties of the system, may change due to variation of a number of macroscopic variables such as spatial dimension, symmetry of spin and the type of coupling interactions. The critical properties of system can also be affected by the presence of randomness. In fact randomness is an important subject to probe as defect or impurity is always present in any real material. There exists
an important theoretical conjecture called Harris criterion [2] which predict the role played by
a randomness in affecting the critical properties of system. According to this criterion, the
critical behavior of disordered system can only be affected by the presence of randomness if the
specific heat exponent $\alpha$ of the corresponding pure system is positive. For $\alpha < 0$, randomness is
irrelevant, in other words, it will not affect the critical properties of the system. The presence
of randomness is called marginal if $\alpha = 0$, meaning that the Harris criterion is inconclusive.

The two dimensional (2D) Ising model [3] has long been the object for benchmarking study in
many fields. The present study is probing whether certain type of randomness is relevant or not
for the existing phase transition. This model is well known to experience SOPT with positive
exponent $\alpha$, hence some type of randomness should be relevant, according to Harris criterion. A
type of randomness by adding extra bonds, i.e., rewiring regular lattices with antiferromagnetic
coupling have been studied for probing the so-called non-canonical spin glasses and the effect
on the existing Neél phase [4, 5, 6, 7]. In the case of bond dilution, There has been several
numerical studies on 2d Ising model, for example the old report by [8, 9]. However, the data are
not very accurate due to the limitation of computer power in the previous decades. The effect of
diluted bonds for system experiencing Kosterlitz-Thouless transition was also studied [10].

In this work, we study diluted bonds of 2D Ising model by using Wang-Landau (WL)
algorithm [11] of Monte Carlo method. This algorithm have been widely used in studying
phase transition of various magnetic models [12, 13]. Typical characteristics of this method is
to obtain the system density of states (DOS) for the calculation of ensemble average of physical
quantity. Recently, the DOS obtained from WL algorithm also used to determine the order
of phase transition, whether first or second order by analysing the difference of DOS between
neighboring energy states [14, 15].

In general, to analyse the critical behavior of the system, one calculates the order parameter,
which is the magnetization for the case of ferromagnetic system. The correlation ratio, i.e.,
the ratio of correlation functions of order parameter for two different distances [16] is another
interesting quantity for probing critical behavior. This compelling physical quantity had been
applied in several previous studies [10, 13, 17]. However, other quantities such as the energy
and the specific heat can also be used to detect the existence of phase transition. In particular,
for system experiencing SOPT, the diverging specific heat can be used to estimate the critical
temperature. The paper is organized as follows: Section II will discribe the model the method
used, Section III presents and discusses the the results and Section IV is devouted for the
summary and concluding remarks.

2. Model and Method

Ising model is the simplest magnetic model yet mostly studied in probing phase transition [3].
The model consists all important concepts related to phase transition, for example, the broken
symmetry, the existence of critical exponents of various physical quantities, order parameters,
etc. The model is represented with the following Hamiltonian

$$H = - \sum_{\langle ij \rangle} J_{ij} s_i s_j$$  \hspace{1cm} (1)

where spins $s_i$ occupy lattice sites; here we consider two dimensional (2D) lattice (square). As
the underlining symmetry for the Ising spin is $Z_2$, the value of $s_i$ can be either +1 or -1,
respectively associated with up and down spins. $J_{ij}$ is the exchange coupling between spin on
site $i$ and $j$. We consider ferromagnetic system, therefore with this notation $J_{ij}$ is positive. We
apply the nearest neighbor interaction and the summation are performed to all pairs of nearest
neighboring spins. However, as we probe diluted problem, some bonds are depleted, i.e., $J_{ij} = 0$.

In this study, Monte Carlo method of Wang-Landau (WL) algorithm [11] is used. It is an
extended ensemble sampling algorithm where the random walk is performed in the whole energy
space, which is essential to obtain the energy density of states (DOS). However, because of a wide range of energy space, two common problems are frequently encountered by the random walker: (i) the random walker tends to be blocked by the edge of the already visited energy states [12], (ii) it takes time from one end of the area to reach the other end, which is a common feature of random walks. The main idea of WL is to get away from the problems and to accelerate the dynamics of the random walk so that the DOS \( g(E) \) can be efficiently and precisely evaluated. This is done through the introduction of the transition probability defined as follows

\[
P(E \rightarrow E') = \min \left[ 1, \frac{g(E)}{g(E')} \right]
\]  

(2)

where \( g(E) \) is the DOS for state \( E \). Since this \( g(E) \) is not known at the beginning of the simulation, it is presumed to be \( g(E) = 1 \) for the whole states. The DOS is then evaluated through iterative random walk and its exact value is obtained when the histogram \( h(E) \) of energy achieves flatness condition i.e. the histogram for all possible \( E \) is not less than some value of the average histogram, say, 0.80. The DOS and \( h(E) \) are updated every time \( E \) is visited through the relation

\[
\ln g(E_i) \rightarrow \ln g(E_i) + f_i
\]  

(3)

\[
h(E_i) \rightarrow h(E_i) + 1
\]  

(4)

where \( f_i \) is the modification parameter which is gradually reduced to zero when the DOS reaches the convergence.

Thermal average of physical quantity \( Q \) is obtained through relation

\[
\langle Q \rangle_\beta = \frac{\int dE \ g(E) \ Q(E) \ \exp(-\beta E)}{\int dE \ g(E) \ \exp(-\beta E)}
\]  

(5)

where \( \beta = 1/kT \), \( k \) and \( T \) respectively being the Boltzmann constant and temperature. The detail steps of the algorithm are as follows

(i) Set (a) initial spin configuration and initial iteration factor \( f_i = 1 \); (b) assume that the initial values of the DOS and histogram as \( \ln g(E_i) = 1 \) and \( h(E_i) = 0, \forall i \).
Figure 2. (Color online) Temperature dependence of energy of system size $L = 8$ for several bond concentrations. It is to be noticed that we used normalized scale, therefore the minimum energy $E_{min} = 1$, instead of 2.

(ii) Update the configuration based on the transition probability (2).

(iii) Update the DOS and the histogram as (3) and go to step 2 until the histogram reaches the flatness condition.

(iv) Refine the iteration factor $f_i = f_i/2$, rescale the DOS by using condition $\sum E_i g(E_i) = 2^N$ (for the case of the Ising model); and reset the histogram $h(E_i) = 0$ before going back to step 2.

(v) Do steps 1 to 4 until the DOS achieves convergence, then perform measurement of physical quantity $Q_i$ with a definite number of MCS’s.

For the application of the WL algorithm to the large system size, one performs window break, where the whole range of the energy is cut into several reasonable widths. The result from each window is later joined to obtain the resultant.

3. Results and discussion

We studied the ferromagnetic Ising model on square lattice with diluted bonds using Wang-Landau algorithm. Several system sizes, namely $L = 8, 10, 12$ and 16 were simulated in order to probe how the size dependent of physical quantities. This is essential for extracting the thermodynamics behavior from the data of finite system sizes. As we are investigating the role played by randomness in the form of bond dilution, we took several number of bond concentrations, namely $p=1.0, 0.9, 0.8, 0.7, 0.6, 0.5$ and $0.45$; where $p=1.00$ corresponds to pure case, i.e., all bonds exist. With $p=0.90$, there are 10% bonds deleted. The density of state (DOS) for the pure and diluted case, i.e., for $P=1.0, 0.9$ and $0.8$ for system size $L=8$, are shown in figure 1.

The ensemble (thermal) average of any physical quantity $\langle Q \rangle$ is calculated according to standard relation in statistical mechanics written as follows

$$\langle Q \rangle = \frac{\int Q(E)g(E)e^{-\beta E}dE}{\int g(E)e^{-\beta E}dE}. \quad (6)$$

Using the density of state we can extract ensemble average energy $\langle E \rangle$ and its $n$-th order moment $\langle E^n \rangle$. Using $\langle E \rangle$ and the second order moment $\langle E^2 \rangle$, we can obtain the specific heat defined as
follows

\[ C_v(T) = \frac{1}{Nk_BT^2}(\langle E^2 \rangle - \langle E \rangle^2) \]  

where \( E \) is the energy in unit of \( J \). All temperatures are expressed in unit of \( J/k_B \) where \( k_B \) is the Boltzmann constant.

The temperature dependence of energy and specific heat for various system sizes as well as for different bond concentrations are plotted in figure 2 and figure 3, respectively. As shown, there is a systematic shift of the energy as well as the peak of specific heat to the lower temperature as concentration decreases. For pure size for example, \( c = 1.0 \), the critical temperature, which is associated with the abscissa of peak as \( L \to \infty \) is roughly estimated around \( T=2.48(3) \), after the energy being rescaled to the original value. For system with \( c = 0.90 \), the estimate of \( T_c \) is \( 2.04(2) \). The complete estimate of our critical temperatures is tabulated in table 1. Our rough estimates are in good agreement with the previous reports although always smaller due to large correction to finite size scaling as we probe quite small sizes. However, this already indicates the elegance of the WL algorithm. We have yet to report our estimate on critical exponents, such as the \( \nu \) and \( \eta \) for the correlation length and magnetization. Our precise estimate and more comprehensive report will be published elsewhere.

It is to be noticed that the typical characteristics of physical quantity extracted from the WL calculation in principle can be continuously temperature dependence, which is different from that of obtained from such microcanonical ensemble methods as the Metropolis algorithm. Therefore, using WL algorithm, we can estimate critical temperatures for each concentration more precisely, compared to all previous results, such as that of reported in [8].

4. Summary and concluding remarks

We have investigated the role played by randomness in affecting the existing phase transition by probing the 2D ferromagnetic Ising model with bond dilution. The macrocanonical ensemble WL algorithm is used. Various concentrations of bond dilution are simulated. W calculated the ensemble average of energy and the specific heat which are extracted from the DOS directly obtained from the simulation using the WL algorithm. Then, we estimate the critical
Table 1. The estimate of critical temperature $T_c$ for each value of $c$. The number in bracket is the error bar of the last digit.

| Bond concentration ($c$) | $T_c$     |
|-------------------------|----------|
| 1.0                     | 2.48(3)  |
| 0.9                     | 2.04(2)  |
| 0.8                     | 1.80(2)  |
| 0.7                     | 1.44(2)  |
| 0.6                     | 1.36(2)  |
| 0.5                     | 1.30(2)  |
| 0.45                    | 1.24(2)  |

temperature for each bond concentration. We start from the pure case (where no bond depleted) down to lower concentration of bonds close to percolation ratio. We observe the shift of critical temperature to the lower side as the bond concentration $c$ decreases.

Our estimate of critical temperatures are tabulated in table 1. These results are consistent with most previous work. We observe SOPT all the way down until it disappear at certain concentration. The concentration bonds $c=0.45$ is close to the critical value where the order phase disappear. This value is related to percolation ratio. For better estimate of our results, we perform a comprehensive study, which is in progress, and calculate the order parameter and consider larger system sizes. The results will be reported elsewhere.

Acknowledgments
The authors wish to thank Bansawang BJ, D. Tahir and A. W. Sandvik for valuable discussions. The extensive computation was performed using parallel computer facility at the Department of Physics, Hasanuddin University and that belongs to GRID-LIPI of the Indonesian Institute of Science. The present work is supported by a research grant of scheme: Priority Research for Tertiary Education, Indonesian Ministry of Research, Technology and Tertiary Education, Fiscal Year 2017.

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