Phase diagram of six-state clock model on rewired square lattices

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Abstract. The six-state clock model (SSCM) on rewired square lattice is studied using Monte Carlo simulation with Wang-Landau algorithm. This is a discrete counterpart of the well-known XY model, the native host of a unique topological phase transition called Kosterlitz-Thouless (KT) transition. The model has two KT transitions, i.e., at temperature $T_1$ and $T_2$, where $T_1 < T_2$. The first transition separates the lower temperature magnetic order and the quasi-long range order (QLRO) also known as KT phase; while the second transition separates the QLRO and the higher temperature paramagnetic phase. It has been established that the presence of KT phase is affected by the presence of randomness in the form of site and bond dilution. This intermediate phase is totally ruled out if bonds or sites of the lattice are no longer percolated. Here different type of randomness is probed, namely the rewired lattices, obtained by randomly adding one extra bond to each lattice site, and connect the site to one of its next-nearest neighbors. As a results, the average number of neighbors $C$ increases. The increase of $C$ affects the existence of KT phase. For each value of $C$, the KT temperatures, $T_1$ and $T_2$, were estimated from the plot of specific heats. Variation of KT temperatures for different values of $C$ is observed, which is plotted with respect to each corresponding $C$ to obtain the system phase diagram.

1. Introduction
Phase transitions are ubiquitous natural phenomena and appear in various realizations. Based on the properties of broken symmetry of the microscopic ingredient of the system, phase transitions are grouped into two main categories, i.e., the discontinuous and continuous phase transitions [1]. The former type also called first order (FO) is characterized by the discontinuous change of the free energy of the system, exemplified by transition of water-ice, one of the well known PVT (Pressure-Volume-Temperature) systems [2]. In this type of transition, two phases co-exist, accompanied by the presence of latent heat. For the second type, the free energy of the system changes continuously and no co-existing phases observed during transition. A firm example of this is a spontaneous magnetization of the ferromagnetic material which changes from paramagnetic to an ordered magnetic phase. It occurs at Curie temperature ($T_c$), commonly referred to as critical point and phenomena nearby this point are referred to as critical phenomena.

The interesting aspect in studying critical phenomena is that the behavior of system (the critical properties) usually indicates universality, where different systems may exhibit identical behavior; characterized by a set of critical exponents. With universality, understanding properties of certain system enables one to comprehend other systems. Values of critical
exponents are usually controlled by a limited number of variables, such as spin symmetry, coupling interaction and lattice structures. Randomness in the form of defect or impurity can be a part of these variables; therefore may change the universality class of certain system. Different set of critical exponents represent different type of universality class.

The effect of randomness, in a variety of forms such as site vacancies and diluted bonds, on phase transition has been intensively investigated. According to Harris criterion [3], randomness is relevant for the pure system experiencing second order phase transition with specific heat exponent $\alpha > 0$, and irrelevant for $\alpha < 0$; otherwise it is marginal (inconclusive). The two dimensional (2D) Ising model is a classic example of system experiencing second order phase transition with positive $\alpha$. Various investigations related to the role of randomness on phase transition of this system had been reported, including the most recent studies probing the critical behaviour of the Ising model on rewired square lattice [4, 5].

Motivated by the studies above mentioned, here we investigate the phase transition of FM $q$-state clock model on rewired square lattices. The pure system of this model is well known to experience Kosterlitz-Thouless (KT) transition, which is a transition from a low temperature quasi long range order (QLRO) called KT phase to high temperature disordered phase. The QLRO (KT phase) which is a topological phase formed by vortex-antivortex pairs [6, 7], is the only type of order allowed by the Mermin-Hohenberg theorem for 2D systems [8]. Due to discrete symmetry of the clock model, additional KT transition occur at lower temperature, separating the ferromagnetic true long range order (TLRO) and the KT phase [9]. The number of vortex-antivortex pairs increases with the temperature until the system experiences the KT transition. The KT transition corresponds to the unbinding of vortex-antivortex pairs, which leads the system to a high-temperature disordered phase. Probing QLRO of planar spin model with randomness is an important subject. As this type of order is not a true long range order, one may question about its vulnerability against impurity. The continuous counterpart of clock model, the XY model (with dilution) found a relevance in the study of superconductivity, particularly for depicting the interaction between vortices and the spatial inhomogeneity due to the impurities.

The effect of randomness in the form of site and bond dilution for system undergoing KT transition has been investigated and found that the KT phase persists so long as the lattice sites and bonds are percolated [10, 11, 12]. In this report, different type of randomness is studied, i.e., the rewired regular lattices. While number of neighbours of each site in a regular lattice is homogeneous, assigned by a definite integer called coordination number, it is in contrast for a rewired lattice where a fractional coordination number may be obtained, depending on the way of rewiring. Rewiring a regular lattices can be considered as increasing lattice spatial dimension, where several extra bonds are added to each lattice site. In the present study, only one extra bond is randomly added to each site, which connects the site to one of its diagonal neighbours. The concentration of bonds added determines the average number of bonds (ANOB). Therefore, a site (spin) may have up to seven bonds. ANOB which is assigned as $C$ varies from 2.0 to 3.0, where $C = 2.0$ and $C = 3.0$ correspond respectively to unrewired and the fully rewired square lattice. One particular realization of these lattices is shown in Fig. 1.

This paper reports the study of six-state clock models on rewired square lattice by using Monte Carlo (MC) method with Wang-Landau algorithm. The subsequent sections of the paper is organized as follows: The model and method are explained in Section 2. Results and discussion are presented in Section 3. Section 4 is devoted to summary and concluding remarks.

2. Model and Method of Simulation
The 6-state clock model is written in the following Hamiltonian

$$H = -\sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j = -\sum_{\langle ij \rangle} J_{ij} \cos(\theta_i - \theta_j),$$

(1)
Figure 1. (Color online) (a) Unrewired square and (b) rewired square lattice where one bond is randomly added to each site.

where $S_i$ and $S_j$ are spins occupying respectively the site $i$-th and $j$-th of the lattice; and $J_{ij}$ is the coupling interaction between them. For a FM six-state clock model, possible spin orientation takes discrete values, $\theta_i = 2\pi q/6$ with $q = 0, \cdots, 5$; and $J_{ij} = J < 0$. The summation is carried out over all directly connecting pairs of spins. For a regular lattice such as a square or a cubic lattice, all sites possess similar number of neighbours, corresponds to a fixed coordination number. We currently consider rewired square lattices with fractional connectivity, i.e., with ANOB $C$ varies from 2.0 to 3.0. A rewired lattice is regarded as a quasi-regular structure as the translational symmetry is (partially) preserved, where the notion of spatial dimension remains. Our procedure of constructing the lattice is by randomly connecting each lattice site to one of its diagonal neighbors. There are 4 nearest neighbors of each site for the original square lattice while 7 neighbors in maximum for a rewired lattice. Therefore, a fractional ANOB may be obtained for a randomly rewired lattice.

Due to the complexity of the energy landscape, which may be difficult to tackle when using the the standard Metropolis MC algorithm, here we used the Wang-Landau (WL) algorithm[13]. It is an extended ensemble sampling algorithm where random walk is performed in the whole energy space. The central quantity to obtain is the energy density of states (DOS). This algorithm can accelerate the dynamics of the random walk so that the DOS $g(E)$ can be efficiently and correctly 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, which set at the beginning of the simulation 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.

It is to be noticed that using the WL algorithm, average energy as well as specific heat can be directly extracted from the DOS, both FM and AF systems. Thermal average of physical quantity $Q$ is obtained from the standard 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 following is the detail steps of the algorithm:

(i) Set (a) random spin configuration and initial iteration factor $f_i = 1$; (b) Set the initial DOS and histogram as $\ln g(E_i) = 1$ and $h(E_i) = 0, \forall i$.

(ii) Based on the transition probability (Eq. 2), update the spin configuration.

(iii) Update the DOS and the histogram as Eq. 3 and go to step (ii) if the flatness condition of the histogram is fulfilled.

(iv) Modify the iteration factor $f_i = f_i/2$, refine the DOS by using condition $\sum E_i g(E_i) = 6^N$ (for the case of the six-state clock model); and reset the histogram $h(E_i) = 0$ before going back to step (ii).

(v) Do steps (i) to (iv) until the DOS is convergent, then measure physical quantity $Q_i$ with a definite number of MCS’s.

For the application of the WL algorithm to the large system size, we perform window break strategy, 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

This paper studies the six-state clock model on rewired square lattices with various concentration of bonds $C$ by using Wang-Landau algorithm of MC method. Several system sizes were
simulated, namely $L = 8, 10, 12$ and $14$, with $N = L^2$ is the total number of sites. As a periodic boundary condition is imposed, each lattice site, for the pure case, has equal number of nearest neighbors. For the rewired lattices, number of nearest neighbours (direct connections) of each site varies from 4 to 7. The lattice structure and the trivial ground state (GS) configuration of the system can be used to check the accuracy of calculation. For example, the density of states (DOS) for the case of pure lattice is normalized using the condition $\sum_E g(E) = 6^N$, and the degeneracy of GS energy, $g(E_{GS}) = 6$. Fig. 2: (a) shows the energy DOS of pure system for several system sizes and (b) the DOS for $L = 8$ for various values of $C$. Here, the energy is represented in units of $J$, and the GS energy is given by $-CNJ$.

According to the standard relation written in 5, the ensemble average of energy $\langle E \rangle$ can be extracted from the DOS, which is the main data obtained from the extensive simulation using WL algorithm. Combined with the second order moment of energy, $\langle E^2 \rangle$, we can define specific heat as follows

$$C_v(T) = \left[ \frac{1}{NkT^2} (\langle E^2 \rangle - \langle E \rangle^2) \right]_{av}$$

where the energy $E$ is in unit of $J$. All temperatures are expressed in unit of $J/k$ where $k$ is the Boltzmann constant. The square bracket symbolizes averaging with respect to a number of diluted lattice realizations. This is a standard procedure in dealing with disorder system, where each realization of a diluted lattice with size $L$ has different configuration of bond dilution. Therefore, for a reliable statistics, we average over several dilution configurations for each specified size, i.e., for $L = 8$, we take 10 realizations.

We plot the temperature dependence of energy $E$ as shown in Fig. 3. There is a systematic increase of the absolute value of energy as concentration increases. This is due to the fact that the number of pair interactions increase, resulted from the presence of extra bonds, where each bond costs energy. The shift may signify an increase of critical temperature $T_c$ for any existing phase transition. In diluted cases, both for the 2D Ising and clock model, $T_c$ decreases as the number of depleted bonds increase. The difference in DOS (DDOS) is another physical quantity which can be directly extracted from DOS. This quantity can be used to analyze the order of phase transition, for example to probe the order of phase transition of $q$-state Potts model as value of $q$ varies [14]. As KT transition is a special type of second order phase transition, it

![Figure 3](image-url)
is interesting to study the characteristics of DDOS for q-state clock model; by which one can distinguish between the KT and the usual second order phase transition. This topic will be considered as prospective subject and be reported the result elsewhere.

A KT phase is a topological ordering in the form of vortex-antivortex pairs [6, 7]. For the continuous planar spin model (XY model), these pairs unbind at high temperature KT transition which separates the paramagnetic phase and the KT phase. This corresponds to the $T_2$ transition of the clock models which have another transition at lower temperature $T_1$. The presence of peaks in the temperature dependence of specific heat could generally signify the existence of phase transitions. As shown in Fig. 4, the specific heat plot possesses two peaks, which correspond to two KT temperature transitions, $T_1$ and $T_2$, each is associated with the abscissa of peak of specific heat as $L \to \infty$. For pure case, i.e., the lattice with $C = 2.0$, $T_1$ and $T_2$, are roughly estimated around 0.55(2) and 1.15(2), respectively, where number in bracket is the error bar of the last digit. The complete estimate of our critical temperatures are tabulated in Table 1. For the pure case, our rough estimates are comparable to the results reported by several previous studies [15, 16, 17], although significantly larger (for $T_2$ estimate) as we presently treat quite small system sizes. The temperature difference of the two peaks tends to be larger for smaller system size. For example, the estimates by Challa and Landau [15] and by Tomita and Okabe [16] are respectively ($T_1 = 0.68(2), T_2 = 0.92(1)$) and ($T_1 = 0.7014(11), T_2 = 0.9008(6)$). Nonetheless, our results have indicated the elegance of the WL algorithm applied to discrete model with multiple integer of energy.

It is to be noticed that the physical quantity extracted from the WL calculation can be presented in any temperature scale without having to perform extra MC simulation, which is different from that of obtained from such microcanonical ensemble methods such as the Metropolis algorithm. Therefore, using WL algorithm, one can obtain critical temperatures with very fine scale, which is more precise as long as the calculated DOS is truly convergent. As explained above, the KT transition temperatures presently reported are rough estimates as they are extracted from the specific heat plot. For a more precise estimate of critical temperature, one should perform finite size scaling of an appropriate order parameter, which is the magnetization for a ferromagnetic system having a TLRO. However, as the 2D XY model and its discrete counterpart q-state clock model have no TLRO (if $q > 4$), the magnetization is not a suitable
order parameter to detect the existence of KT phase (QLRO). A more precise quantity to detect the existence and analyze the KT transition is the correlation ratio, as used in previous studies \cite{16, 17, 18}. Our calculation on correlation ratio is still in progress and the analysis of its results will be reported elsewhere.

4. Summary and Conclusion
This paper reports the study of the six-state clock model on rewired square lattices with various average number of bonds (ANOB). The lattices are obtained by randomly adding an extra bond to each site of the original square lattice, lead the rewired lattices to have fractional ANOB, symbolized as $C$, varied from 2.0 to 3.0. ANOB is analogous to coordination number for regular lattices. An added bond is constrained to connect one of the diagonal neighbors to the site. Rewiring the square lattice is associated with an increase in lattice dimension, which affects the existing QLRO (KT phase). Due to the increasing average number of bonds, spins become more cooperative; which may lead the system to possess a true long range order at certain value of $C$, in particular if we allow the rewiring not limited to nearest neighbors.

Monte Carlo method with Wang-Landau algorithm is used to study the physical properties of the system. This algorithm is considered to be very powerful in dealing with models with multiple integer of energy, such as Ising and six-state clock model. From the DOS, the energy and its second moment were extracted then used to calculate the specific heat. A clear indication of the effect of randomness on the existing KT phase is observed, which shifts the KT phase to higher temperature side. This result suggest that randomness in the form of irregular connectivity

### Table 1. The estimate of KT temperatures $T_1$ and $T_2$ for each value of $C$. The number in bracket is the error bar of the last digit.

| ANOB ($C$) | $T_1$   | $T_2$   |
|------------|---------|---------|
| 2.0        | 0.55(2) | 1.15(2) |
| 2.2        | 0.60(2) | 1.30(2) |
| 2.4        | 0.75(2) | 1.45(2) |
| 2.6        | 0.80(1) | 1.48(2) |
| 2.8        | 0.83(2) | 1.65(2) |
| 3.0        | 0.92(2) | 1.98(2) |

![Figure 5.](image_url) (Color online) Phase diagram of rewired six-state clock model. The QLRO is in between of the two solid lines. The true magnetic order is below the red line, while the paramagnetic phase is above the blue line.
of lattices, which is weak type of randomness, does not change the universality of the system. Therefore, an interesting aspect to probe is the interplay between randomness rendered by rewiring procedure and the partially frustrated state, which is the case for the anti-ferromagnetic system not for FM. In addition, to find the lower dimension (smallest ANOB) and the higher dimension (largest ANOB) for the existence of KT phase on rewired lattices is still desirable. It will be our next topic to probe, for example searching for spin glass phase of AF six-state clock model on rewired lattices.

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