Geometric Upper Critical Dimensions of the Ising Model

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(Received 12 June 2022; accepted manuscript online 5 July 2022)

The upper critical dimension of the Ising model is known to be $d_c = 4$, above which critical behavior is regarded to be trivial. We hereby argue from extensive simulations that, in the random-cluster representation, the Ising model simultaneously exhibits two upper critical dimensions at ($d_c = 4$, $d_p = 6$), and critical clusters for $d \geq d_p$, except the largest one, are governed by exponents from percolation universality. We predict a rich variety of geometric properties and then provide strong evidence in dimensions from 4 to 7 and on complete graphs. Our findings significantly advance the understanding of the Ising model, which is a fundamental system in many branches of physics.

DOI: 10.1088/0256-307X/39/8/080502

The Ising model[1] is one of the most fundamental models in statistical physics and condensed matter, and has great influence in almost every branch of modern physics. When introduced in 1925, the Ising model was shown to have no finite-temperature phase transition in one dimension (1D).[2] In 1944, a milestone was achieved by Onsager[3,4] who obtained the exact free energy density on the square lattice without external field. In 1952, Yang derived that, close to the critical temperature, the spontaneous magnetization vanishes as a power law with exponent $\beta = 1/8$.[5] In 1970s, the renormalization group (RG) theory was established, which is now the foundation of the modern theory of critical phenomena.[6–9] An important result of the RG theory is that the Ising model has the upper critical dimension $d_c = 4$, above which its critical behavior is controlled by the Gaussian fixed point (GFP). In 3D, extensive numerical studies have been available,[10–12] and recently, the conformal bootstrap program has led to new insights and an unprecedented precision of critical exponents.[13,14]

Percolation[15,16] has been intensively studied since 1950s due to its richness in both physics and mathematics. In bond percolation, the edges of a lattice are occupied with probability p, or vacant. Two sites are connected if there is a path of occupied bonds from one to the other. A maximal set of connected sites is called a cluster. The upper critical dimension of percolation is known to be $d_p = 6$,[17] and, for $d \geq 11$,[18,19] many rigorous results have been obtained. Besides their fundamental roles, both percolation and the Ising model are widely applied to many fields, including material science, neuroscience, complex network, epidemiology, ecology and biology, etc.[20–27]

In 1972, Fortuin and Kasteleyn (FK) derived the so-called random-cluster (RC) representation[28] for the Q-state Potts model,[29] in which the Ising and percolation models are simply the special cases for $Q = 2$ and $Q \to 1$, respectively. This geometric representation has led to many exact results in 2D and efficient simulation algorithms.[30–33] A natural question arises: what is the upper critical dimension d_u of the general RC model? In 1970s, the RG analysis suggested that, depending on the inclusion of the ϕ^3 term or not, d_u could be 6 or 4 for general Q. Special attention was paid to the FK-Ising model. On the Bethe lattice and complete graph (CG),[34] both of which can be regarded as the $d \to \infty$ limit, $d_u = 6$ was conjectured from a hyperscaling relation.[35] On CGs, a percolation-like scaling window was rigorously shown,[36] and a recent study revealed that, at criticality, medium-size clusters are CG-percolation-like.[37] In 5D, interesting two-scale scaling behaviors were observed.[38]

In this Letter, we carry out extensive simulations for the Ising model on periodic hypercubic lattice of linear size L in dimensions from 4 to 7 and on CGs, as well as for bond percolation in 7D. The simulation is up to be of more than 10^8 lattice sites. We observe a surprisingly rich variety of finite-size and thermodynamic critical behaviors, and on this basis, argue that, in the RC representation, the Ising model simultaneously exhibits two upper critical dimensions at $d_c = 4$ and $d_p = 6$, respectively.

On the one hand, as long as $d \geq 4$, a bunch of geometric quantities display finite-size scaling (FSS) behavior governed by a uniform set of mean-field exponents. For instance, the L-dependent scaling exponent for the largest cluster is $D_{L1} = 3d/4$ from the CG-Ising asymptotics, while it is $D_{L2} = 1 + d/2$ for the second-largest cluster from the GFP in the RG framework. On the other hand, critical clusters exhibit different geometric structures for $4 \leq d < 6$ and $d \geq 6$. Consider the thermodynamic fractal

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dimension $D_{\rm F}$, as defined from the asymptotic power-law dependence of the size of a cluster on its gyration radius. For $4 \le d < 6$, one has $D_{\rm F1} = 3d/4$ for the largest cluster and $D_{\rm F2} = 1+d/2$ for all the remaining ones. However, for $d \ge 6$, one has $D_{\rm F1} = 9/2$ and $D_{\rm F2} = 4$; the latter is from high-d percolation universality. This is summarized in Table 1. A variety of other critical behaviors are observed. For instance, for $d \ge 6$, the number of spanning clusters and the winding number of the largest cluster are both divergent as L increases, while they are of $\mathcal{O}(1)$ in lower dimensions. Further, there exist two scaling windows: the leading one is of CG-Ising type, and the other is of Gaussian type for $4 \le d < 6$ and of percolation type for $d \ge 6$, align with rigorous result for CGs.

Table 1. Conjectured exact fractal dimensions for $4 \le d < 6$ and $d \ge 6$, as inspired by CG-Ising asymptotics (asy.), Gaussian fixed point (f.p.) and results for high-d percolation (perc.).

	$4 \le d < 6$			$d \ge 6$
$D_{\rm L1}$	$3d/4$		$\Leftarrow$	same
$D_{\rm F1}$	$3d/4$	(CG-Ising asy.)		$9/2$
$D_{\rm L2}$	$1+d/2$		$\Leftarrow$	same
$D_{\rm F2}$	$1+d/2$	(Gaussian f.p.)		4 (perc.)

Models. The Hamiltonian of the Ising model reads

$$\mathcal{H} = -K \sum_{i\sim j} S_i S_j, \quad (S_i = \pm 1), \tag{1}$$

where $K > 0$ represents the ferromagnetic coupling and the summation is over all neighboring pairs. By the FK transformation, it can be mapped onto the Q-state RC model with $Q = 2$, with the partition function

$$\mathcal{Z} = \sum_{A\subseteq G} p^{|A|}(1-p)^{|E\setminus A|} Q^{c(A)}, \tag{2}$$

where the lattice is denoted as $G \equiv (V, E)$, the summation is over all spanning subgraphs $A \subseteq G$, $|A|$ and $c(A)$ respectively represent the numbers of occupied bonds and of clusters, and the bond probability is $p = 1 - e^{-2K}$.

We simulate the FK-Ising model on d-dimensional tori with $4 \le d \le 7$ and on CGs, at and near the critical points as in Refs. [39,40]. A combination of the Wolff and Swendsen–Wang algorithms [30,31] is applied, and the latter is mainly used to generate FK-bond configurations. The maximum system volume is $V = 48^4, 51^5, 24^6, 16^7, 2^{22}$ for $d = 4, 5, 6, 7$ and CGs, respectively. We also simulate bond percolation in 7D at criticality. [41]

We sample the number $n(s, V)$ of clusters of size s per site, and the sizes of the largest- and the second-largest clusters as $C_1 = \langle \mathcal{C}_1 \rangle$ and C_2, respectively, with $\langle\cdot\rangle$ for ensemble average. Further, to study geometric fractal structures, we use the breadth-first search method to grow FK clusters and measure their gyration radius in an *unwrapped* way, effectively taking into account periodic boundary effects. [38] Given a cluster $\mathcal{C}$, we randomly choose a seed site and assign it a d-dimensional *zero* coordinate ($\boldsymbol{x} \equiv 0$), and each newly included site v is assigned by an unwrapped coordinate as $\boldsymbol{x}_v = \boldsymbol{x}_{\rm u} + \boldsymbol{e}_i$ $(-\boldsymbol{e}_i)$, if v is grown from u along (against) the ith direction, with $\boldsymbol{e}_i$ the corresponding unit vector. The unwrapped gyration radius is calculated as $\mathcal{R} \equiv \sqrt{\langle|\boldsymbol{x}_{\rm u}|^2\rangle - \langle|\boldsymbol{x}_{\rm u}|\rangle^2}$, where the average is over all sites in cluster $\mathcal{C}$. We also measure the unwrapped expansion distance $\mathcal{U}$ along the first-coordinate direction for each cluster.

Evidence for $d_{\rm c} = 4$ from Finite-Size Scaling. In the spin representation, $d_{\rm c} = 4$ is widely known for the Ising model. Nevertheless, finite-size scaling behavior for $d \ge 4$ has been a long-standing debate. [38,42–45] It is now believed [38,39,46] that the critical free energy on high-d tori contains two scaling terms, i.e., RG exponents ($y_t = 2, y_h = 1+d/2$) from the GFP and ($y_t^* = d/2, y_h^* = 3d/4$) from the CG-Ising asymptotics. An important consequence is that the critical two-point function behaves as $G(\boldsymbol{x}, L) \approx \|\boldsymbol{x}\|^{2-d} + L^{-d/2}$, algebraically decaying with distance $\|\boldsymbol{x}\|$, with exponent $2-d$ from GFP, and then saturating to a plateau of height $L^{-d/2}$ from CG-Ising asymptotics. [47–49] This implies that the magnetic susceptibility, which is exactly the average cluster size in the FK representation, scales as $L^{d/2}$.

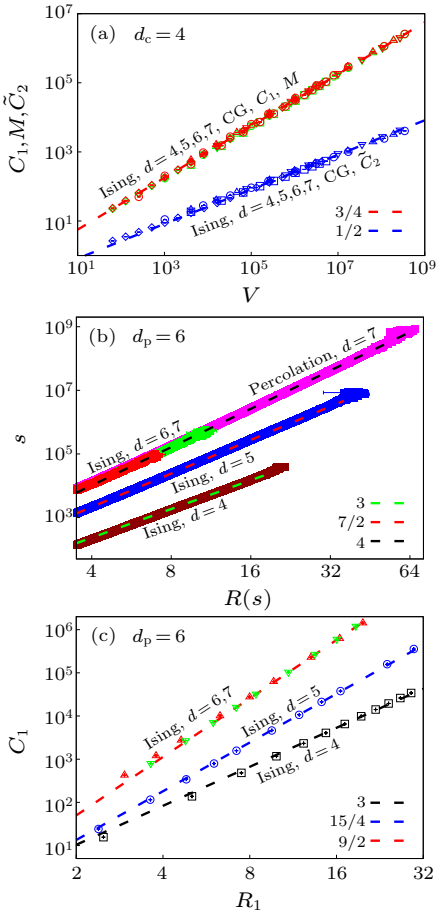

Fig. 1. Evidence for the two upper critical dimensions, with power-law scaling illustrated by approximately straight lines in the log-log scale. (a) Evidence for $d_{\rm c} = 4$ from finite-size scaling. The largest-cluster size C_1, the rescaled second-largest-cluster size $\tilde{C}_2$ and the magnetization M are plotted versus system volume V. Up to non-universal constants, data of C_1 and M collapse well onto a line with slope 3/4 for $d = 4, 5, 6, 7$ and on CGs, and data of $\tilde{C}_2$ collapse onto a line of slope 1/2. (b) Evidence for $d_{\rm p} = 6$ from geometric fractals. Size s of medium clusters is shown versus gyration radius R, and the fractal dimension $D_{\rm F2}$ is $1+d/2$ for $4 \le d < 6$ and 4 for $d \ge 6$ (percolation universality). (c) Evidence for $d_{\rm p} = 6$ from the largest cluster, which has fractal dimension $D_{\rm F1} = 3d/4$ for $4 \le d < 6$ and $D_{\rm F1} = 9/2$ for $d \ge 6$.

Figure 1(a) shows the critical magnetization $M \equiv \langle|\sum_i S_i|\rangle$ versus volume V. The good data collapsing for $d = 4, 5, 6, 7$ and on CGs, displaying $M \sim V^{3/4}$. Moreover, the C_1 data collapse well onto those for M. This confirms the conventional upper dimension $d_c = 4$, and demonstrates the uniform scaling $\sim V^{3/4}$ for $d \geq d_c$, which can be proved for CGs.[36,50]

From extensive simulations and results in Ref. [38], we conjecture that, for $d > 4$, the FSS of C_2 behaves as $C_2 \sim L^{1+d/2} = \sqrt{V}V^{1/d}$, corresponding to the GFP. This is seemingly consistent with the scaling $C_2 \sim \sqrt{V}\ln V$ for CGs,[36] where $\ln V$ may be related to the term $V^{1/d}$ for finite d. Rescaled quantities are then defined as $\tilde{C}_2 \equiv C_2/L$ for $d \geq 4$ and $\tilde{C}_2 \equiv C_2/\ln V$ for CGs. Indeed, the $\tilde{C}_2$ data for $d = 4, 5, 6, 7$ and on CGs collapse well on a line with slope 1/2, as shown in Fig. 1(a).

At the upper critical dimensions, logarithmic corrections are usually expected. For the Ising model in the spin representation, field theory predicts the form of logarithmic corrections for many quantities at $d_c = 4$,[51,52] such as the magnetization $M \sim L^3(\ln L)^{1/4}$, and the susceptibility $\chi \sim L^2(\ln L)^{1/2}$. We now examine the effect of logarithmic corrections to C_1 and C_2. In Fig. 2, we plot in log-log scale C_1 and C_2, rescaled by their expected power-law scaling, versus $\ln L$. Our data suggest that $C_1 \sim L^3(\ln L)^{1/4}$, consistent with the field-theory prediction for M, and $C_2 \sim L^3(\ln L)^{-1/4}$, which has no direct counterpart in the spin representation.

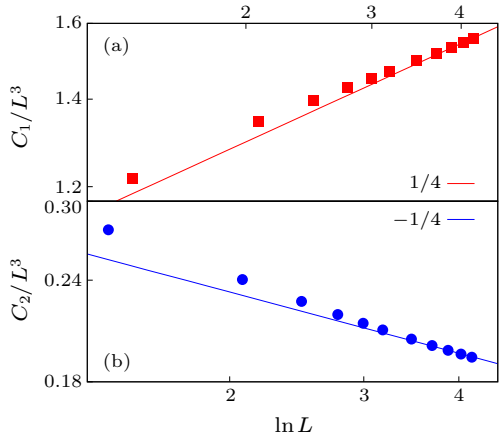

Fig. 2. Log-log plot of the rescaled sizes of the largest and second largest clusters at $d = 4$ versus $\ln L$.

Evidence for $d_p = 6$ from Geometric Fractals. In comparison with FSS, intrinsic geometric properties of clusters are better characterized by the power-law dependence of cluster size on gyration radius as $s \sim R^{D_F}$, which is shown in Fig. 1(b) for medium-size clusters, i.e., clusters with size $1 \ll s \ll C_1$. Distinct fractal structures are revealed: the fractal dimension D_{F2} is $1+d/2$ for $4 \leq d < 6$, and becomes constant 4 for $d \geq 6$. While the former is from the GFP, the latter is consistent with percolation universality,[53] as well illustrated by the 7D-percolation data in Fig. 1(b).

Actually, the largest cluster also has different fractal dimensions below and above $d_p = 6$. The plot of the C_1 data against the gyration radius R_1 in Fig. 1(c) gives $D_{F1} = 3d/4$ for $4 \leq d < 6$ and 9/2 for $d \geq 6$, with 9/2 calculated from $3d/4$ with $d = 6$.

Therefore, we conclude that $d_p = 6$ is also an upper critical dimension for the FK-Ising model.

Evidence for $d_p = 6$ from Topological Properties. The essential assumption of the standard FSS theory is that the divergent correlation length, e.g., as characterized by R_1, is cut off as $\mathcal{O}(L)$, resulting in the phenomenon that the number of percolating clusters is of $\mathcal{O}(1)$. This has been widely used as a powerful tool in numerical study of critical phenomena.

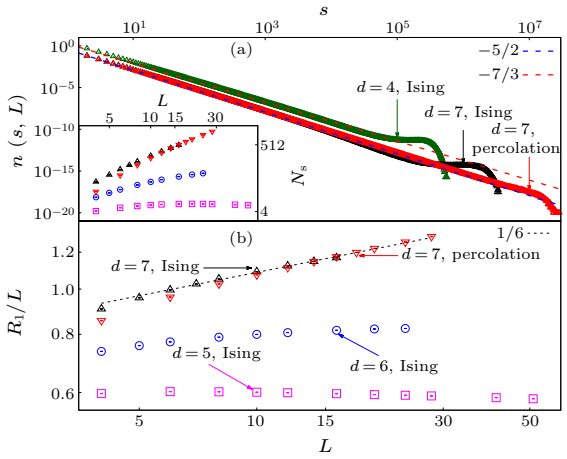

Fig. 3. Evidence for $d_p = 6$ from topological properties. (a) Cluster-number density $n(s, L)$ versus s, where the Fisher exponent τ is clearly different for $d = 4$ and 7. The inset is for the number N_s of spanning clusters. (b) Winding number of the largest cluster as represented by R_1/L. Both the winding number and the spanning-cluster number are of size $\mathcal{O}(1)$ for $d < 6$ but diverge for $d > 6$.

We first look at the cluster-number density $n(s, L) \sim s^{-\tau}\tilde{n}(s/L^{D_{L1}})$, where τ is the Fisher exponent, D_{L1} is the finite-size fractal dimension and $\tilde{n}$ is a universal function. The hyperscaling relation $\tau = 1 + d/D_{L1}$ is further believed to hold, giving $\tau = 7/3$ for $d \geq 4$. As shown in Fig. 3(a), while being indeed true for 4D, the hyperscaling relation is broken for 7D, which has $\tau \approx 5/2$. From the data collapsing for the FK-Ising and percolation models in 7D, it can be restored by using $D_{LP} = 2d/3$ for percolation universality.

To illustrate the emergence of clusters with nontrivial topology, we measure the number N_s of spanning clusters, of which the unwrapped expansion distance $\mathcal{U} \geq L$. The inset of Fig. 3(a) shows that, while $N_s = \mathcal{O}(1)$ for $d < 6$, it diverges as L increases for $d > 6$. From the scaling $s \sim R^4$ in Fig. 1(b), it is suggested that the typical size of spanning clusters must be $s > L^4$, and thus, N_s can be calculated as $L^d \int_{L^4} n(s, L)\, ds$. With $\tau = 5/2$ for $d > 6$, this gives $N_s \sim L^{d-6}$, consistent with the inset of Fig. 3(a).

Topological properties can be further illustrated by the winding number, as characterized by ratio R_1/L. As shown in Fig. 3(b), one has $R_1/L = \mathcal{O}(1)$ for $d < 6$, consistent with the observation of $D_{L1} = D_{F1}$, i.e., the finite-size and thermodynamic fractal dimensions are identical. For $d > 6$, however, one has $C_1 \sim L^{3d/4} \sim R_1^{9/2}$ (Table 1), and thus expects $R_1 \sim L^{d/6}$. In other words, as L increases, the largest cluster winds around the tori for more and more times. This is well confirmed in Fig. 3(b).

Percolation-Like Scaling for the Largest Cluster. The above scaling behaviors at criticality also hold within a

scaling window of size $\mathcal{O}(1/L^{y_t^*})$, with $y_t^* = d/2$ from the CG-Ising asymptotics. As an example, the inset of Fig. 4 shows the scaling $C_1(t,V) \sim V^{3/4}\tilde{C}_1(tV^{1/2})$ for the largest cluster of the Ising model with $d = 6, 7$ and CG, where $t \equiv (K_c - K)/K_c$ and $t \geq 0$ is for the high-temperature phase. This has also been observed for the 5D FK Ising model in Ref. [38].

Actually, in each dimension $d \geq 4$, there also exists another scaling window, which is less sharp and thus can survive slightly further away from K_c. For $4 \leq d < 6$, it is of size $\mathcal{O}(1/L^{y_t})$, with $y_t = 2$ from the GFP, where all the clusters, including the largest one, would scale as $s \sim L^{y_h} \sim R^{y_h}$ with $y_h = 1 + d/2$.

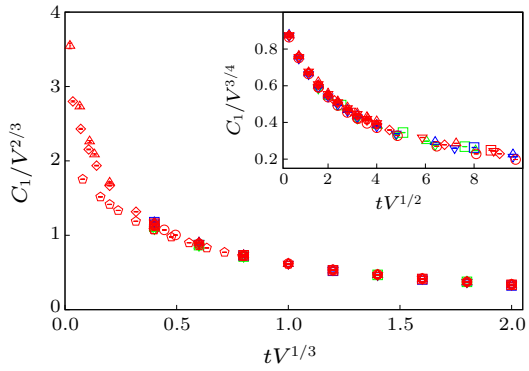

Fig. 4. Percolation scaling window for $d \geq 6$. Within window $t \sim \mathcal{O}(V^{-1/3})$, the largest cluster scales percolation-like as $C_1 \sim V^{2/3}$. The data points of various shapes are for different system sizes V, and the colors are for 6D (blue), 7D (red) and CGs (green). The inset demonstrates the CG-Ising scaling window of $\mathcal{O}(V^{-1/2})$, in which $C_1(t,V) \sim V^{3/4}\tilde{C}_1(tV^{1/2})$.

For $d > 6$, the second scaling window is of size $\mathcal{O}(1/L^{d/3})$, with exponent $d/3$ from high-d percolation, where all the clusters, including the largest one, are expected to be percolation-like as $s \sim R^4 \sim L^{2d/3}$. This is illustrated by Fig. 4, displaying $C_1(t,V) \sim V^{2/3}\tilde{C}_1(tV^{1/3})$. Note that, unlike the CG-Ising scaling window, the percolation scaling window only occurs at the high temperature side. The scattering for small values of $tV^{1/3}$ is due to the CG-Ising scaling window. On CGs, the existence of the percolation scaling window has been rigorously proved [36] and an RG-like argument has been provided. [37]

The second-largest cluster scales as $C_2 \sim L^{1+d/2}$ in the CG-Ising scaling window (including K_c). It is therefore expected for $d > 6$ that the maximum of C_2 would occur in the percolation scaling window and diverge as $\sim L^{2d/3}$.

Other interesting phenomena emerge. For instance, as criticality is approached from the low-temperature side, i.e., $t \to 0^-$, one can expect that the second-largest cluster scales as $C_2(t,V) \sim L^{1+d/2}\tilde{C}_2(tL^{d/2})$. Suppose that the relation $C_2 \sim R_2^4$ holds within the scaling window, then we have $R_2 \sim L^{(d+2)/8}\tilde{R}_2(tL^{d/2})$ for $d \geq 6$. To recover the thermodynamic critical behavior, one expects $\tilde{R}_2(x) \sim x^{-(d+2)/4d}$, such that $R_2 \sim |t|^{-\nu_2'}$ with $\nu_2' = (d+2)/4d$. Thus $\nu_2' = 1/3$ for $d = 6$ and converges to $1/4$ as $d \to \infty$. The exponent $1/4$ was also obtained on the Bethe lattice with fixed boundary conditions. [35] In addition, it was observed on CGs [37] that a tiny sector emerges in the whole configuration space and slowly vanishes as L increases. Conditioned on being in this sector, quantities are observed to exhibit CG-percolation behavior. On lattices, our preliminary simulations suggest that there exists a tiny sector for all $d \geq 4$, which is of Gaussian and percolation types for $4 \leq d < 6$ and $d \geq 6$, respectively.

Based on a combination of extensive simulations from $d = 4$ to 7 and insights from RG theory, and rigorous and numerical results for CG, we propose that, in the FK random-cluster representation, the Ising model simultaneously has two upper critical dimensions at $(d_c = 4, d_p = 6)$. Besides being an answer for the long-standing debate, dated back to 1970s, this picture provides a counter-intuitive and advanced understanding for the Ising model, which is probably the most fundamental system in statistical and condensed-matter physics. Note that the scenario of two upper critical dimensions was also proposed in the field-theoretical treatment of the CP^1 model. [54]

In FK-Ising clusters for $d \geq 4$, the thermodynamic and finite-size scaling behaviors are surprisingly rich, partially summarized in Tables 1 and 2. Two pronounced features can be seen: (1) As long as $d \geq 4$, there exist two-scale properties, two scaling windows and two configuration sectors. (2) For $d > 6$, the scaling behaviors of all clusters, except the largest one, are in percolation universality, unexpected from the first sight. Interestingly, while the geometric properties are very sophisticated, critical behaviors in the spin representation are much simpler: no percolation-like behaviors exist and the upper critical dimension $d_p = 6$ cannot be seen.

Table 2. Some scaling behaviors for $4 \leq d < 6$ and $d \geq 6$, including Fisher exponent τ, finite-size scaling of the gyration radius R_1 and the number N_s of spanning clusters, and two scaling windows.

	$4 \leq d < 6$	$d \geq 6$
$\tau - 1$	$d/(1+d/2)$	$3/2$
R_1	$\sim L$	$\sim L^{d/6}$
N_s	$\mathcal{O}(1)$	$\sim L^{d-6}$
Scaling windows	CG-Ising + GFP	CG-Ising + perc.

Several open questions arise. First, what are the precise forms of logarithmic corrections in critical FK clusters at $d_c = 4$ and $d_p = 6$? In this work, we study the logarithmic corrections of sizes of the largest two clusters, but it will be interesting to carry out a systematic study of the effect of logarithmic corrections to various geometric quantities, especially at $d_p = 6$. Second, in the loop representation of the Ising model, which is another geometric representation and can be coupled to the RC model via the loop-cluster joint model, [33] what would be geometric effects for $d \geq 4$? Finally, most of the exact exponents in Tables 1 and 2 are conjectured and rigorous proofs remain elusive.

Acknowledgements. This work was supported by the National Natural Science Foundation of China (Grant No. 11625522), the Science and Technology Committee of Shanghai (Grant No. 20DZ2210100), the National Key R&D Program of China (Grant No. 2018YFA0306501). We thank Eren M. Elçi, Jens Grimm, Timothy Garoni, Martin Weigel and Jonathan Machta for valuable discussions, in particular for Jesper Jacobsen. When finalizing the collection and analysis of our Monte Carlo data, we learned from private communications that Jesper Jacobsen and Kay Wiese (ENS, Paris) are working on the same topic using a field-theoretical approach and propose an-

other scenario, i.e., for $4 \leq d < 6$, the scaling behavior of some geometric observables could be described by non-trivial critical exponents other than those from the CG-Ising asymptotic and from the GFP. Taking into account the logarithmic correction for the scaling of the second-largest cluster, which is conjectured solely based on simulations, this interesting scenario cannot be ruled out.

We dedicate this work to Professor Henk W. J. Blöte, who passed away on June 10, 2022. Blöte was internationally renowned for his numerous contributions to statistical mechanics, holding official positions at Delft University of Technology and Leiden University until his retirement in 2008, as well as a lifetime service to physics. Since his first paper on the specific heat singularities of Ising antiferromagnets in 1967, Blöte has maintained a particular passion for the Ising model among his research interests in different physical topics. As this work demonstrates, he has successfully conveyed his spirit to his students (Y.D.) and his second-generation students (S.F. and Z.Z.). Blöte has maintained a very close relationship with China over the past few decades, even learning to speak the Chinese language. Blöte gave enormous guidance to the students and researchers he supervised, treating them as his children. His research fellows, especially his two Chinese PhD students (Youjin Deng and Xiaofeng Qian) and his Chinese postdoc Wen'an Guo are so grateful for having had Blöte as their supervisor. Blöte was very generous, kind, and always ready to provide us with support and love. Blöte was our physics mentor and remains our lifetime mentor. The seed of physics he sowed in China has grown into academic trees of several generations; the seed of love he planted in China has grown into a sea of sunflowers that warms the hearts of countless people.

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