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Finite-size scaling of the free energy levels in the Ising and Potts $q=3$ universality

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Abstract. The finite-size scaling of the free energy levels of Privman and Fisher is tested numerically on two-dimensional lattice strips in the Ising and $q=3$ Potts universality. The universal amplitudes and the free energy per site are obtained.

1. Introduction

Privman and Fisher (1984) have recently argued that the singular part of the free energy density of a system with size L (either hypercubical with $V=L^d$ or cylinder-shaped with $V=L^{d-1}\times\infty$) near the critical point $t=0$, $h=0$ ($t=(T-T_c)/T_c$), $h=H/k_BT$) and below the upper critical dimension $d_>$ may be written as

$$f^{(s)}(t,h,L)=-F^{(s)}/Vk_BT\approx L^{-d}Y(x_1,x_2)$$
$$x_1=C_1tL^{y_t}\qquad x_2=C_2hL^{y_h}\tag{1.1}$$

where $Y(x,y)$ is a universal function (for cubes and cylinders, respectively); y_t and y_h are the thermal and magnetic exponents such that $y_t=1/\nu$ and $y_h/y_t=\beta+\gamma=\Delta$. The non-universal metric factors C_1 and C_2 enter the scaled variables x_1 and x_2 but no further non-universal prefactor is needed.

On an $L^{d-1}\times\infty$ cylinder built up of $L^{d-1}\times l$ slices, the free energy density is given by

$$f_0(t,h,L)=(1/lL^{d-1})\ln\Lambda_0(t,h,L)\tag{1.2}$$

where Λ_0 is the largest eigenvalue of the transfer matrix. Free energy levels f_j may be defined through

$$f_j(t,h,L)=(1/lL^{d-1})\ln\Lambda_j(t,h,L)\tag{1.3}$$

where Λ_j is any one of the subdominant eigenvalues of the transfer matrix $\Lambda_0>\Lambda_1\geqslant\Lambda_2\geqslant\ldots$. At the critical point infinitely many of the eigenvalues $\Lambda_j(L)$ approach $\Lambda_0(L)$ when $L\to\infty$ and the corresponding correlation lengths

$$\xi_{\parallel j}(t,h,L)=l[\ln(\Lambda_0/\Lambda_j)]^{-1}\tag{1.4}$$

diverge. When $j=1$ $\xi_{\parallel j}$ is the spin-spin correlation length and when $j=2$, the energy-energy correlation length. A finite-size scaling relation for the correlation lengths may

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be written in analogy with (1.1)

$$\xi_{\parallel j}(t, h, L) \approx L S_j(x_1, x_2). \tag{1.5}$$

With the same scaled variables as in (1.1) $S_j(x, y)$ is a universal function. Privman and Fisher (1984) then speculate that (1.1) may be generalised for the singular part of the lowest free energy levels. Then, one may write

$$f_j^{(s)}(t, h, L) \approx L^{-d} Y_j(x_1, x_2) \tag{1.6}$$

with $Y_j(x, y)$ a universal function.

The singular part of the free energy densities $f_j(t, h, L)$ may be defined as

$$f_j^{(s)}(t, h, L) = f_j(t, h, L) - f_\infty(t, h) \tag{1.7}$$

where the analytic background $f_\infty(t, h)$ must be the same for all the levels in order to recover (1.5) from (1.3), (1.4) and (1.6). The scaling functions of the correlation lengths $S_j(x_1, x_2)$ are then given by

$$S_j(x_1, x_2) = [Y_0(x_1, x_2) - Y_j(x_1, x_2)]^{-1}. \tag{1.8}$$

The universal amplitude of the correlation length at the critical point $S_j(0, 0)$ which is related to the decay exponent η_j of the corresponding correlation function (Pichard and Sarma 1981, Luck 1982, Cardy 1984) has been extensively studied on two-dimensional models in recent years. Derrida and de Sèze (1982) confirm this relation for the percolation problem and mention unpublished results for the q-state Potts model when $j = 1$ (spin-spin correlations). Nightingale and Blöte (1983) have performed a numerical study on various two-dimensional models (eight-vertex, Potts and N-component cubic models) for $j = 1$ and $j = 2$, looking at the influence of anisotropy.

In the present work the finite-size scaling of the free energy levels at the critical point ($t = h = 0$) is studied numerically on two-dimensional systems which are believed to belong either to the Ising or to the Potts $q = 3$ universality. Although the eigenvalues of the transfer matrix of the spin-$\frac{1}{2}$ Ising model are known on two-dimensional lattices in the principal directions (Domb 1960) allowing an exact evaluation of the universal amplitudes (see for example Derrida and de Sèze (1982) for the square lattice and Privman and Fisher (1984) for the honeycomb lattice in the case of the correlation length amplitude) we have made a numerical study of the square and triangular spin-$\frac{1}{2}$ Ising models in order to test the extrapolation procedure which is used to extract the free energy levels' universal amplitudes. The numerical results are presented in § 2 and discussed in § 3.

2. Numerical results

We have studied the universal properties of the free energy levels by looking either at the lattice universality (i.e. the same model on different lattices) or at the model universality (different models which are believed to belong to the same class of universality). Results are presented for the spin-$\frac{1}{2}$ Ising model on the square and triangular lattices, the spin-1 Ising model on the square lattice and the hard square lattice gas in the Ising universality and for the $q = 3$ Potts model on the square and triangular lattices and the hard hexagon lattice gas in the $q = 3$ Potts universality.

The first three free energy levels at the critical point of the infinite system are obtained for strips with size $L \times \infty$ and periodic boundary conditions through the diagonalisation of the row-to-row transfer matrix sketched in figure 1 for the different lattices. According to (1.6) and (1.7), at the critical point, the free energy levels scale with L as

$$f_j(L) = A_j L^{-2} + B \tag{2.1}$$

where $A_j = Y_j(0, 0)$ is a universal amplitude and $B = f_\infty(0, 0)$ gives the critical value of the free energy density in the infinite system. In order to compare the different lattices one has to use the same unit length u which has been chosen as

$$u = (\text{surface per site})^{1/2}. \tag{2.2}$$

$f_j(L)$ is then a free energy per site. Let N be the number of sites in the transverse direction on the strip (figure 1), then $L = \alpha N$ where α is a geometrical constant which takes the values $\alpha = \sqrt{2}$, $(2\sqrt{3})^{1/2}$, $(\sqrt{3}/2)^{1/2}$ for the transfer matrices (a), (b) and (c) respectively.

For the critical couplings (K_c, z_c, table 1) we have used the known exact values for the spin-$\frac{1}{2}$ Ising model (Syozi 1972), the $q = 3$ Potts model (Wu 1982) and the hard hexagon lattice gas (Baxter 1980). The approximate values for the spin-1 Ising model and the hard square lattice gas were taken from Adler and Enting (1984) and Baxter *et al* (1980).

The first three non-degenerate levels were calculated for strips with width $N = 2$–8 for the spin-$\frac{1}{2}$ Ising model and the hard square lattice gas, $N = 2$–5 for the spin-1 Ising model and the $q = 3$ Potts model and $N = 2$–10 for the first level of the hard hexagon lattice gas. In this case only even N values were used in order to satisfy the symmetry of the ground state.

The free energy per site at the critical point B and the universal amplitudes A_j were estimated by a two-point fit of equation (2.1) for pairs of successive strips $(N-1, N)$. These values are given in table 2. When possible they were extrapolated to infinite width by assuming power law corrections to scaling, through a three-point fit of $\ln(G(N-1, N) - G_\infty)$ against $\ln(N)$. In other cases we used a three-point fit of $G(N-1, N)$ against $1/N$; the extrapolated values obtained in this way are marked

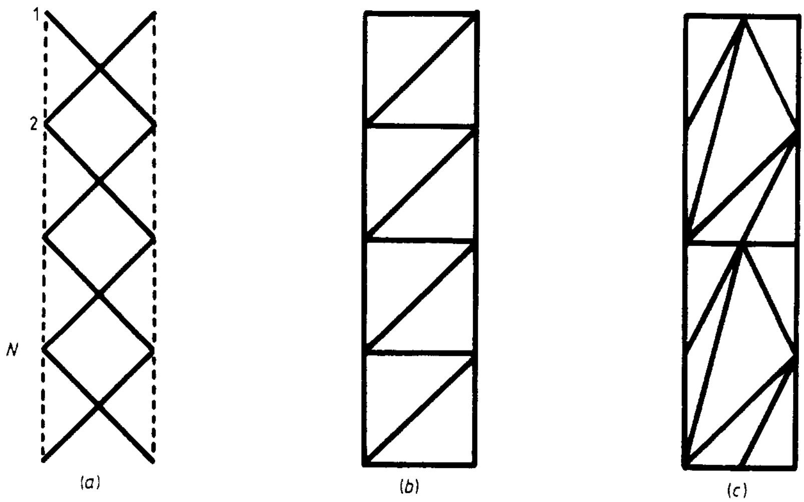

Figure 1. Transfer matrix for the square (a) and triangular (b) lattices and for the hard hexagon lattice gas (c).

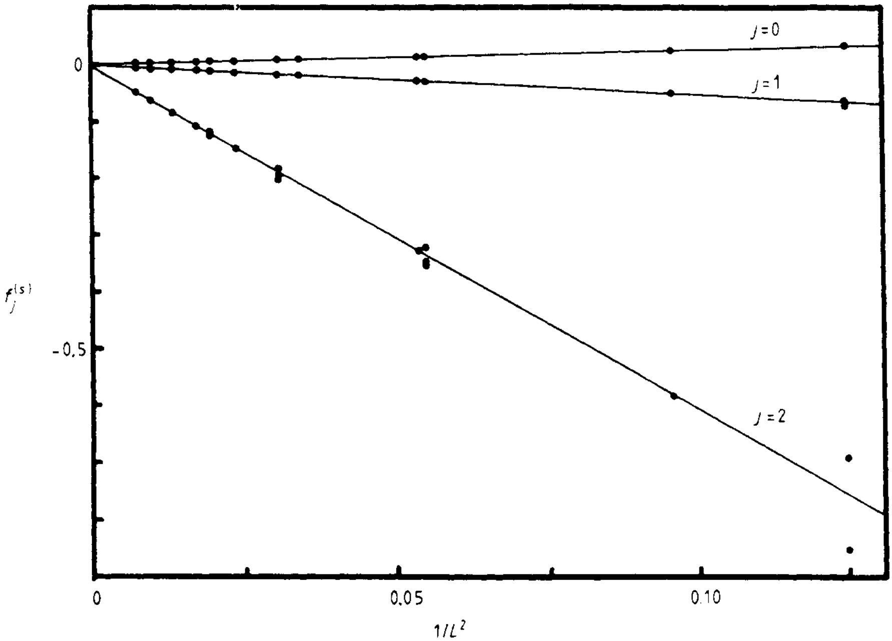

Figure 2. Scaling of the free energy levels with the strip width L in the Ising universality.

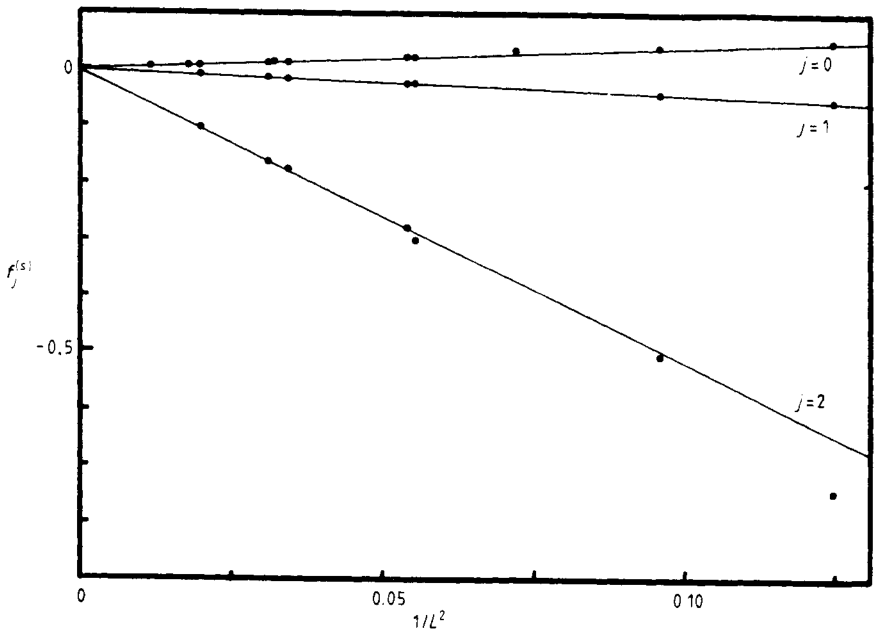

Figure 3. As in figure 2 for the $q = 3$ Potts universality.

Table 1. Models and lattices studied in this paper and their critical couplings. The last two lines give the correlation exponents estimated through finite-size scaling of the free energy levels.

Model	Ising $s=\frac{1}{2}$	Ising $s=\frac{1}{2}$	Ising $s=1$	Hard square
Lattice	Square	Triangular	Square	Square
Transfer matrix	(*a*)	(*b*)	(*a*)	(*a*)
K_c, z_c	$\frac{1}{2}\ln(1+\sqrt{2})$	$\frac{1}{4}\ln 3$	0.590 48	3.7962
η	0.2499	0.2500	0.2499	0.2500
η_{EE}	2.0028	2.0000	1.9974	2.0000
Model	Potts $q=3$	Potts $q=3$	Hard hexagon	
Lattice	Square	Triangular	Triangular	
Transfer matrix	(*a*)	(*b*)	(*c*)	
K_c, z_c	$\ln(1+\sqrt{3})$	$\ln(2\cos\pi/9)$	$\frac{1}{2}(11+5\sqrt{5})$	
η	0.2700	0.269	—	
η_{EE}	1.738	1.723	—	

by an asterisk. In figures 2 and 3 we have collected all the results obtained for the singular part of the free energy levels $f_j(L)-B$ as functions of L^{-2} in the Ising and $q=3$ Potts universality, respectively.

3. Discussion

According to (1.8) and (1.5), the universal amplitude of the correlation length $\xi_{\|j}$ is given by $(A_0-A_j)^{-1}$ at the critical point. An heuristic argument (Pichard and Sarma 1981; see also Luck 1982, Derrida and de Sèze 1982, Nightingale and Blöte 1983, Penson and Kolb 1984) and conformal covariance may be used to show (Cardy 1984) that this amplitude is related to the decay exponent η_j of the corresponding correlation function through

$$A_0-A_j=\pi\eta_j \tag{3.1}$$

where $j=1$ corresponds to the spin-spin correlations ($\eta_1=\eta=d+2-2y_h$) and $j=2$ to the energy-energy correlations ($\eta_2=\eta_{EE}=d+2-2y_t$) so that the knowledge of the first three energy levels is sufficient to obtain the thermal and magnetic exponents. The values obtained in this way are given in table 1. They are to be compared with the known exact values (see for example Wu 1982):

$$\eta=0.25 \qquad \eta_{EE}=2 \qquad \text{(Ising)} \tag{3.2}$$

$$\eta=\tfrac{4}{15}\simeq 0.2667 \qquad \eta_{EE}=1.6 \qquad (\text{Potts } q=3). \tag{3.3}$$

The agreement is excellent in the Ising universality but wider strips would be necessary to improve the Potts results.

The $1/L$ expansion of the free energy per site has been given by Ferdinand and Fisher (1969) for the spin-$\frac{1}{2}$ Ising model on the square lattice with periodic boundary conditions and reads

$$f_0(L)=(2G/\pi)+\tfrac{1}{2}\ln 2+(\pi/12)L^{-2}+O(L^{-4}\ln^3(L)) \tag{3.4}$$

where $G=(1/1^2)-(1/3^2)+(1/5^2)-\ldots\simeq 0.915\,965\,594$, which is Catalan's constant. It

Table 2. Universal amplitudes A_j of the free energy levels and free energy per site B_j deduced from the eigenvalues Λ_j of the transfer matrix on strips with width N and periodic boundary conditions at the critical point.

Ising $s=\frac{1}{2}$ square

$N-1, N$	A_0	A_1	A_2	B_0	B_1	B_2
5, 6	0.256 993	−0.518 074	−6.207 061	0.929 734	0.929 651	0.931 232
6, 7	0.258 325	−0.519 611	−6.152 230	0.929 716	0.929 672	0.930 470
7, 8	0.259 174	−0.520 587	−6.118 707	0.929 707	0.929 682	0.930 128
Extrap	0.2617	−0.5235	−6.0304	0.929 70	0.929 70	0.929 71

Ising $s=\frac{1}{2}$ triangular

$N-1, N$	A_0	A_1	A_2	B_0	B_1	B_2
5, 6	0.262 184	−0.523 996	−6.026 930	0.879 578	0.879 593	0.879 689
6, 7	0.261 988	−0.523 793	−6.024 183	0.879 583	0.879 588	0.879 623
7, 8	0.261 904	−0.523 706	−6.022 948	0.879 584	0.879 586	0.879 601
Extrap	0.2618	−0.5236	−6.0215	0.879 59*	0.879 58*	0.879 59

Ising $s=1$ square

$N-1, N$	A_0	A_1	A_2	B_0	B_1	B_2
2, 3	0.245 899	−0.496 469	−5.329 075	1.318 183	1.316 657	1.292 181
3, 4	0.253 197	−0.508 610	−5.659 414	1.317 778	1.317 332	1.310 533
4, 5	0.256 453	−0.514 106	−5.801 069	1.317 676	1.317 503	1.314 960
Extrap	0.2618	−0.5234	−6.0132	1.3176	1.3176	1.3175

Hard square lattice gas

$N-1, N$	A_0	A_1	A_2	B_0	B_1	B_2
5, 6	0.265 850	−0.535 305	−6.477 047	0.791 562	0.791 697	0.795 469
6, 7	0.264 548	−0.531 579	−6.333 859	0.791 580	0.791 645	0.793 480
7, 8	0.263 805	−0.529 413	−6.250 318	0.791 588	0.791 623	0.792 628
Extrap	0.2618	−0.5236	−6.0215	0.791 63	0.791 60	0.791 69

follows that the regular part of the free energy per site is

$$B \simeq 0.929\,695\,398. \tag{3.5}$$

Our numerical value (table 2) is in fairly good agreement with this result. Using (3.1) and (3.2) one may deduce the universal amplitudes

$$A_0 = \pi/12 \simeq 0.261\,799\,388 \tag{3.6}$$

$$A_1 = -\pi/6 \simeq -0.523\,598\,776 \tag{3.7}$$

$$A_2 = -\tfrac{23}{12}\pi \simeq -6.021\,385\,920 \tag{3.8}$$

which compare well with the extrapolated values of the Ising universality in table 2.

Table 2. (continued)

Potts $q = 3$ square

$N-1, N$	A_0	A_1	A_2	B_0	B_1	B_2
2, 3	0.387 276	−0.423 368	−6.400 178	2.071 340	2.069 952	2.126 508
3, 4	0.402 139	−0.427 653	−5.659 033	2.070 514	2.070 190	2.085 333
4, 5	0.408 635	−0.428 498	−5.376 275	2.070 311	2.070 216	2.076 497
Extrap	0.4188	−0.4289	−5.0406	2.0702	2.0707*	2.0721

Potts $q = 3$ triangular

$N-1, N$	A_0	A_1	A_2	B_0	B_1	B_2
2, 3	0.437 749	−0.454 720	−5.699 869	1.960 837	1.963 847	2.006 725
3, 4	0.426 405	−0.443 318	−5.395 145	1.961 929	1.962 750	1.977 403
4, 5	0.422 444	−0.437 944	−5.253 002	1.962 143	1.962 459	1.969 709
Extrap	0.4184	−0.4280	−4.9956	1.9623	1.9623	1.9647

Hard hexagon lattice gas

$N-2, N$	A_0	B_0
4, 6	0.496 045	0.838 168
6, 8	0.488 519	0.838 410
8, 10	0.466 804	0.838 801
Extrap	0.4300*	0.8397*

Since A_0 is not known in this case, the Potts results provide estimates for the universal amplitudes in the $q = 3$ Potts universality:

$$A_0 \simeq 0.4186 \pm 0.005 \tag{3.9}$$

$$A_1 \simeq -0.4285 \pm 0.005 \tag{3.10}$$

$$A_2 \simeq -5.0 \pm 0.4. \tag{3.11}$$

The hard hexagon results, which could not be correctly extrapolated, were not taken into account there.

Equations (3.9) and (3.10) lead to $A_m = A_0 - A_1 \simeq 0.847 \pm 0.01$, in good agreement with the estimate of Nightingale and Blöte (1983) $A_m = \simeq 0.843$, and with the conjectured exact result $A_m = 0.837\,76$.

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