

## Universal finite-size scaling functions with exact nonuniversal metric factors

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Using exact partition functions and finite-size corrections for the Ising model on finite square, plane triangular, and honeycomb lattices and extending a method [J. Phys. **19**, L1215 (1986)] to subtract leading singular terms from the free energy, we obtain universal finite-size scaling functions for the specific heat, internal energy, and free energy of the Ising model on these lattices with exact nonuniversal metric factors.

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Finite-size scaling has been of interest to scientists working on a variety of critical systems, including superfluids, spin models, percolation models, lattice gauge models, spin glass, etc. [1–4]. Universal finite-size scaling and finite-size corrections in finite critical systems have attracted much attention in recent decades [2–9]. Using renormalization group arguments, in 1984 Privman and Fisher first proposed the concepts of universal finite-size scaling functions (UFSSF's) and nonuniversal metric factors [2]. Using Monte Carlo methods [10] and choosing aspect ratios of the square (SQ), plane triangular (PT), and honeycomb (HC) lattices so that these have the relative proportions  $1:\sqrt{3}/2:\sqrt{3}$  [11], Hu *et al.* and Okabe *et al.* found UFSSF's for the percolation and the Ising models on two-dimensional lattices [3,4]. Since these studies were based on numerical simulations, there is always some numerical uncertainty in the obtained results. Here, we use the exact partition functions of the Ising model on finite SQ, PT, and HC lattices with periodic-a-periodic boundary conditions [12,13] and an exact expansion method [8] to obtain exact finite-size corrections of the free energy  $f^B$ , the internal energy  $E^B$ , and the specific heat  $C^B$  of the critical Ising model on these lattices with periodic-periodic ( $pp$ ), periodic-antiperiodic ( $pa$ ), antiperiodic-periodic ( $ap$ ), and antiperiodic-antiperiodic ( $aa$ ) boundary conditions (BC's), where  $B$  denotes BC's. Using these coefficients and extend a method [14] to subtract leading singular term from the free energy, we subtract leading singular terms from  $C^B$ ,  $E^B$ , and  $f^B$  and find that the corresponding residuals  $\Delta^B$ ,  $\Gamma^B$ , and  $W^B$  [see Eqs. (7)–(9) below] have a very good finite-size scaling behavior. Choosing aspect ratios of the SQ, PT, and HC lattices so that these have the relative proportions  $1:\sqrt{3}/2:\sqrt{3}$  [11] and calculating exact nonuniversal metric factors from exact partition functions and finite-size corrections, we find that  $\Delta^B$ ,  $\Gamma^B$ , and  $W^B$  of the SQ, PT, and HC lattices have very nice universal finite-size scaling behavior.

The partition function of the Ising model is given by

$$Z = \sum_{\{\sigma\}} \exp \left[ \beta J \sum_{\langle ij \rangle} \sigma_i \sigma_j \right], \quad (1)$$

where  $J$  is the coupling constant,  $\beta = 1/(k_B T)$  with  $k_B$  being the Boltzmann constant and  $T$  being the absolute temperature,  $\sigma_i = \pm 1$  is the Ising spin at site  $i$ , the first sum is over all spin states and the second sum is over the nearest-neighbor pairs  $\langle i, j \rangle$  of the spins. The exact partition functions for  $L_1 \times L_2$  SQ, PT and HC lattices for various periodic-a-periodic BC's are [13]

$$Z^B = \frac{1}{2} 2^{L_1 L_2} [\cosh(\beta J)]^{z L_1 L_2 / 2} \sum_{i=1}^4 \varepsilon_i^B \Omega_i, \quad (2)$$

where  $z$  is the coordination number of the lattice and  $\varepsilon_i^B$  shown in Table I are sign factors specified by BC's, and  $\Omega_1 = \Omega_{(1/2)(1/2)}$ ,  $\Omega_2 = \Omega_{(1/2)0}$ ,  $\Omega_3 = \Omega_{0(1/2)}$ ,  $\Omega_4 = -\text{sgn}(\theta/\theta_c - 1)\Omega_{00}$ , with

$$\Omega_{\mu\nu} = \prod_{p=0}^{gL_1-1} \prod_{q=0}^{L_2-1} \left\{ A_0 - A_1 \left[ \cos \frac{2\pi(p+\mu)}{gL_1} + \cos \frac{2\pi(q+\nu)}{L_2} \right] - A_2 \cos \left( \frac{2\pi(p+\mu)}{gL_1} - \frac{2\pi(q+\nu)}{L_2} \right) \right\}^{1/2}. \quad (3)$$

Here  $g$ ,  $A_0$ ,  $A_1$ ,  $A_2$ , and the critical values of  $\beta J$ ,  $\beta_c J$ , are listed in Table II.

To calculate the specific heat, we write  $Z^B$  as

$$Z^B = \frac{1}{2} [2 \sinh(2\eta)]^{L_1 L_2 / 2} \sum_{i=1}^4 \varepsilon_i^B Z_i(\tau, R, L), \quad (4)$$

TABLE I. Sign factors  $\varepsilon_i^B$  in Eq. (2) for various BC's.

BC	$\varepsilon_1^B$	$\varepsilon_2^B$	$\varepsilon_3^B$	$\varepsilon_4^B$
$pp$	+	+	+	+
$pa$	+	+	-	-
$ap$	+	-	+	-
$aa$	-	+	+	-

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TABLE II. Expressions for  $g$ ,  $A_0$ ,  $A_1$ ,  $A_2$  in Eq. (3) and  $\beta_c J$  for various lattices,  $t = \tanh(\beta J)$ .

Lattice	$g$	$A_0$	$A_1$	$A_2$	$\beta_c J$
SQ	1	$(1+t^2)^2$	$2t(1-t^2)$	0	$\frac{1}{2}\ln(1+\sqrt{2})$
PT	1	$(1+t^2)^3+8t^3$	$2t(1-t^2)^2$	$2t(1-t^2)^2$	$\frac{1}{2}\ln\sqrt{3}$
HC	$\frac{1}{2}$	$1+3t^4$	$2t^2(1-t^2)$	$2t^2(1-t^2)$	$\frac{1}{2}\ln(2+\sqrt{3})$

where  $\eta = \beta J$ ,  $Z_i(\tau, R, L) = \Omega_i / (A_1/2)^{g L_1 L_2 / 2}$ ,  $\tau = D_2 L \epsilon$ ,  $D_2$  is a nonuniversal metric factor [15],  $L = (L_1 L_2)^{1/2}$ ,  $\epsilon = (T - T_c) / T_c$ , and  $R = L_1 / L_2$  is the aspect ratio. Then, the specific heat  $C^B / k_B \equiv (\eta^2 / L^2) (\partial^2 \ln Z^B / \partial \eta^2)$  near  $\tau = 0$  can be written as

$$\frac{C^B}{k_B} = \left[ C_{0,0} \ln L + C_0^B(R) + \frac{C_1^B(R)}{L} + O\left(\frac{1}{L^2}\right) \right] + \frac{1}{D_2} \left[ A_0^B(R) + \frac{A_{0,0}(R)}{L} \ln L + O\left(\frac{1}{L}\right) \right] \tau + O(\tau^2). \quad (5)$$

Here  $C_{0,0} = c_{0,0} \eta_c^2$ ,  $C_0^B(R) = \eta_c^2 [c_{0,1} - 2c_{0,0} f_1 - c_{0,2} R f_2^2 - \frac{1}{2} c_{0,0} \ln R]$ ,  $C_1^B(R) = -c_1 \sqrt{R} \eta_c^2 f_2$ ,  $A_{0,0}(R) = a_{0,0} \sqrt{R} \eta_c^3 - 2c_{0,0} \eta_c^2$ ,  $A_0^B(R) = -(a_0 \sqrt{R} \eta_c^3 / \pi) f_2 + a_1 f_1 - \frac{1}{3} a_1 f_3$ , where  $\eta_c = \beta_c J$ ,  $f_1 = (\epsilon_1^B |\theta_3| \ln |\theta_3| + \epsilon_3^B |\theta_4| \ln |\theta_4| + \epsilon_2^B |\theta_2| \ln |\theta_2|) / F$ ,  $f_2 = (\epsilon_4^B |\theta_2| |\theta_3| |\theta_4|) / F$ ,  $f_3 = \ln(4 |\theta_2| |\theta_3| |\theta_4|)$ ,  $F = (\epsilon_1^B |\theta_3| + \epsilon_3^B |\theta_4| + \epsilon_2^B |\theta_2|)$ , with  $\theta_i = \theta_i(0, q)$  the Elliptic  $\theta$  functions of modulus  $q$ , and  $c_{0,0}$ ,  $c_{0,1}$ ,  $c_{0,2}$ ,  $c_1$ ,  $a_{0,0}$ ,  $a_0$ ,  $a_1$ , and  $q$  are listed in Table III.

Based on Ref. [14], we write the free energy  $f^B \equiv (1/L^2) \ln Z^B$  near  $\epsilon = 0$  as

$$f^B \approx F_0^B + F_1^B \epsilon - \frac{1}{2} [C_0^B(R) + C_{0,0} \ln L] \epsilon^2 - (D_2 L)^{-2} W^B(\tau, R, L), \quad (6)$$

with scaling function  $W^B$ . Here  $F_0^B = f_{0,0} + f_{0,1} / L^2 + O(L^{-4})$  and  $F_1^B = \beta_c E_{0,0} + \beta_c E_{0,1} / L + O(L^{-2})$ , where  $f_{0,0} = 0.9296954 \dots$  for SQ,  $0.8795854 \dots$  for PT, and

 TABLE III. Expressions for  $c_{0,0}$ ,  $c_{0,1}$ ,  $c_{0,2}$ ,  $c_1$ ,  $a_{0,0}$ ,  $a_0$ ,  $a_1$ ,  $q$ , and  $E_{0,0}$ ;  $\gamma_E (= 0.5772156649 \dots)$  is the Euler constant.

Lattice	$c_{0,0}$	$c_{0,1}$	$c_{0,2}$	$c_1$	$a_{0,0}$	$a_0$	$a_1$	$q$	$E_{0,0}$
SQ	$\frac{8}{\pi}$	$\frac{8}{\pi} \left( \ln \frac{4\sqrt{2}}{\pi} + \gamma_E - \frac{\pi}{4} \right)$	4	$2\sqrt{2}$	$\frac{24\sqrt{2}}{\pi}$	16	6	$e^{-\pi R}$	$-\sqrt{2}$
PT	$\frac{12\sqrt{3}}{\pi}$	$\frac{12\sqrt{3}}{\pi} \left( \ln \frac{4\sqrt{3}}{\pi} + \gamma_E - \frac{\sqrt{3}\pi}{6} \right)$	9	6	$\frac{72\sqrt{3}}{\pi}$	54	$4\sqrt{3}$	$e^{-\pi(\sqrt{3}-i)R/2}$	-2
HC	$\frac{2\sqrt{3}}{\pi}$	$\frac{2\sqrt{3}}{\pi} \left( \ln \frac{4\sqrt{3}}{\pi} + \gamma_E - \frac{\sqrt{3}\pi}{9} \right)$	$\frac{3}{4}$	$\frac{1}{\sqrt{2}}$	$\frac{6\sqrt{2}}{\pi}$	$\frac{3\sqrt{3}}{4}$	$8\sqrt{3}$	$e^{-\pi(\sqrt{3}-i)R/4}$	$-\frac{2}{\sqrt{3}}$

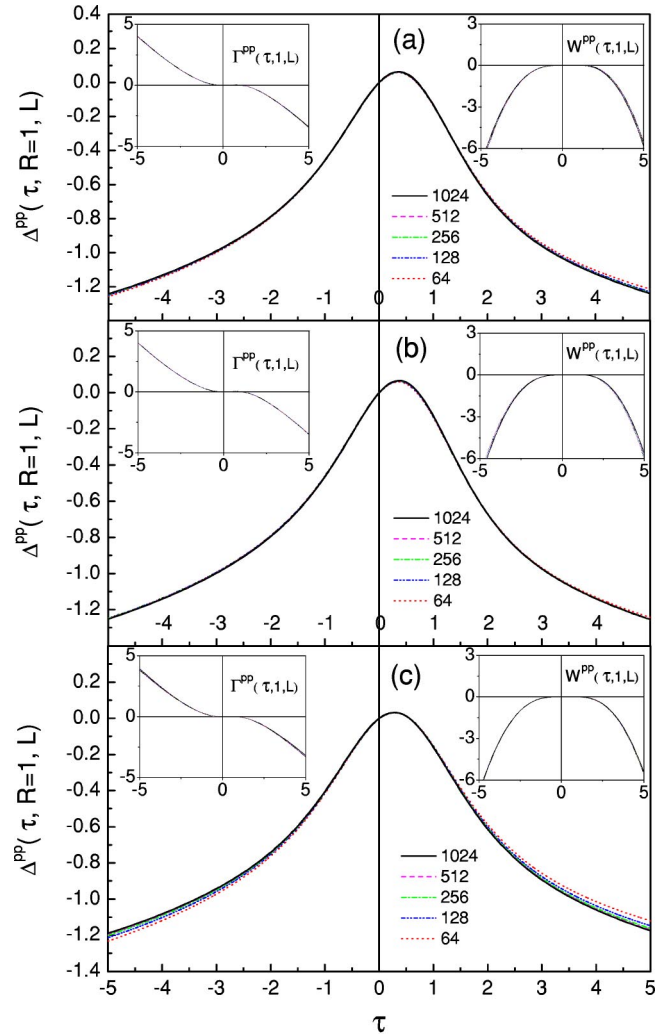


FIG. 1. The scaling functions  $\Delta^{pp}(\tau, R=1, L)$ ,  $\Gamma^{pp}(\tau, R=1, L)$ , and  $W^{pp}(\tau, R=1, L)$  as a function of  $\tau$  with  $D_2=1$  for (a) SQ, (b) PT, (c) HC lattices under periodic-periodic ( $pp$ ) BC's.  $\Gamma^{pp}$  and  $W^{pp}$  are shown as left and right insets, respectively.

$1.0250591 \dots$  for HC lattices,  $f_{0,1}^B = \ln F - \frac{1}{3} \ln f_3$ ,  $E_{0,0}$  for the SQ, PT, and HC lattices are listed in Table III, and  $E_{0,1}^B = -\sqrt{c_{0,2} R} f_2$ .

To study finite-size scaling, we define the scaling function for the specific heat,  $\Delta^B$ , as

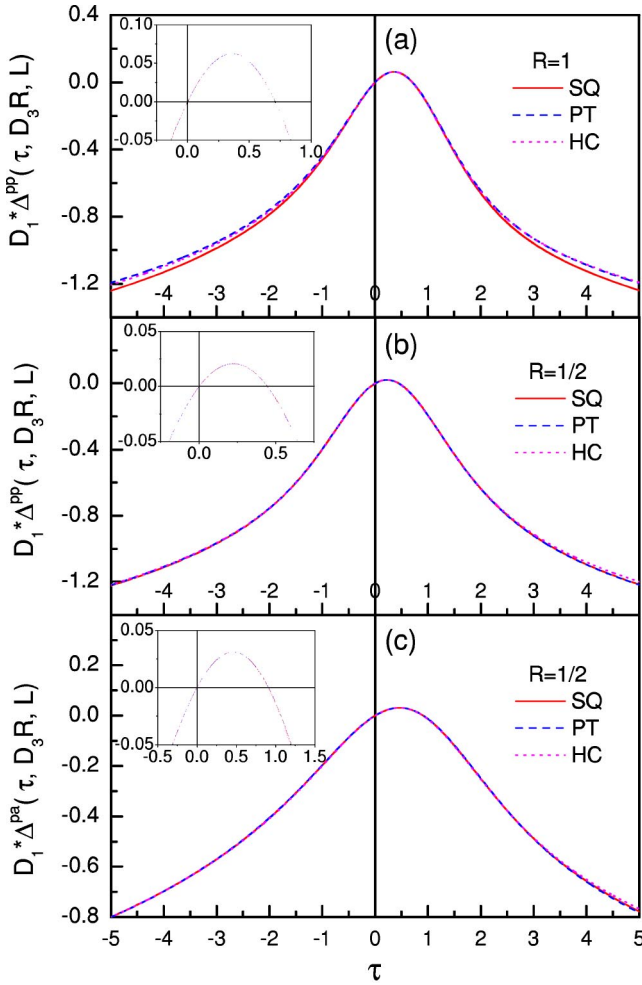


FIG. 2. The scaling function  $D_1 \Delta^B(\tau, D_3 R, L)$  as a function of  $\tau$  for SQ, PT, and HC lattices, and  $D_3$  is defined in the text. (a)  $R=1$ ,  $pp$  BC's,  $L_1=1024$ ,  $D_1^{PT}=0.957\dots$ , and  $D_1^{HC}=0.9896\dots$ , (b)  $R=1/2$ ,  $pp$  BC's,  $L_1=768$ ,  $D_1^{PT}=0.9898\dots$ , and  $D_1^{HC}=1.018\dots$ , and (c)  $R=1/2$ ,  $pa$  BC's,  $L_1=768$ ,  $D_1^{PT}=0.9997\dots$ , and  $D_1^{HC}=1.0167\dots$ . The insets show curves near  $\tau=0$  in more detail.

$$\begin{aligned} \Delta^B(\tau, R, L) &= \frac{\partial^2 W^B(\tau, R, L)}{\partial \tau^2} = \frac{c^B}{k_B} - [C_0^B(R) + C_{0,0} \ln L] \\ &= \frac{1}{D_2} \left[ A_0^B(R) + \frac{A_{0,0}(R)}{L} \ln L + O\left(\frac{1}{L}\right) \right] \tau + O(\tau^2) \\ &\quad + \frac{C_1^B(R)}{L} + O\left(\frac{1}{L^2}\right). \end{aligned} \quad (7)$$

According to the definition of internal energy  $E^B = -(1/L^2)(\partial \ln Z^B)/(\partial \eta)$ , we define the scaling function for the internal energy,  $\Gamma^B$ , as

$$\begin{aligned} \Gamma^B(\tau, R, L) &= \frac{\partial W^B(\tau, R, L)}{\partial \tau} = -D_2 L \beta_c \left\{ E^B - \left( E_{0,0} + \frac{E_{0,1}^B}{L} \right) \right. \\ &\quad \left. + \frac{1}{\beta_c} [C_0^B(R) + C_{0,0} \ln L] \epsilon \right\} \simeq \Delta^B \tau + O(\tau^2). \end{aligned} \quad (8)$$

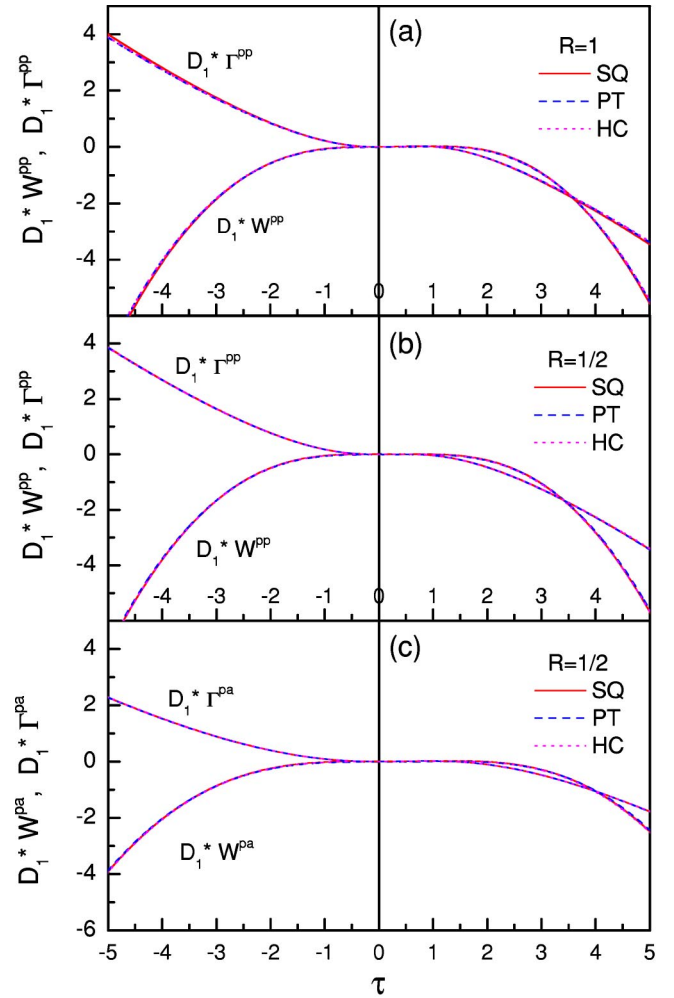


FIG. 3. The scaling functions  $D_1 W^B(\tau, D_3 R, L)$  and  $D_1 \Gamma^B(\tau, D_3 R, L)$  as a function of  $\tau$  for SQ, PT, and HC lattices. Boundary conditions and the values of  $R$ ,  $L_1$ ,  $D_1^{PT}$ , and  $D_1^{HC}$  for (a), (b), and (c), respectively, are the same as the corresponding parts in Fig. 2.

Similarly, the scaling function for the free energy,  $W^B$ , is

$$\begin{aligned} W^B(\tau, R, L) &= -(D_2 L)^2 \left\{ \frac{\beta_c}{\beta} \left[ f^B - \left( f_{0,0} + \frac{f_{0,1}^B}{L^2} \right) \right] \right. \\ &\quad \left. + \beta_c \left( E_{0,0} + \frac{E_{0,1}}{L} \right) \epsilon + \frac{1}{2} [C_0^B(R) + C_{0,0} \ln L] \epsilon^2 \right\} \\ &\simeq \frac{1}{2} \Delta^B \tau^2 + O(\tau^3). \end{aligned} \quad (9)$$

In the scaling function  $\Delta^B$ ,  $C_1^B(R)$  is the leading term in finite-size corrections. Thus, the finite-size effect for the  $pp$  boundary condition is the smallest in comparison with the  $pa$ ,  $ap$ , and  $aa$  BC's. The behaviors of  $\Delta^B(\tau, R=1, L)$ ,  $\Gamma^B(\tau, R=1, L)$ , and  $W^B(\tau, R=1, L)$  as a function of  $\tau$  with  $D_2=1$  for the SQ, PT, and HC lattices with  $pp$  BC's are shown in Figs. 1(a), 1(b) and 1(c), respectively, which show that these quantities have very nice finite-size scaling behavior.

To study the UFSSF's of  $\Delta^B(\tau, R, L)$ , we take aspect ratios of the SQ, PT, and HC lattices to have the relative proportions  $1: \sqrt{3}/2: \sqrt{3}$ . Equation (7) implies that for large lattices, the slope of  $\Delta^B$  as a function of  $\tau$  at  $\tau=0$  is determined by  $A_0^B$ . We can further multiply the scaling function by another nonuniversal metric factor  $D_1$  to obtain

$$D_1 \Delta^B(\tau, R, L) = \frac{D_1}{D_2} \left[ A_0^B(R) + \frac{A_{0,0}(R)}{L} \ln L + O\left(\frac{1}{L}\right) \right] \tau + O(\tau^2) + O\left(\frac{1}{L}\right). \quad (10)$$

We can take values of  $D_1/D_2$  so that the leading terms in the right-hand sides of Eq. (10) have the same slope for SQ, PT, and HC lattices. Accordingly, we take  $(D_1/D_2)_{\text{SQ}}=1$  for the SQ lattice,  $(D_1/D_2)_{\text{PT}}=A_{0,\text{SQ}}^B(R_{\text{SQ}})/A_{0,\text{PT}}^B(R_{\text{PT}})$  for the PT lattice, and  $(D_1/D_2)_{\text{HC}}=A_{0,\text{SQ}}^B(R_{\text{SQ}})/A_{0,\text{HC}}^B(R_{\text{HC}})$  for the HC lattice. To explore the behaviors of the amplitude  $A_0^B$  as a function of  $R$ , we consider  $A_0^B(D_3 R)$  with scale factors  $D_3 = 1, \sqrt{3}/2, \sqrt{3}$  for the SQ, PT, and HC lattices, respectively. The sign of the  $A_0^B(D_3 R)$ , in general, gives the information about the location ( $\tau_{\text{max}}$ ) of the maximum of the specific heat. When  $A_0^B(D_3 R)$  is positive,  $\tau_{\text{max}} > \tau_c = 0$ , and when  $A_0^B(D_3 R)$  is negative,  $\tau_{\text{max}} < \tau_c$ . For the *pp* and *pa* BC's, the behaviors of  $A_0^B(D_3 R)$  for the SQ, PT, and HC lattices are roughly in a similar feature in the region of  $0 < R \leq 1$ . However, for the *ap* and *aa* BC's, the curves of  $A_0^B(D_3 R)$  for the SQ lattice are quite different from those for PT and HC lattices.

To show examples of  $(D_1/D_2)$  and UFSSF's, we note that for  $R=1$ ,  $(D_1/D_2)_{\text{PT}}=0.9688 \dots (pp)$ ,  $1.0297 \dots (pa)$ , and  $(D_1/D_2)_{\text{HC}}=1.0332 \dots (pp)$ ,  $1.0981 \dots (pa)$ . For  $R=1/2$  and  $1/3$ , we have  $(D_1/D_2)_{\text{PT}}=0.9864 \dots (pp)$ ,  $0.9864 \dots (pa)$ , and  $(D_1/D_2)_{\text{HC}}=1.0520 \dots (pp)$ ,  $1.0520 \dots (pa)$ . We find that the values of  $D_1/D_2$  are roughly  $0.9864 \dots, 1.0520 \dots$  for the PT and HC lattices in the range  $0.05 \leq R \leq 0.75$  and the values are same for the *pp* and *pa* BC's. Using these values and calculating  $D_1$  based on exact specific heat for such finite lattices, we plot the  $D_1 \Delta^B(\tau, D_3 R, L)$  for the SQ, PT, and HC lattices in Figs. 2(a), 2(b), and 2(c), respectively, which show that the residual specific heats have very nice universal finite-size scaling behavior. Based on  $\Delta^B$ ,  $\Gamma^B$ , and  $W^B$  in Eqs. (7)–(9), we can further multiply the scaling functions of the internal energy and the free energy by the same  $D_1$ , and obtain UFSSF's for  $D_1 \Gamma^B(\tau, D_3 R, L)$  and  $D_1 W^B(\tau, D_3 R, L)$ , which are plotted in Figs. 3(a)–3(c). These figures also show very nice universal finite-size scaling behavior.

Although the results of this paper are based on analytic expressions for the physical quantities of the Ising model, our formulations can be extended to numerical or experimental studies of finite critical systems [16]. For example, the coefficients  $C_0^B(R)$  and  $C_{0,0}$  of Eq. (7) can be evaluated by using extrapolation techniques to analyze simulation or experimental data, then one can define the scaling function of the specific heat similar to that in Eq. (7). As a result, the UFSSF for the specific heat can be obtained.

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