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Shape effects of finite-size scaling functions for anisotropic three-dimensional Ising models

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Abstract. The finite-size scaling (FSS) functions for anisotropic three-dimensional (3D) Ising models of size $L_1 \times L_1 \times aL_1$ (a: anisotropy parameter) are studied by Monte Carlo simulations. We study the a dependence of FSS functions of the Binder parameter g and the magnetization distribution function $p(m)$. We have shown that the FSS functions for $p(m)$ at the critical temperature change from a two-peak structure to a single-peak one by increasing or decreasing a from 1. We also study the FSS near the critical temperature of the layered square-lattice Ising model, when the systems have a large two-dimensional (2D) anisotropy. We have found the 3D and 2D FSS behaviour depending on the parameter which is fixed; a unified view of 3D and 2D FSS behaviour has been obtained for the anisotropic 3D Ising models.

1. Introduction

Finite-size scaling (FSS) has been increasingly important in the study of critical phenomena [1, 2]. This is partly due to the progress in the theoretical understanding of finite-size effects, and partly due to the application of FSS in the analysis of simulational results.

Recently, more attention has been paid to the universality of FSS functions [3] for both percolation models [4–7] and Ising models [8–10]. It has been shown that several quantities including distribution functions on various lattices have universal FSS functions by choosing appropriate metric factors. It should be noted that universal FSS functions depend on boundary conditions and the shape of finite systems.

In the percolation problem it was considered, until quite recently, that there exists only one percolating cluster on two-dimensional (2D) lattices at the percolating threshold. However, the importance of the number of percolating clusters for anisotropic systems, which was pointed out by Hu and Lin [5], has captured current interest [5,11–13]. Aizenman [11] derived the upper and lower bounds of the probability for the appearance of n percolating clusters, W_n, for 2D percolation at criticality. His result was later confirmed by Monte Carlo simulations [12]. By use of conformal field theory, Cardy [13] proposed an exact formula for W_n at the percolation threshold for the systems with large aspect ratios [13]. The aspect ratio L_1/L_2 is an important quantity in the FSS functions for anisotropic 2D systems of size $L_1 \times L_2$. The 'nonuniversal scaling' of the low-temperature conductance peak heights for Corbino discs in the quantum Hall effect has been discussed in terms of the number of the percolating clusters [14].

For the Ising model, the aspect ratio dependence of the Binder parameter [15] at the critical temperature was studied by Kamieniarz and Blöte [16]. Binder and Wang discussed anisotropic

FSS [17]. The aspect ratio dependence of the universal FSS functions for the Binder parameter and magnetization distribution function was discussed by Okabe *et al* [10] for the 2D Ising model with tilted boundary conditions. For a fixed set of the aspect ratio and the tilt parameter, the FSS functions were shown to be universal [10]. Quite recently, based on the connection between the Ising model and a correlated percolation model, Tomita *et al* [18] studied the FSS properties of distribution functions for the fraction of lattice sites in percolating clusters in subgraphs with n percolating clusters, $f_n(c)$, and the distribution function for magnetization in subgraphs with n percolating clusters, $p_n(m)$. They studied the change of the structure of the magnetization distribution function for the 2D system with a large aspect ratio in terms of percolating clusters.

Almost all the results above for the shape effects on FSS functions are for 2D systems except for some works on the percolation problem [6, 7]. It is quite important to extend these arguments for higher-dimensional systems. Conformal invariance plays a role in 2D systems [19], but is not so powerful for three-dimensional (3D) systems as for 2D ones. Moreover, there are two limiting cases for anisotropic 3D systems, that is, the one-dimensional (1D) limit and the 2D limit. It is interesting to study various types of scaling for anisotropic 3D systems.

In this paper, we study the FSS functions for anisotropic 3D systems by Monte Carlo simulations. We are concerned with the ferromagnetic Ising model on the $L_1 \times L_1 \times aL_1$ simple cubic lattices with the periodic boundary conditions, where a is regarded as the anisotropy parameter. Attention is paid mainly to the effect of anisotropy, and we study the a dependence of the FSS functions for quantities such as the Binder parameter and the magnetization distribution function.

At the critical temperature for the 3D Ising model, we find that FSS functions for the magnetization distribution function change from a two-peak structure to a single-peak one, when the anisotropy parameter a is varied from 1. This behaviour is observed both for the systems with 2D and 1D anisotropy. When a system has a large 2D anisotropy, we find that finite-size systems with a fixed anisotropy parameter show good FSS behaviour as 3D systems near the critical temperatures for the layered square-lattice Ising models. In contrast, when we fix a number of layers and apply the FSS analysis for layered systems, these systems are scaled as 2D ones.

We organize the rest of the paper as follows. In section 2, we define the FSS functions and describe the quantities we treat in this paper. In section 3, we present our simulational results. In section 4, our results are summarized and discussed.

2. Finite-size scaling

If a quality Q has a singularity of the form $Q(t) \sim t^{\omega}$ ($t = T - T_c$) near the criticality $t = 0$, then the corresponding quantity $Q(L, t)$ for finite systems with the linear size L has the following scaling form:

$$Q(L, t) \sim L^{-\omega/\nu} f(tL^{1/\nu}) \tag{1}$$

where ν is the correlation-length critical exponent and $f(x)$ is the scaling function. Of course, the corrections to FSS are not negligible for smaller L. The FSS is also applicable to the distribution function of Q. At the criticality $t = 0$, and the FSS function has the following form:

$$p(Q; L, t = 0) \sim L^{\omega/\nu} F(QL^{\omega/\nu}). \tag{2}$$

In this paper we focus on the Binder parameter and the magnetization distribution function. The Binder parameter [15] is given by

$$g = \frac{1}{2}\left(3 - \frac{\langle m^4\rangle}{\langle m^2\rangle^2}\right) \tag{3}$$

and serves as a measure of the non-Gaussian nature of the distribution function. The FSS functions for these quantities are given by

$$g(L,t) \sim g(tL^{1/\nu}) \tag{4}$$

$$p(m; L, t=0) \sim L^{\beta/\nu} p(mL^{\beta/\nu}) \tag{5}$$

where β is the magnetization exponent.

3. Results

We used the Metropolis Monte Carlo method to simulate the ferromagnetic Ising model on $L_1 \times L_1 \times aL_1$ simple cubic lattices with different values of L_1 and a, implementing periodic boundary conditions.

First, we show the results for $a \leqslant 1$, that is, a 2D anisotropic case. We plot the temperature dependence of the Binder parameter g for $a = 1$, $\frac{1}{2}$, and $\frac{1}{4}$ of various sizes in figure 1(*a*). Error bars are within the size of the plotted symbols unless specified otherwise. We give the FSS plots in figure 1(*b*); g is plotted as a function of $(T - T_c)L^{1/\nu}$, where L is given by $(L_1 \times L_1 \times aL_1)^{1/3}$. For T_c, β and ν, we use the numerically estimated values for the 3D Ising model [20], that is, $T_c = 4.5114$, $\beta = 0.320$ and $\nu = 0.625$. From now on, we represent the temperature in units of J. From figure 1(*b*) we see that the FSS functions have a dependence in 3D systems, which is similar to the case of 2D systems.

We can get more information on the a dependence from the magnetization distribution function $p(m)$. In figure 2, we show the scaling plot of the magnetization distribution function $p(m)$ at $T = T_c$ for various sizes with different anisotropy parameters ($a \leqslant 1$). From the figure we find good FSS behaviour and also a large a dependence. By decreasing the anisotropy parameter a from 1, the FSS functions for the magnetization distribution function change from a two-peak structure to a single-peak one.

Next, we turn to the case of $a \geqslant 1$, that is, a 1D anisotropic case. We plot the temperature dependence of g for $a = 1$, 2 and 4 of various sizes in figure 3(*a*). The FSS plots are given in figure 3(*b*). We see similar behaviour of the FSS functions for $a \geqslant 1$, that is, g takes smaller values if we change a from 1. We show the a dependence of the FSS functions of the magnetization distribution functions at $T = T_c$ for $a \geqslant 1$ in figure 4. By increasing a from 1, FSS functions for $p(m)$ change from a two-peak structure to a single-peak one again.

If we compare the results of figures 1(*b*) and 3(*b*), and also those of figures 2 and 4, it seems that there could be a set of the anisotropy parameters $a < 1$ and $a > 1$ which give the same FSS functions. However, more careful calculations are needed to clarify this universality.

Let us consider the origin of the a dependence of FSS functions. This problem is related to the multiple percolating clusters. The connection between critical phenomena of spin models and percolation problems has been studied for a long time [21–23]. Quite recently, Tomita *et al* [18] used the cluster formalism to investigate the percolating properties of the 2D Ising model. They elucidated that the existence of several percolating clusters for anisotropic finite systems leads to the change of the structure of $p(m)$. That is, the combination of up-spin clusters and down-spin clusters gives the contribution of $m \sim 0$ in $p(m)$ for anisotropic case. The a dependence of $p(m)$ for the 3D systems can be understood in the same way as the 2D systems. We can apply this argument to cases for both 2D anisotropy ($a < 1$) and 1D

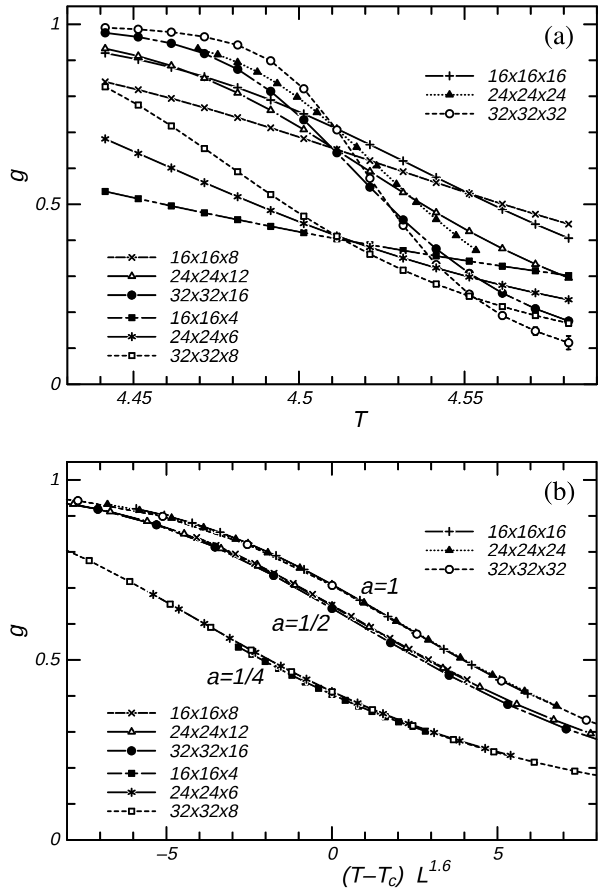

Figure 1. (*a*) Temperature dependence of g for several lattices with $a = 1, \frac{1}{2}$ and $\frac{1}{4}$. The temperature is represented in units of J. (*b*) Plot of g as a function of $(T - T_c)L^{1/\nu}$.

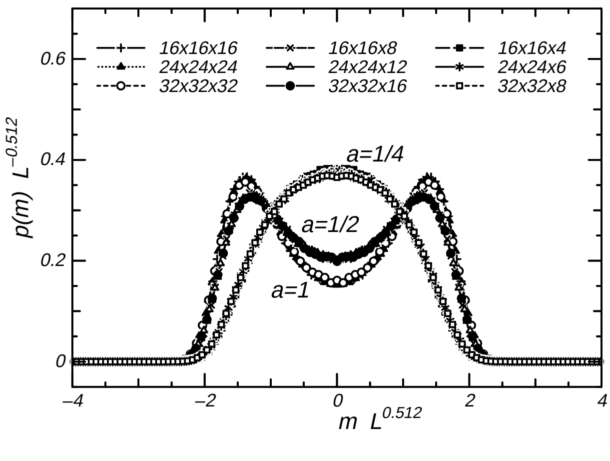

Figure 2. $p(m)L^{-\beta/\nu}$ at $T = T_c$ as a function of $mL^{\beta/\nu}$ for several lattices with $a = 1, \frac{1}{2}$ and $\frac{1}{4}$.

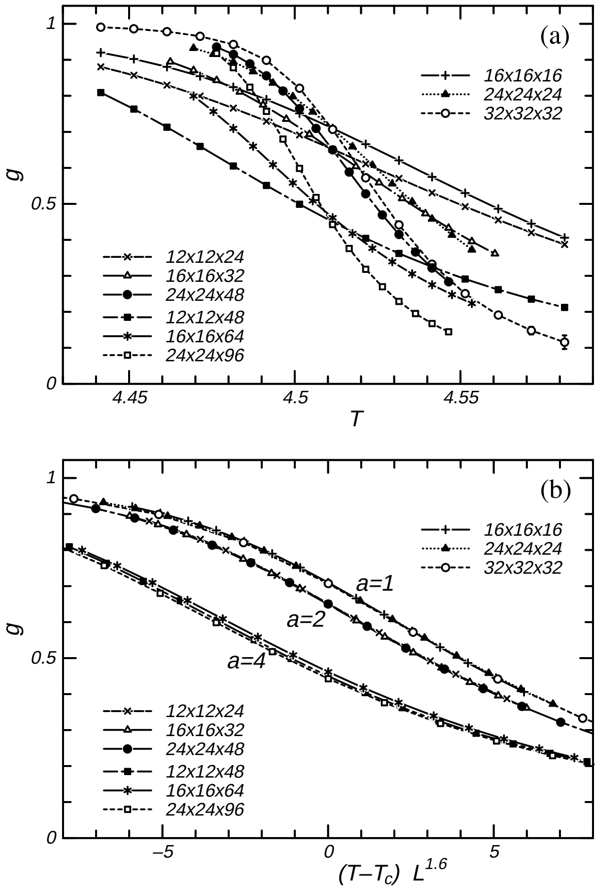

Figure 3. (*a*) Temperature dependence of g for several lattices with $a = 1$, 2 and 4. (*b*) Plot of g as a function of $(T - T_c)L^{1/\nu}$.

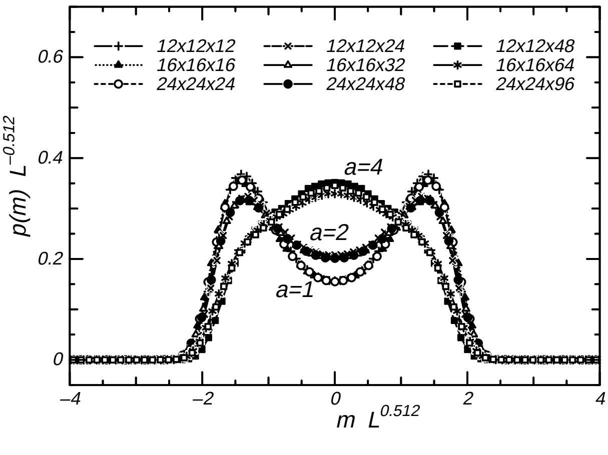

Figure 4. $p(m)L^{-\beta/\nu}$ at $T = T_c$ as a function of $mL^{\beta/\nu}$ for several lattices with $a = 1$, 2 and 4.

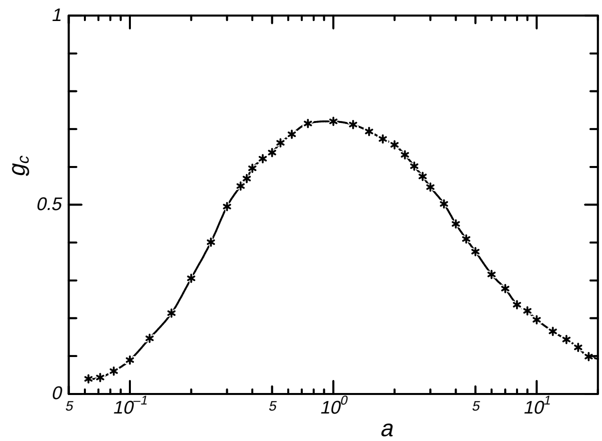

Figure 5. g at $T = T_c$, g_c, as a function of a. We use a semi-logarithmic scale.

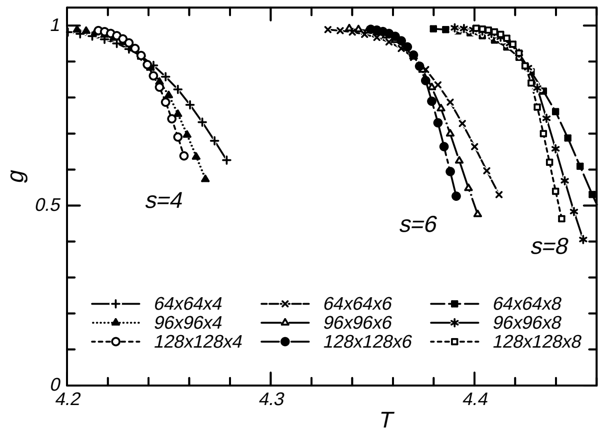

Figure 6. Temperature dependence of g for several systems. The numbers of layers are 4, 6 and 8.

anisotropy ($a > 1$). The value of Binder parameter g at $T = T_c$, of course, reflects upon the structure of the distribution function $p(m)$.

In order to see the anisotropy parameter dependence more clearly, we plot the a dependence of the Binder parameter g at criticality, g_c, in figure 5. Here, we use the semi-logarithmic scale for our plot. We add several data other than those given in figures 1 and 3. For large enough a or small enough a, the corrections to FSS become larger. From figure 5, we find that g_c takes the maximum value at $a = 1$ and decreases gradually in both directions, $a < 1$ and $a > 1$. For very large or very small a, g_c tends to vanish, which indicates that the distribution function $p(m)$ approaches the Gaussian distribution. This behaviour is consistent with above-mentioned multiple-percolating-cluster argument. Such an a dependence of g at criticality for 1D anisotropy of the 2D Ising model has already been discussed [16].

It is also interesting to consider the relation to the layered square-lattice Ising model for the case of large 2D anisotropy. The critical temperatures and the shift exponent for the layered square-lattice Ising model were studied by Kitatani *et al* [24]. In figure 6, we give the temperature dependence of g for several lattices, where the number of layers, s, is 4, 6 and 8.

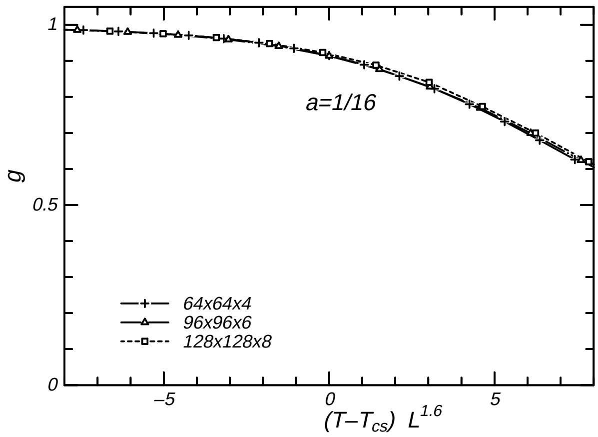

Figure 7. Scaling plot of g for fixed $a(=\frac{1}{16})$. The scaled variable is $(T - T_{cs})L^{1/\nu}$ for each s. The values of T_{cs} are $T_{c4} = 4.2364$, $T_{c6} = 4.3701$ and $T_{c8} = 4.4222$. We use the 3D exponent, $\nu = 0.625$.

If we make the system size large by fixing s, the system becomes the layered square-lattice Ising model. We can estimate the s-dependent critical temperature T_{cs} from the crossing point of the curves for fixed s in figure 6. Our estimates, $T_{c4} = 4.2364(4)$, $T_{c6} = 4.3701(4)$ and $T_{c8} = 4.4222(4)$, are consistent with those of [24].

Picking up the data for $a = \frac{1}{16}$ from figure 6, we plot g as a function of $(T - T_{cs})L^{1/\nu}$ in figure 7. Here we treat $T - T_{cs}$ for each s and ν is chosen as 0.625, that is, the 3D value. We have good FSS behaviour in figure 7, but this FSS plot is different from that given in figure 1(*b*), where $T - T_c$ has been treated. We should note that $T - T_{cs}$ can be rewritten as $T - T_{cs} = (T - T_c) + (T_c - T_{cs})$ and $T_c - T_{cs} \propto s^{-\lambda}$. Here λ is the shift exponent and is shown to be $1/\nu_{3D}$ [24]. Thus, for fixed a, we have 3D FSS for $T - T_{cs}$. In this case, the value of g_c at $T = T_{cs}$ is $\sim$0.92, which is simply the g_c value for the isotropic 2D Ising model. It is different from the g_c value of $\sim$0.04 for the anisotropic 3D Ising model for $a = \frac{1}{16}$, which is given in figure 5. In figure 8, we also show the scaling plot of the magnetization distribution function $p(m)$ at $T = T_{cs}$ for each s, fixing a as $\frac{1}{16}$. We have good FSS behaviour using 3D exponents. There are two distinct peaks in $p(m)$, which is a typical character of $p(m)$ at T_c for the isotropic 2D Ising model. In contrast, if we pick up the data for fixed s, for example, $s = 6$, these systems are expected to be scaled by using 2D critical exponents. Since we fix $s(= aL_1)$, the scaled variable is given by $(T - T_{cs})L_1^{1/\nu}$. Using the 2D exponent, $\nu_{2D} = 1$, we get a very good scaling plot, shown in figure 9. Of course, the critical value g_c at $T = T_{c6}$ is $\sim$0.92, that is, the g_c value for the isotropic 2D system.

4. Summary and discussions

To summarize, we have studied the FSS functions for anisotropic 3D Ising model by Monte Carlo simulations. The anisotropy parameter, a, dependence of the FSS functions on the Binder parameter and the magnetization distribution function has been investigated. We have shown that the magnetization distribution functions change from two-peak structures to single-peak ones as a increases or decreases from 1. This change of distribution functions may be attributed to the combination of up-spin percolating clusters and down-spin percolating clusters for anisotropic systems, which is the same as the case of 2D systems [18]. We should also note

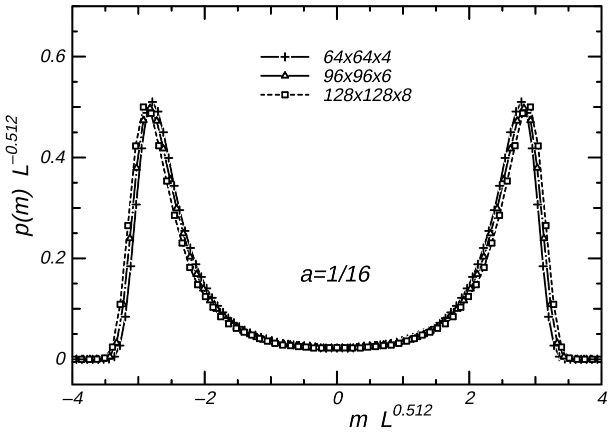

Figure 8. Scaling plot of $p(m)$ at $T = T_{cs}$ for fixed $a(=\frac{1}{16})$; $p(m)L^{-\beta/\nu}$ as a function of $mL^{\beta/\nu}$. The values of T_{cs} are $T_{c4} = 4.2364$, $T_{c6} = 4.3701$ and $T_{c8} = 4.4222$. We use the 3D exponents, $\beta = 0.320$ and $\nu = 0.625$.

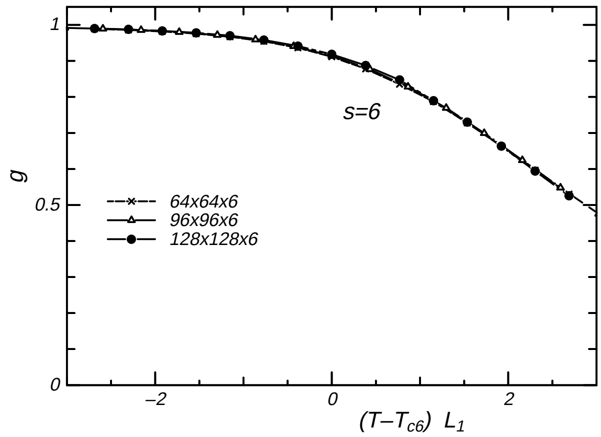

Figure 9. Scaling plot of g for fixed $s(= 6)$. The scaled variable is $(T - T_{c6})L_1^{1/\nu}$ and $T_{c6} = 4.3701$. We use the 2D exponent, $\nu = 1$.

that the distribution function $p(m)$ approaches the Gaussian distribution for large anisotropy, which is another indication of the multiple-percolation-cluster argument. In a future study, it would be interesting to calculate the probability for the appearance of n percolating clusters, W_n, for the anisotropic 3D Ising model and to make cluster analysis.

Moreover, we have considered the relation to the layered square-lattice Ising models for large 2D anisotropy. We have obtained 3D FSS behaviour near the critical temperature of the layered square-lattice Ising models, T_{cs}, for fixed a. In contrast, when we fix the number of layers, we have shown 2D FSS behaviour near T_{cs}. Thus, we have obtained a unified view of 3D and 2D FSS behaviour for the anisotropic 3D Ising models.

We have studied the shape effects of FSS functions for 3D Ising models. FSS functions also depend on boundary conditions. Extension of the 2D results for various boundary conditions, for example, tilted boundary conditions [10], to 3D systems will be interesting. This study is now in progress.

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References

[1] Fisher M E 1971 *Proc. E Fermi International School of Physics (Varenna, 1970)* vol 51, ed M S Green (New York: Academic) p 1
[2] Cardy J L (ed) 1988 *Finite-Size Scaling* (New York: North-Holland)
[3] Privman V and Fisher M E 1984 *Phys. Rev.* B **30** 322
[4] Hu C-K, Lin C-Y and Chen J-A 1995 *Phys. Rev. Lett.* **75** 193
Hu C-K, Lin C-Y and Chen J-A 1995 *Phys. Rev. Lett.* **75** 2786E
[5] Hu C-K and Lin C-Y 1996 *Phys. Rev. Lett.* **77** 8
[6] Lin C-Y, Hu C-K and Chen J-A 1998 *J. Phys. A: Math. Gen.* **31** L111
[7] Lin C-Y and Hu C-K 1998 *Phys. Rev.* E **58** 1521
[8] Okabe Y and Kikuchi M 1996 *Int. J. Mod. Phys.* C **7** 287
[9] Wang F-G and Hu C-K 1997 *Phys. Rev.* E **56** 2310
[10] Okabe Y, Kaneda K, Kikuchi M and Hu C-K 1999 *Phys. Rev.* E **59** 1585
[11] Aizenman M 1997 *Nucl. Phys.* B **485** 551
[12] Shchur L N and Kosyakov S S 1997 *Int. J. Mod. Phys.* C **8** 473
[13] Cardy J L 1998 *J. Phys. A: Math. Gen.* **31** L105
[14] Cooper N R, Halperin B I, Hu C-K and Ruzin I M 1997 *Phys. Rev.* B **55** 4551
[15] Binder K 1981 *Z. Phys.* B **43** 119
[16] Kamieniarz G and Blöte H W J 1993 *J. Phys. A: Math. Gen.* **26** 201
[17] Binder K and Wang J-S 1989 *J. Stat. Phys.* **55** 87
[18] Tomita Y, Okabe Y and Hu C-K 1999 *Phys. Rev.* E **60** 2716
[19] Cardy J L 1987 *Phase Transitions and Critical Phenomena* vol 11, ed C Domb and J L Lebowitz (New York: Academic) p 55
[20] Ferrenberg A M and Landau D P 1991 *Phys. Rev.* B **44** 5081
[21] Kasteleyn P W and Fortuin C M 1969 *J. Phys. Soc. Japan Suppl.* **26** 11
Fortuin C M and Kasteleyn P W 1972 *Physica* **57** 536
[22] Coniglio A and Klein W 1980 *J. Phys. A: Math. Gen.* **12** 2775
[23] Hu C-K 1984 *Phys. Rev.* B **29** 5103
1984 *Phys. Rev.* B **29** 5109
[24] Kitatani H, Ohta M and Ito N 1996 *J. Phys. Soc. Japan* **65** 4050