Ising Criticality of the Clock Model from Density of States Obtained by the Replica Exchange-Wang-Landau Method

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Abstract. We performed extensive simulations, using the Replica Exchange-Wang-Landau method, of the clock model for orders 3 and 4 on a square lattice, where critical behaviors are expected to belong to the Ising universality class. Though order 2 represents the Ising model, thus, being exactly solvable in two-dimensions, we still provide such results for comparison to the other two orders. Results for various energy related quantities such as the mean energy per spin, specific heat, as well as logarithm scaling of the peak of the specific heat are presented and shown to follow Ising behavior. Additionally, we also present results related to magnetic quantities, such as the magnetization, magnetic susceptibility, and corresponding scaling behavior of the peak of the magnetic susceptibility. Again, our results show scaling in conformity to Ising critical behavior.

1. Introduction

At the essence of the Wang-Landau method, [1, 2, 3] a random walk in energy space is performed, while building the density of states of a particular system. Concomitantly, an histogram of visited energy values is also built providing a way to warrant its flatness at some specified level of quality. Once the flatness of the histogram has been signaled, the histogram is reset and the simulation proceeds to the next iteration level using a smaller factor for the buildup of the density of states, until a pre-defined, small enough value is reached.

Since its debut, the Wang-Landau method has been shown to consistently produce high-quality density of states of several model systems, such as lattice spin and biological systems. [1, 2] In its present version, the Replica Exchange-Wang-Landau (RE-WL), the method builds the density of states without little or prior knowledge of the physical properties of the system, under a set of, well-defined, quality factors. In most systems, a simulation can be carried out by selecting an overall energy window and splitting it into several smaller, equally sized, energy windows, but in some systems additional knowledge of the proper window sizes for energy windows near the energy of the fundamental state(s) of the system may become a requirement.

One such class of possible applications of the RE-WL method is provided by (magnetic) lattice spin systems of wide interest in statistical physics. These systems, typically exhibit critical behavior, in the thermodynamic limit, which the method appropriately addresses. The critical behavior may include well-defined temperatures of first and second order phase transitions or a critical line of temperatures as in the case of the Berenzynski-Kosterlitz-Thouless transition. [4]

An example of such a system, it is provided by the clock model, where, depending on its order, the model can exhibit either Ising or BKT behavior at criticality. As the name implies,
an order \( n \), clock model proposed by Cyril Domb in the early fifties of the last century, \([5, 6]\) possible, equally-distributed spin orientations are provided by the *hand of a clock*. Consequently, the possible states of a lattice spin can be expressed as

\[
\sigma = \left( \cos \left( \frac{2\pi s}{n} \right), \sin \left( \frac{2\pi s}{n} \right) \right),
\]

where \( s \) takes values \( 0, 1, \ldots, n-1 \). The Hamiltonian is of the form

\[
H = -J \sum_{\langle i,j \rangle} \sigma_i \cdot \sigma_j,
\]

where \( J > 0 \) is a constant representing the strength of the interaction, \( \sigma_i \) represents a spin positioned at lattice site \( i \), \( \sigma_i \cdot \sigma_j \) represents the scalar product between spins \( i \) and \( j \), and \( \langle i,j \rangle \) denotes sum over nearest-neighbor spin pairs. In this work, we provide initial results of the clock model for orders 3 and 4, i.e., of orders within the Ising universality class. \([7, 8, 9]\) Results for order 2, the Ising model, are also included to provide direct comparison to the other two orders.

**2. Clock Model**

As above-mentioned, depending on the order of the clock, its critical behavior can change from the Ising class to the BKT class. \([10]\) Within the scope of the present work, we restrict ourselves to the Ising class, which implies clock orders of 2 to 4. Orders \( n \geq 5 \) are within the BKT universality class and, therefore, outside the scope of the present work. The critical temperatures for \( n = 2, 3, \) and 4 were exactly derived, by renormalization group studies, \([10]\) to be, respectively, \( 2/\ln(1 + \sqrt{2}) \), \( 3/(2 \ln(1 + \sqrt{3})) \), and \( 1/\ln(1 + \sqrt{2}) \). Note that the critical temperature for \( n = 4 \) is just half of the Ising model, as it represents two mutually orthogonal Ising models.

Let us, now, consider a square lattice, where spins \( \sigma_i \) lie at each of its sites and the subscript labels \( i \)-th site of the lattice. In the case of the clock model of order \( n \), each spin can assume \( n \) possible states (orientations) given by Eq. (1) and the Hamiltonian for the clock model of order \( n \) is defined by Eq. (2).

Finally, it is pedagogical to note that in the limit \( n \to \infty \), the clock model is expected to behave as the planar rotator model, in which, each spin can continuously vary its orientation, but we will not address here such case.

**3. Simulations and Results**

Extensive Monte Carlo simulations, using the RE-WL method of the clock model within an overall energy window, per spin, of \([-2,0]\) were performed for orders 2, 3, and 4 with a flatness criterium for the minimum value of the histogram set to 70% of its average value and a stop criterium set to \( \ln(f) = 10^{-8} \).

Each of the clock orders above were simulated for system sizes of \( L = 20, 40, 80, 100, \) and 200 lattice constants with a number of samples of 10, 2, 2, 2, and 1, respectively. The number of energy windows varied with the system size being 4, 4, 10, 20, 40, respectively, for the previous sequence of system sizes. In all cases, the overall energy window of each simulation per spin for the various orders of the clock model, i.e., the physical energy interval per spin, was set to be \([-2,0]\), which provides ample energy variation, allowing proper description of various quantities up to including the fundamental state along with its critical behavior.

We start presenting our results by providing the results of a sample of the fundamental quantity \( g(\epsilon) \), the density of states, in Fig. 1 for a system with \( 100 \times 100 \) spins on a square

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1 Please refer to references \([1, 2, 3]\) for detailed descriptions of the Wang-Landau method and clarification on the meaning of the parameters.
lattice. We note that the error bars associated are smaller than the thickness of the lines for this and remaining (not shown) system sizes. In the following, the Ising model will be solely included for comparison purposes, since the model is exactly solvable in two dimensions. The (logarithm of the) density of states grows substantially with the order of the clock model. In fact, near the maximum value of $g(e)$, the values are about $2.88 \cdot 10^3$, $4.76 \cdot 10^3$, and $6 \cdot 10^3$ orders of magnitude greater than $g(-2)$, i.e., the density of states at energy of the fundamental state. Additionally, order 3, at the maximum has a factor of about 1.65 greater of the number of orders of magnitude of the corresponding value of the Ising model, while order 4 the number of orders of magnitude is just 1.26 times larger of those of order 3.

The mean energy per spin is defined
$$\langle e \rangle = \langle E \rangle / L^2,$$
where $\langle E \rangle$ is the average energy of the system. The canonical partition function
$$Z(T) = \sum_E g(E) e^{-\beta E},$$

Figure 1. Plots of the (decimal) logarithm of the density of states, $\log g(e)$, of orders 2 (red), 3 (green), and 4 (blue) of systems with $100 \times 100$ spins. Error bars (not provided) are smaller than line thickness of the plots.

Figure 2. Plots of quantities associated with the energy for the three clock orders 2 (red), 3 (green), and 4 (blue). In parts (a) and (b) the plots are for a square lattice of $100 \times 100$ spins. (a) Average energy per spin, $\langle e \rangle$, as a function of temperature. (b) Plots of the specific heat $c_V$. 

\[ Z(T) = \sum_E g(E) e^{-\beta E}, \]
where $\beta = 1/k_B T$, and $k_B$ is the Boltzmann constant, can be utilized to define the mean energy, per spin,

$$\langle e \rangle = Z^{-1} \sum_{E} \frac{E}{N} e^{-\beta E}. \quad (4)$$

Next, we present in Fig. 2(a) the mean energy per spin over a broad interval of temperatures, $T$, in the range $[0,8]$. Notice that the Ising model does not merge its mean energy values, per spin, with those of the other two cases, even at the highest temperature of the interval. In contrast, it is somewhat surprising that reasonably merged mean energy values, for $T > 4$, with solely 3 or 4 states per spin. Once again, error bars are not included as they are smaller than line thicknesses.

Next, we show plots of the specific heat (per spin) defined as

$$c_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{N k_B T^2}, \quad (5)$$

in Fig. 2(b). Of notice, it is the enhanced $c_V$ of the order 3 clock relatively to the other two orders. The clock orders 2 and 4 also have a logarithmic dependence of the peak of the specific heat with size shown in Fig. 3(a), while order 3 has a power-law dependence as shown in Fig. 3(b).
Figure 4. Plots of quantities associated with the magnetization for the three clock orders 2 (red), 3 (green), and 4 (blue). In parts (a) and (b) the plots are for a lattice of 100 \times 100 spins. (a) Magnetization, $m$, as a function of temperature. (b) Plots of the magnetic susceptibility $\chi$. (c) Log-log plot showing the scaling of the magnetic susceptibility peaks, $\chi_{\text{max}}$, with system size. Solid, black line shows expected slope of $1/3$ for Ising behavior.

Values of the slopes of orders 2 and 4 are not universal, so their values vary. The computed slope of the log-log plot is 0.47, which differs from the expected 1/3. [6]

Now, we move on to show results of magnetic related quantities. We start with the
magnetization, the order parameter, defined as

\[ m = \frac{\sqrt{\left(\sum_{i=1}^{N} \sigma_{xi}\right)^2 + \left(\sum_{i=1}^{N} \sigma_{yi}\right)^2}}{N}, \]  

(6)

where \( \sigma_{\alpha i} \) represents the corresponding coordinate, given by \( \alpha = \{x, y\} \), of the spin at site \( i \). The above definition in the case of orders 2 and 4 boils down to

\[ m = \frac{|\sum_{i=1}^{N} \sigma_i|}{N}, \]

(7)

for both cases. In the case of the Ising model (order 2) we just need to associate \( \sigma_i \) to \( \sigma_{yi} \) as this is the only non-zero coordinate. Now, order 4 represents two Ising models at orthogonal directions, i.e., the magnetization can be formally written as

\[ m = \frac{|\sum_{i=1}^{N} (a_i \sigma_{xi} + (1 - a_i) \sigma_{yi})|}{N}, \]

(8)

where \( a_i \) takes value 1 (one) if the spin is aligned along the \( x \)-direction and 0 (zero) if the spin is aligned along the \( y \)-direction. We observe in Fig. 4(a) plots of the magnetization for temperatures in the interval \([0,4]\). As expected, the increased number of states per spin with the order, leads to the transitioning of the magnetization, from its maximum to approximately zero, occurring at a lower temperatures, i.e., the critical behavior occurs at a lower critical temperature with increasing orders (within the set 2, 3, and 4).

Another quantity of interest is the magnetic susceptibility defined as

\[ \chi = N \frac{(m^2) - (m)^2}{k_B T}. \]  

(9)

Plots of the magnetic susceptibility are shown in Fig. 4(b). The results corroborate the higher response, at criticality, of order 3 as observed for \( c_V \). Scaling of the maximum of the magnetic susceptibility follows a dependence of the form

\[ \chi \approx L^{\gamma/\nu}. \]

(10)

Since the exponent associated with the correlation length, \( \nu = 1 \), for the Ising model in two dimensions, we are directly observing the value of \( \gamma \) (see references [12, 11]). This is, in fact, observed in Fig. 4(c) where the three curves have the expected slope of 7/4 illustrated by the solid (black) line.

4. Concluding Remarks

We presented preliminary results of the clock model restricted to orders 3 and 4, where its critical behavior belongs to the Ising universality class.

The results fully corroborate expected properties of the Ising universality class, such as the logarithmic divergence of the specific heat (per spin) and the power-law divergence of the magnetic susceptibility. In particular, our results on the critical temperatures, not included in the present work, are in close agreement with exact results from renormalization group studies. [10]

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