The Critical Finite Size Scaling Relation of the Order-Parameter Probability Distribution for the Three-Dimensional Ising Model on the Creutz Cellular Automaton

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We study the order parameter probability distribution at the critical point for the three-dimensional spin-1/2 and spin-1 Ising models on the simple cubic lattice with periodic boundary conditions. The finite size scaling relation for the order parameter probability distribution is tested and verified numerically by microcanonical Creutz cellular automata simulations. The state critical exponent $\delta$, which characterizes the far tail regime of the scaling order parameter probability distribution, is estimated for 3-d Ising models using the cellular automaton simulations at the critical temperature. The results are in good agreement with the monte carlo calculations.

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A quantity of central importance for the finite-size scaling analyses of the critical phenomena is the order parameter probability distribution $P(M)$. The knowledge of the finite size scaling function for $P(M)$ of the Ising model makes it possible to calculate all the moments of the order parameter and all its cumulants.$^{[1-5]}$ Most properties of $P(M)$ are known from computer simulations.$^{[6-14]}$ For $d=3$, the corresponding finite size scaling function do
not exist in the analytical form. There are effort to get simple analytical functions by fitting to Monte Carlo results at the critical temperature for the infinite lattice.\textsuperscript{[10–13]} The main purpose of these study is to test the finite size scaling relations for the order parameter probability distribution of the three-dimensional spin-1/2 and spin-1 Ising models by the microcanonical Creutz cellular automaton algorithm on the simple cubic lattice and to obtain the value of the state critical exponent $\delta$. The Creutz cellular automaton (CCA) for the Ising model has been proven to be successful in producing the values of the universal statical critical exponents and the critical temperature in two and higher dimensions.\textsuperscript{[15–20]} The CCA algorithm, which was first introduced by Creutz,\textsuperscript{[20]} is a microcanonical algorithm interpolating between the canonical Monte Carlo and Molecular dynamics techniques.

In this paper, the probability distribution of order parameter is obtained for the two variants of the Ising model on the CCA. The first model is the 3-d spin-1/2 Ising model on the simple cubic lattice. For the zero external magnetic field ($H = 0$), the Hamiltonian of the model is given by

$$H_I = -J \sum_{<ij>} S_i S_j$$

(1)

where $S_i = \pm 1$ and the sum is carried out over all nearest-neighboring (nn) spin pairs. The parameter $J$ ($J > 0$) is the ferromagnetic coupling constant. The simulations are carried out on simple cubic lattice $LxLxL$ of linear dimensions $L = 16, 18, 20, 24$ and $40$ with periodic boundary conditions. The second model is the Blume-Capel (BC) model without single-ion anisotropy parameter ($D = 0$). The BC model is a spin-1 Ising model.\textsuperscript{[21,22]} It has
the same Hamiltonian with spin-1/2 Ising model for the $H = 0$. Here, the spins can take three discrete values -1, 0 and 1. The BC model is simulated using an improved algorithm\cite{18} from CCA for simple cubic lattice $L \times L \times L$ of linear dimensions $L = 16, 20, 24, 28$ and 32 with periodic boundary conditions. The data are averages over the lattice and the number of time steps (1,000,000) during which the cellular automaton develops. The simulations are done 20 times with different initial configurations at the critical point for the Ising models.

The infinite lattice critical temperature values for spin-1/2 and spin-1 Ising models are estimated from the temperature variation of the Binder forth-order cumulant for the finite lattices. The Binder forth-order cumulant of the order parameter, which is used to estimate the infinite lattice critical temperature, is given by

$$g_L = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}$$

The temperature variations of the Binder cumulant are illustrated in Fig.1 (a) for spin-1/2 and (b) in Fig.1(b) for spin-1 Ising model. The infinite lattice critical temperatures are obtained from the intersection of the finite lattice Binder cumulant curves. The critical temperature value for spin-1/2 Ising model is estimated as $kT_c/J = 4.511 \pm 0.002$ which is in good agreement with Monte Carlo calculations.\cite{23–26} For the spin-1 Ising model, the estimated critical temperature ($kT_c/J = 3.197 \pm 0.002$) is also in a good agreement with a series expansion results.\cite{27–29} The behavior of the order parameter probability distribution at the critical point is investigated at these estimated
critical temperatures.

The order parameter probability distribution $P_L(M)$ is calculated by

$$P_L(M) = \frac{N_M}{N_{CCAS}}$$

where $N_M$ is the number of times that magnetization $M$ appears, and $N_{CCAS}$ is total number of Creutz cellular automaton steps. Histograms of 200 bins are used in plotting $P_L(M)$ at critical point for finite lattice sizes which are shown in Fig.2 (a) for spin-1/2 and in Fig.2(b) for spin-1 Ising model. The simulations have been performed for the twenty different initial configurations with a constant total energy at critical point. The data of $P_L(M)$ are obtained from averages of data for different initial configurations. The relative standard deviation (RSD) of the average $P_L(M)$ values is approximately in the interval 5% – 10%.

The finite size scaling hypothesis for the probability distribution of order parameter for Ising model can be expressed generally as follows

$$P_L(M) = bP^*(M^*)$$

where $b = b_0L^{\beta/\nu}$, $\beta$ and $\nu$ are critical exponents, $M^* = bM$, $b_0$ is a constant, and $P^*(M^*)$ is a universal scaling function. To compute the normalized distribution $P^*(M^*)$ via Eq.4 one has evaluate the pre-factor $b$. The value of $b$ for each lattice sizes can be easily calculated by

$$b = 1/(\langle M^2 \rangle - \langle M \rangle^2)^{1/2}$$
Thus, we used the Eq.4 for obtained of the universal function $P^*(M^*)$ as in Ref.[8]. At the critical point, the plots of finite size scaling for $P(M)$ are illustrated in Fig.3 (a) for spin-1/2 and in Fig. 3(b) for spin-1 models. The microcanonical simulations have been done on simple cubic lattices at $kT_c/J = 4.511$ for spin-1/2 and at $kT_c/J = 3.197$ for spin-1. For both models, the universality at critical point can be easily seen from Fig.3(a) and (b). The scaling probability distributions $P^*(M^*)$ for spin-1/2 and spin-1 Ising models coincided with each other for all $M^*$ values. These results verify the finite size scaling relation given in Eq. 4 for the order parameter probability distribution of the three dimensional Ising model. On the other hand, the log-log plots of the pre-factor $b$ against $L$ are shown in Fig.4. The slopes of the data line a single curve are given the values of $\beta/\nu=0.498\pm0.003$ for spin-1/2 and $\beta/\nu=0.492\pm0.003$ for spin-1. Furthermore, the $\beta/\nu$ values for both models are estimated using the scaling relation of the order parameter at the critical temperature[Fig.4(b)]. The slopes of the log-log plots of $M(T_c)$ against to $L$ are given the values the $\beta/\nu=0.50\pm0.01$ for spin-1/2 and $\beta/\nu=0.51\pm0.01$ for spin-1. All estimated values of $\beta/\nu$ are in good agreement with universal value$^{[5,30]}$.

On the other hand, for the $|M^*| > 1$ and the periodic boundary conditions, the scaling function of the order parameter probability distribution is expected to have the following exponential form$^{[13]}$

$$P^*(M^*) \propto \exp (-AM^*^{\delta+1})$$

(6)

where $\delta$ denotes the equation of state exponent. Its value can be obtained from the log-log plot of $\ln P^*(M^*)$ against to $M^*$. In the far tail regions, the
slopes of data line a single curve gives approximately $\delta + 1 = 5.8$ for spin-$1/2$ and $\delta + 1 = 5.7$ for spin-$1$ on the right and left tails. The behavior of tails for large $M^*$ are shown in Fig.5 (a) and (b) for spin models. The estimated values of $\delta + 1$ are in good agreement with Monte Carlo results ($\delta = 4.8$) \cite{6,13} for 3-d Ising model. Finally, the finite size scaling relation for the order parameter probability distributions of the Ising models is verified by Creutz cellular automaton simulations numerically.

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**Figure Captions**

Fig.1 The variations of Binder cumulant against to $kT/J$ for (a) spin-1/2 and (b).spin-1 Ising model.

Fig.2. The order parameter probability distribution at the critical point for (a) spin-1/2 and (b).spin-1 Ising model on the simple cubic lattices. Simulations were performed at $kT_C/J = 4.511$ for spin-1/2 and at $kT_C/J = 3.197$ for spin-1 model.

Fig.3. Scaling functions $P^*(M^*)$ for (a) three-dimensional spin-1/2 and (b) spin-1 Ising model on simple cubic lattices.

Fig.4.(a ) The Log-log plot of $b$ against to $L$ for spin-1/2 and spin-1 Ising models. (b) The log-log plots of $M(T_c)$ against to $L$ . The values of slopes are in good agreement with the universal $\beta/\nu$ value.

Fig.5. The log-log plots of $\ln(P^*(M^*))$ against to $M^*$ for (a) spin-1/2 and (b) spin-1 Ising model. The slopes are equal to $\delta + 1 = 5.8$ for spin-1/2 and $\delta + 1 = 5.7$ for spin-1 model in the far tail regions.
(a) spin-1/2 Ising model

- $L=8$
- $L=10$
- $L=12$
- $L=14$
- $L=16$
- $L=18$
- $L=20$
- $L=24$

$kT_c/J = 4.511 \pm 0.002$

(b) spin-1 Ising model

- $L=8$
- $L=10$
- $L=12$
- $L=16$
- $L=20$
- $L=24$
- $L=28$
- $L=32$

$kT_c/J = 3.197 \pm 0.002$
spin 1/2 Ising model
$kT_c/J = 4.511$

(a)

spin-1 Ising model
$kT_c/J = 3.197$

(b)
(a) spin-1/2 Ising model

(b) spin-1 Ising model
\[ \beta/\nu = 0.492 \pm 0.001 \]

(a)  

\[ \beta/\nu = 0.498 \pm 0.001 \]

\[ \text{spin-1} \quad (\text{slope}=0.492) \]

\[ \text{spin-1/2} \quad (\text{slope}=0.498) \]

\[ \text{Log}(L) \]

\[ \text{Log}(b) \]

\[ \text{Log}(M(T_c)) \]

(b)  

\[ \beta/\nu = 0.50 \pm 0.01 \]

\[ \beta/\nu = 0.51 \pm 0.01 \]

\[ \text{spin-1} \quad (\text{slope}=-0.51) \]

\[ \text{spin-1/2} \quad (\text{slope}=-0.50) \]

\[ \text{Log}(L) \]
**spin-1/2 Ising model**

\[(\delta + 1) = 5.8\]

- L=16
- L=18
- L=20
- L=24
- L=28
- L=32
- L=40

Linear (slope=5.8) for right tail

**spin-1 Ising model**

\[(\delta + 1) = 5.71\]

- L=16
- L=20
- L=24
- L=28
- L=32
- L=40

Linear (slope=5.71) for left tail