The Finite-Size Scaling Study of the Specific Heat and the Binder Parameter of the Two-Dimensional Ising Model for the Fractals Obtained by Using the Model of Diffusion-Limited Aggregation

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The two-dimensional Ising model with nearest-neighbour pair interactions is simulated on the Creutz cellular automaton by using the finite-size lattices with the linear dimensions L = 80, 120, 160, and 200. The temperature variations and the finite-size scaling plots of the specific heat and the Binder parameter verify the theoretically predicted expression near the infinite lattice critical temperature. The approximate values for the critical temperature of the infinite lattice T_c = 2.287(6), T_c = 2.269(3), and T_c =2.271(1) are obtained from the intersection points of specific heat curves, Binder parameter curves, and the straight line fit of specific heat maxima, respectively. These results are in agreement with the theoretical value (T_c =2.269) within the error limits. The values obtained for the critical exponent of the specific heat, α = 0.04(25) and α = 0.03(1), are in agreement with α = 0 predicted by the theory. The values for the Binder parameter by using the finite-size lattices with the linear dimension L = 80, 120, 160, and 200 at T_c = 2.269(3) are calculated as $g_L(T_c) = -1.833(5)$, $g_L(T_c) = -1.834(3)$, $g_L(T_c) = -1.832(2)$, and $g_L(T_c) = -1.833(2)$, respectively. The value of the infinite lattice for the Binder parameter, $g_L(T_c) = -1.834(11)$, is obtained from the straight line fit of $g_L(T_c) = -1.833(5)$, $g_L(T_c) = -1.834(3)$, $g_L(T_c) = -1.832(2)$, and $g_L(T_c) = -1.833(2)$ versus L = 80, 120, 160, and 200, respectively.

Key words: Ising Model; Cellular Automaton; Finite-Size Scaling; Scanning Method.
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1. Introduction

The application of fractal concepts, first introduced by Mandelbrot et al. to describe complex natural shapes and structures as well as mathematical sets and functions having an intricately irregular form, has been studied [1 – 4]. The aggregation of particles to form cluster has, for a long time, been one of the central phenomena in natural science with important implications for physical problems such as air pollution, dielectric breakdown, bacterial colony growth, and natural formations (snowflakes and manganese dendrites). The model allow an exploration of the process of pattern formation in real physical systems which is based mostly on the model of diffusion-limited aggregation. This model describes the most important morphology patterns observed in various non-equilibrium systems, such as diffusion-limited aggregation-like, dendrite, needle, tree-like, dense-branching, compact, stingy, spiral, and chiral structures [5 – 14].

The Creutz cellular automaton [15] has simulated the two dimensional Ising model successfully near the critical region, and has reproduced its critical exponents within the framework of the finite-size scaling theory [16, 17]. This algorithm is an order of magnitude faster than the conventional Monte Carlo method and it does not need high quality random numbers. These features of the Creutz cellular automaton would make the Ising model simulations in higher dimensions more practical. Compared to Q2R cellular automaton [18] it has the advantage of allowing the specific heat to be computed from the internal energy fluctations.

The purpose of this study is to test the finite-size scaling study of the specific heat and the Binder parameter of the two-dimensional Ising model for the fractals obtained by using the model of diffusion-limited aggregation. However, the test studies in $d = 2$ dimensions are not available. The simulations are carried out on the Creutz cellular automaton, which has success-

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fully arisen as an alternative research tool for Ising models in the dimensionalities $2 \leq d \leq 8$ [19].

The model is described in Section 2, the results are discussed in Section 3, and a conclusion is given in Section 4.

2. Model

In the model of diffusion-limited aggregation, the central particle is placed in the closed square lattice. Another new particle is started to move on the edge of the lattice site. If this fragment passes by the neighbouring site of the central particle during the random moving, it fixes there. The same conditions are applied to the other particles. However, when the particle or a group of particles goes out of the determined lattice site, at which the particle is cancelled, then another particle is suggested. The operation is repeated until the suggested number of particles in the aggregate, i. e. the behaviour of a particle or a particle group, is obtained.

At the Creutz cellular automaton, four binary bits are associated with each site of the lattice. The value for each site is determined from its value and those of its nearest neighbours at the previous time step. The updating rule, which defines a deterministic cellular automaton, is as follows: Of the four binary bits on each site, the first one is the Ising spin B_i. Its value may be "0" or "1". Ising spin energy (internal energy) of the lattice, H_{I}, is given (in units of the nearest neighbour coupling constant J) by

$$H_{\mathrm{I}} = -J \sum_{\langle i,j \rangle} S_i S_j, \tag{1}$$

where $S_i = 2B_i - 1$, and $\langle i, j \rangle$ denotes the sum over all nearest neighbour pairs of sites. The second and the third bits are for the momentum variable conjugate to the spin (the demon). These two bits form an integer which can take on the value 0, 1, 2, or 3. The kinetic energy (in units of J) associated with the demon can take on four times these integer values. The total energy

$$H = H_{\mathrm{I}} + H_{\mathrm{K}} \tag{2}$$

is conserved; here H_{K} is the kinetic energy of the lattice. For a given total energy the system temperature T (in units of J/k_{B} where k_{B} is the Boltzmann constant) is obtained from the average value of the kinetic energy. The fourth bit provides a checkerboard style updating, and so it allows the simulation of the Ising model on a cellular automaton. The black sites of the checkerboard are updated and then their color is changed into white: the white sites are changed into black without being updated.

The updating rules for the spin and the momentum variables are as follows: For a site to be updated its spin is flipped and the change in the Ising energy (internal energy), H_{I}, is calculated. If this energy change is transferable to or from the momentum variable associated with this site, such that the total energy, H, is conserved, then this change is done and the momentum is appropriately changed. Otherwise the spin and momentum are not changed.

As the initial configuration all spins are taken ordered (up or down). The initial kinetic energy is randomly given to the lattice via the second bits of the momentum variables in the white sites. The quantities computed are averages over the lattice and the number of time steps during which the cellular automaton develops.

The simulations are carried out on simple hypercubic lattices L^2 of linear dimensions $80 \leq L \leq 200$ with periodic boundary conditions by using two-bit demons. The cellular automaton develops $9.6 \cdot 10^5$ ($L = 80, 120, 160, 200$) sweeps for each run with seven runs for each total energy.

3. Results and Discussion

The fractals obtained by using the model of diffusion-limited aggregation are illustrated in Figure 1 for the lattice with $L = 80$, 120, 160, and 200. In $d = 2$ dimension, the finite-size scaling relation for the specific heat C_L is derived below [16, 20]. The finite-size scaling relations for the critical temperatures and the free-energy density are given as [16, 20]:

$$(T_{\mathrm{c}} - T_{\mathrm{c}}(L)) \propto L^{-1/\nu}, \tag{3}$$

$$f_L = L^{-d} F(tL^{y_t}, hL^{y_h}), \quad h \to 0, \quad L \to \infty, \tag{4}$$

where $y_t = \frac{1}{\nu}$ and $y_h = \frac{\Delta}{\nu}$, with $d\nu = 2 - \alpha$ and $\Delta = \gamma + \beta$, $t = (T - T_{\mathrm{c}})/T_{\mathrm{c}}$ is the reduced temperature with $t > 0$ for $T > T_{\mathrm{c}}$ and $t < 0$ for $T < T_{\mathrm{c}}$, h is the reduced external magnetic field, α, β, and γ are the critical exponents for the specific heat, order parameter, and the magnetic susceptibility of the infinite lattice, respectively. Thus, f_L takes the following form:

$$f_L = L^{-d} F(tL^{1/\nu}, hL^{(\gamma+\beta)/\nu}). \tag{5}$$

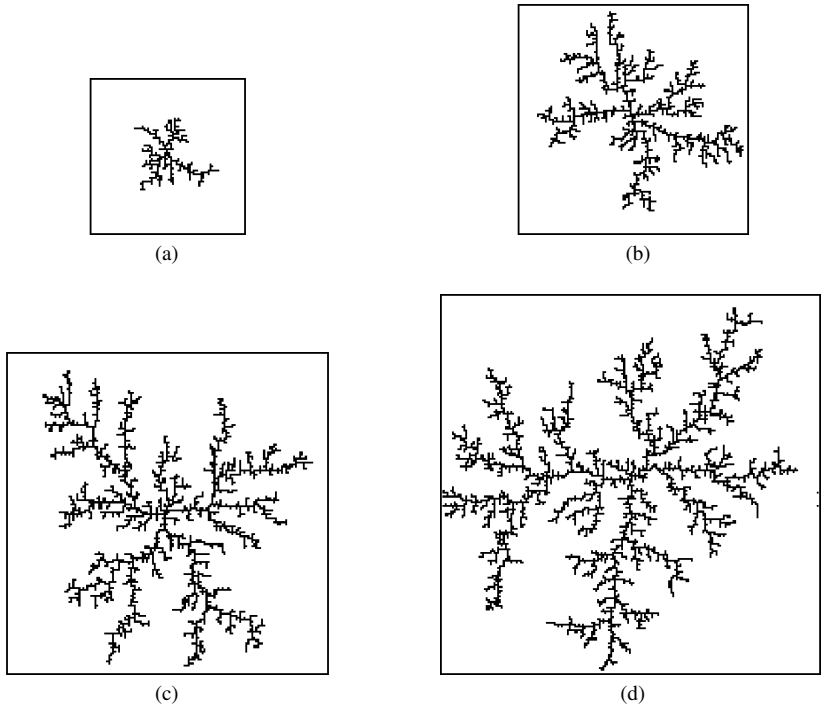

Fig. 1. Images of the fractals obtained by using the model of diffusion-limited aggregation for lattices with the linear dimensions (a) $L = 80$, (b) $L = 120$, (c) $L = 160$, and (d) $L = 200$.

Table 1. The critical temperature and the maximum values of the specific heat for the finite lattices and the values $T_c = 2.269$.

L	$T_c^C(L)$	$C_L^{\max}$	$C_L(T_c)$
80	2.2624(3)	0.575(6)	0.561(12)
120	2.2646(2)	0.593(12)	0.574(14)
160	2.2669(2)	0.598(24)	0.591(22)
200	2.2678(3)	0.602(39)	0.598(40)

By using the definition $C_L = -\frac{\partial^2 f_L}{\partial t^2}$ the following equation is obtained:

$$C_L = L^{\alpha/\nu} F(tL^{1/\nu}, hL^{(\gamma+\beta)/\nu}). \tag{6}$$

Since $\alpha = 0$, $\beta = \frac{1}{8}$, and $\gamma = \frac{7}{4}$ in $d = 2$ dimension, C_L takes the following form:

$$C_L = F(tL^{1/\nu}, hL^{(\gamma+\beta)/\nu}). \tag{7}$$

At $h = 0$ (7) becomes

$$C_L = F(tL^{1/\nu}), \tag{8}$$

where $F = F(x)$ is the finite-size scaling function (the shape function) for the specific heat. This is the relation to be tested. The plots of C_L versus temperature (T) and corresponding temperatures of specific heat maxima $(T_c^C(L))$ listed in Table 1 versus $L^{-1/\nu}$ are illustrated in Figures 2 and 3, respectively. The intersec-

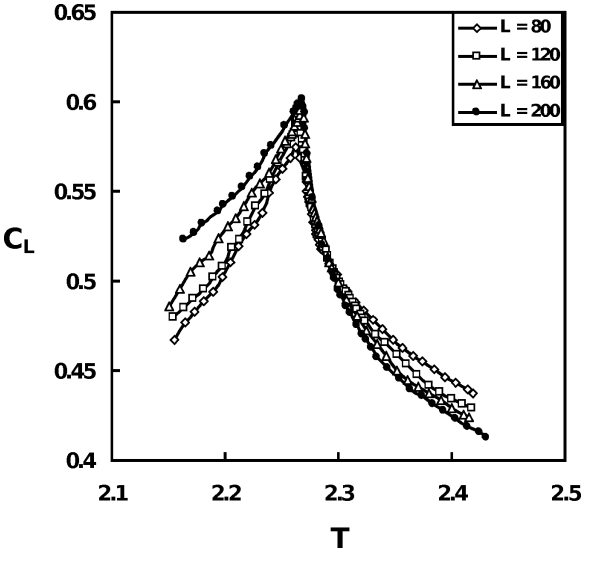

Fig. 2. Specific heat C_L as a function of the temperature T for sizes $80 \leq L \leq 200$.

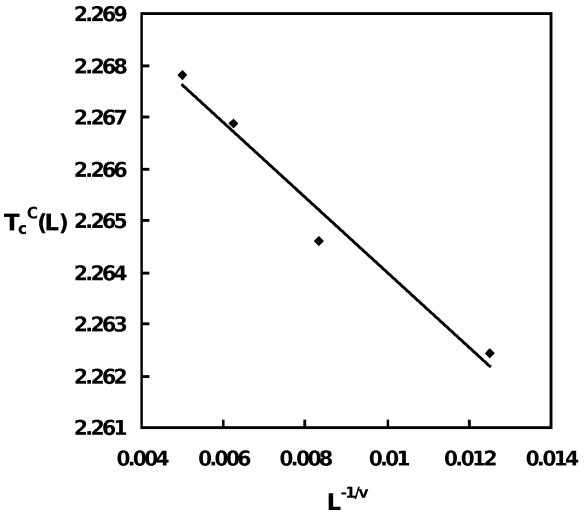

Fig. 3. The value of the infinite-lattice critical temperature for the specific heat C_L, $T_c = 2.271(1)$ obtained by extrapolating the straight line fitted to critical temperatures of the lattice with linear dimensions $80 \leq L \leq 200$ as $L \to \infty$.

tion of the curves in Figure 2 for $80 \leq L \leq 200$ gives the critical temperature of $T_c = 2.287(6)$ at which the specific heat maxima occur when $L \to \infty$. The straight line fit in the plot of $T_c^C(L)$ vs. $L^{-1/\nu}$ also implies $T_c = 2.271(1)$ as $L \to \infty$, seen in Figure 3. These results are in agreement with the value of the Creutz cellular automaton result of $T_c = 2.263$ [17] and the theoretical prediction of $T_c = 2.269$ [22]. In order to calculate the critical exponent for the specific heat we use the general relation for C_L at $h = 0$ and $t = 0$. Thus, (6) reduces to the following form:

$$C_L \propto L^{\alpha/\nu}. \tag{9}$$

This relation is also used for the maxima of the finite lattices. By using the data of Table 1 in getting the log-log plots of $C_L(T_c)$ and $C_L^{\max}$ vs. L, the following values of α are obtained: $\alpha = 0.04(25)$ and $\alpha_{\max} = 0.03(1)$, the average of which is $\alpha = 0.03(25)$. These result is in agreement with $\alpha = 0$ results predicted by the theory.

In Figure 4 we show the finite-size scaling plot of the specific heat. In this figure, not all of the data points for a given L fall on the finite-size scaling curve which is formed by the overlapping parts of the plots for different L. Since all the scaled quantities of C_L for different L values overlap above T_c, the finite-size scaling relations for C_L is valid only in the region above T_c. Therefore, this scaling for C_L is verified only in the region $tL^{1/\nu} > 0$, but not in the region $tL^{1/\nu} < 0$. It should

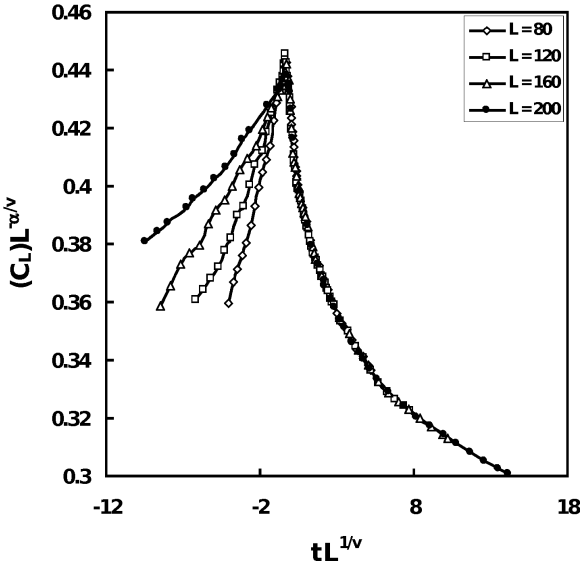

Fig. 4. The data for C_L shown in Figure 2 plotted vs the scaling variable $tL^{1/\nu}$, where $T_c = 2.269(3)$.

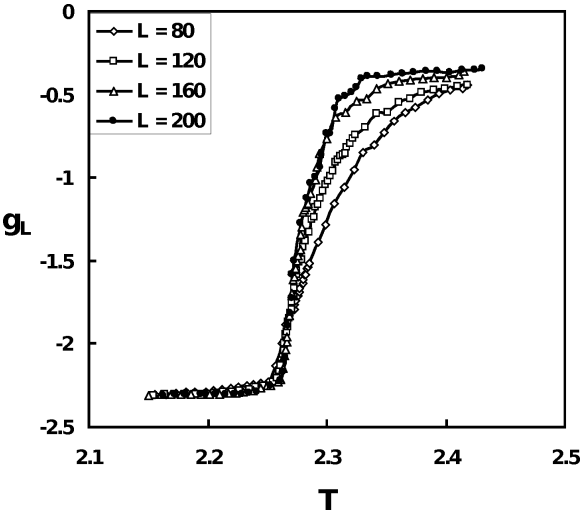

Fig. 5. Same as Figure 2, but for Binder parameter g_L.

be mentioned that the contribution to C_L from the regular part is not considered in this plot. That is, the values of the specific heat computed in the simulations are used directly in the plots.

The $h = 0$ finite size renormalized coupling g_L (Binder parameter or Binder cumulant) introduced by Binder [16, 20, 21]

$$g_L = \frac{\langle s^4 \rangle_L}{\langle s^2 \rangle_L^2} - 3 = \left[\frac{\chi_L^{(4)}}{L^4 \chi_L^4} \right]_{h=0}, \tag{10}$$

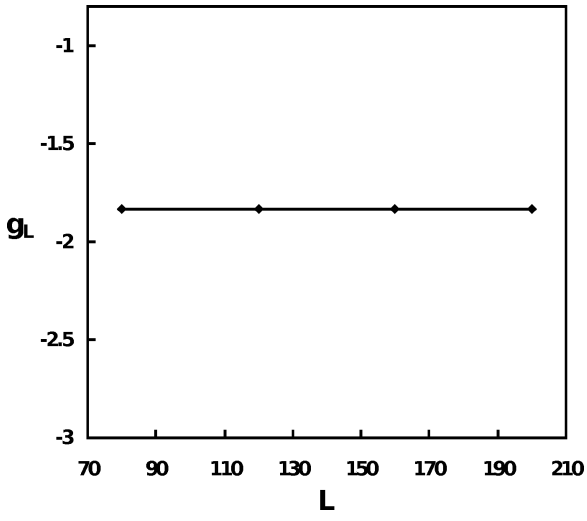

Fig. 6. L-dependence of the data in Figure 5.

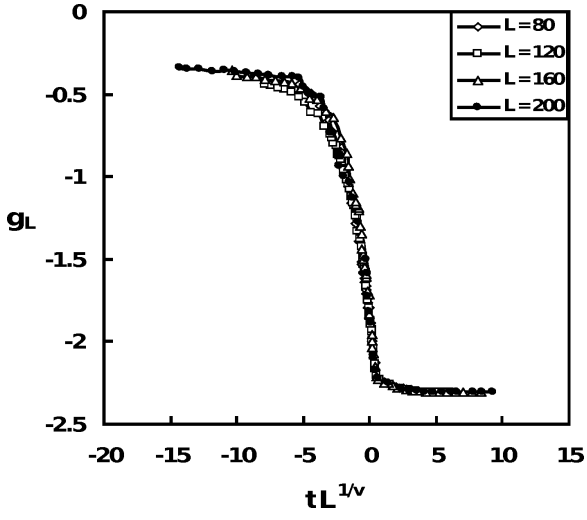

Fig. 7. Same as Figure 4, but for Binder parameter g_L.

where χ_L is the susceptibility and $\chi_L^{(4)}$ is the fourth field derivate; the subcript L denote the corresponding finite-size quantities. In the method of Binder [16, 20, 21], the critical point T_c is located by finding the common crossing point of plots of g_L vs. temperature for a range of different system sizes L [16, 20, 21]. The temperature variation of the Binder parameter for $L = 80$, 120, 160, and 200 is shown in Figure 5. In this figure, the intersection point of the curves for $80 \leq L \leq 200$ gives $T_c = 2.269(3)$ which is in good agreement with the theoretical prediction of $T_c = 2.269$ [22]. From Figure 5 the values for the Binder parameter by using the finite-size lattices with the linear dimension $L = 80$, 120, 160, and 200 at $T_c = 2.269(3)$ are calculated as $g_L(T_c) = -1.833(5)$, $g_L(T_c) = -1.834(3)$, $g_L(T_c) = -1.832(2)$ and $g_L(T_c) = -1.833(2)$, respectively. From Figure 6 and Table 2 the value of the infinite lattice for the Binder parameter, $g_L(T_c) = -1.834(11)$, is obtained from the straight line fit of $g_L(T_c) = -1.833(5)$, $g_L(T_c) = -1.834(3)$, $g_L(T_c) = -1.832(2)$, and $g_L(T_c) = -1.833(2)$ versus $L = 80$, 120, 160, and 200, respectively. This result is in good agreement with the Monte Carlo simulations results of $g_L(T_c) = -(1.830 - 1.835)$ [23–27].

L	$g_L(T_c)$
80	$-1.833(5)$
120	$-1.834(3)$
160	$-1.832(2)$
200	$-1.833(2)$

Table 2. The values of the Binder parameter for the finite lattices.

The finite-size scaling relation for the Binder parameter has the following form:

$$g_L = G(tL^{1/\nu}), \quad h \to 0, \quad L \to \infty, \tag{11}$$

where $t > 0$ for $T > T_c$ and $t < 0$ for $T < T_c$. We illustrate g_L vs. $tL^{1/\nu}$ in Figure 7. Since all the scaled quantities of g_L for different L values overlap above T_c, the finite-size scaling relations for g_L is valid only in the region above T_c. Therefore, this scaling for g_L is verified only in the region $tL^{1/\nu} > 0$, but not in the region $tL^{1/\nu} < 0$.

4. Conclusion

Creutz cellular automaton computer simulations are a tool in scientific fields such as condensed-matter physics, including surface-physics and applied-physics problems (metallurgy and diffusion, etc.). With the increasing ability of this method to deal with quantum-mechanical problems such as quantum spin systems or many-fermion problems, it may become useful to answer some questions in the fields of elementary-particle and nuclear physics as well.

In this work, the two-dimensional Ising model is simulated on the Creutz cellular automaton using the finite-size lattices with the linear dimension $L = 80$, 120, 160, and 200 for the fractals obtained by using the model of diffusions-limited aggregation. Since all the scaled quantities of C_L and g_L for different L values overlap above T_c, the finite-size scaling relations for C_L and g_L are valid only in the region above T_c.

The computer used was an Intel(®) Core(TM) 2 Duo CPU E6550 at 2.33 GMhz. The CPU time invested was 1140 hours for all the simulations.

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