Universal functions in finite-size scaling: a numerical study in the Ising and Potts q=3 universality class

1987 J. Phys. A: Math. Gen. 20 1819

(http://iopscience.iop.org/0305-4470/20/7/027)

J. Phys. A: Math. Gen. 20 (1987) 1819-1827. Printed in the UK

Universal functions in finite-size scaling: a numerical study in the Ising and Potts $q = 3$ universality class

Jean-Marc Debierre and Loïc Turban

Laboratoire de Physique du Solide†, Université de Nancy I, BP 239, F-54506 Vandoeuvre-lès-Nancy, France

Received 29 July 1986, in final form 3 October 1986

Abstract. The universality of the correlation length, order parameter and susceptibility amplitudes is studied in the vicinity of the critical point of two-dimensional models on strips with periodic boundary conditions for the Ising and Potts $q = 3$ universality class. The results confirm the Privman-Fisher conjecture.

1. Introduction

According to a recent conjecture (Privman and Fisher 1984), the free energy levels f_j on a cylinder-shaped system with size $V = L^{d-1} \times \infty$ near the critical point $t = 0$, $h = 0$ ($t = (T - T_c)/T_c$, $h = H/k_B T$) and below the upper critical dimension may be written as

$$f_j(t, h, L) = f_\infty(t, h) + L^{-d} Y_j(x_1, x_2)$$
$$x_1 = c_1 L^{y_t} t \qquad x_2 = c_2 L^{y_h} h \tag{1.1}$$

where f_∞, the analytic background, is the same for all the levels. $Y_j(x_1, x_2)$ is a universal function, y_t and y_h are the thermal and magnetic exponents and c_1, c_2 are non-universal metric factors in the scaled variables x_1 and x_2.

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

$$f_j(t, h, L) = \frac{1}{lL^{d-1}} \ln \Lambda_j(t, h, L) \tag{1.2}$$

where the Λ_j are the eigenvalues of the transfer matrix $\Lambda_0 > \Lambda_1 \geqslant \Lambda_2 \ldots$. The first free energy level ($j = 0$) gives the free energy density. At the critical point infinitely many of the eigenvalues $\Lambda_j(L)$ approach $\Lambda_0(L)$ when $L \to \infty$ so that the corresponding correlation lengths:

$$\xi_{\parallel j}(t, h, L) = l[\ln(\Lambda_0/\Lambda_j)]^{-1} \tag{1.3}$$

diverge.

Using equations (1.1)-(1.3) one gets

$$\xi_{\parallel j} = L[Y_0(x_1, x_2) - Y_j(x_1, x_2)]^{-1}$$
$$= LS_j(x_1, x_2) \tag{1.4}$$

with $S_j(x_1, x_2)$ a universal function of the scaled variables.

† Laboratoire associé au CNRS no 155.

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) has been extensively studied in two-dimensional models (Derrida and de Seze 1982, Nightingale and Blöte 1983) and one-dimensional quantum chains (Penson and Kolb 1984). The relation between S_j and η_j has been deduced from the conformal invariance at the critical point (Cardy 1984). The free energy amplitude at the critical point $Y_0(0,0)$ has been studied numerically in the Ising and Potts $q=3$ universality class (Turban and Debierre 1986a) and an analytic expression for the Potts universality class has been conjectured (Turban and Debierre 1986b) and derived from conformal invariance (Blöte *et al* 1986, Affleck 1986).

In the present paper the universality of the scaling functions on strips with periodic boundary conditions is tested numerically near the critical point of two-dimensional systems belonging to the Ising and Potts $q=3$ universality class. The numerical methods are presented in § 2 and the results are given and discussed in § 3.

2. Numerical methods

Let us consider two systems α and β belonging to the same universality class. Then the scaled variables

$$x_1 = c_{1\alpha} L_\alpha^{y_t} t_\alpha = c_{1\beta} L_\beta^{y_t} t_\beta \tag{2.1}$$

$$x_2 = c_{2\alpha} L_\alpha^{y_h} h_\alpha = c_{2\beta} L_\beta^{y_h} h_\beta \tag{2.2}$$

remain unknown due to the presence of the unknown prefactors c_1 and c_2. This difficulty may be overcome by choosing α as a reference system for this universality class and using the new scaled variables:

$$X_1 = \frac{x_1}{c_{1\alpha}} = L_\alpha^{y_t} t_\alpha = \frac{c_{1\beta}}{c_{1\alpha}} L_\beta^{y_t} t_\beta \tag{2.3}$$

$$X_2 = \frac{x_2}{c_{2\alpha}} = L_\alpha^{y_h} h_\alpha = \frac{c_{2\beta}}{c_{2\alpha}} L_\beta^{y_h} h_\beta. \tag{2.4}$$

The ratio $c_{1\beta}/c_{1\alpha}$ and $c_{2\beta}/c_{2\alpha}$ may be obtained as follows.

Taking derivatives of the spin–spin correlation length $\xi_\parallel = LS(x_1, x_2)$ at the critical point, one gets

$$\left.\frac{\partial \xi_{\parallel\alpha(\beta)}}{\partial x_1}\right|_c = L_{\alpha(\beta)} \left.\frac{\partial S}{\partial x_1}\right|_c = \frac{1}{c_{1\alpha(\beta)} L_{\alpha(\beta)}^{y_t}} \left.\frac{\partial \xi_{\parallel\alpha(\beta)}}{\partial t_{\alpha(\beta)}}\right|_c \tag{2.5}$$

and making use of the universality of $(\partial S/\partial x_1)_c$ one gets the ratio

$$\frac{c_{1\beta}}{c_{1\alpha}} = \left(\frac{L_\alpha}{L_\beta}\right)^{y_t+1} \left.\frac{\partial \xi_{\parallel\beta}/\partial t_\beta}{\partial \xi_{\parallel\alpha}/\partial t_\alpha}\right|_c \tag{2.6}$$

and, in the same way,

$$\frac{c_{2\beta}}{c_{2\alpha}} = \left(\frac{L_\alpha}{L_\beta}\right)^{y_h+1} \left.\frac{\partial \xi_{\parallel\beta}/\partial h_\beta}{\partial \xi_{\parallel\alpha}/\partial h_\alpha}\right|_c. \tag{2.7}$$

In the Ising universality class $\partial\xi_\parallel/\partial h$ vanishes and the ratio $c_{2\beta}/c_{2\alpha}$ may be deduced in the same way from the behaviour of $\partial^2\xi_\parallel/\partial h^2$.

Using the new variables and α as a reference, one gets the universal function

$$s(X_1, X_2) = S(x_1, x_2) = \xi_{\parallel\beta}/L_\beta \tag{2.8}$$

for the correlation length. The singular part of the free energy density is

$$f_{0\beta}^{(s)}(t_\beta, h_\beta, L_\beta) = L_\beta^{-d} Y_0(x_1, x_2) = L_\beta^{-d} y_0(X_1, X_2). \tag{2.9}$$

Since the analytic background $f_\infty(t_\beta, h_\beta)$ cannot contribute to the singular behaviour of field derivatives, one may obtain a universal expression for the order parameter:

$$\begin{aligned} m(X_1, X_2) &= \frac{\partial y_0}{\partial X_2} = L_\beta^d \frac{\partial f_{0\beta}}{\partial X_2} = L_\beta^d \frac{\partial f_{0\beta}}{\partial h_\beta}\frac{\partial h_\beta}{\partial X_2} \\ &= \frac{c_{2\alpha}}{c_{2\beta}} L_\beta^{d-y_h} \frac{\partial f_{0\beta}}{\partial h_\beta} \end{aligned} \tag{2.10}$$

and the susceptibility

$$\begin{aligned} \chi(X_1, X_2) &= \frac{\partial m}{\partial X_2} = \frac{\partial m}{\partial h_\beta}\frac{\partial h_\beta}{\partial X_2} = \frac{c_{2\alpha}}{c_{2\beta}} L_\beta^{-y_h} \frac{\partial m}{\partial h_\beta} \\ &= \left(\frac{c_{2\alpha}}{c_{2\beta}}\right)^2 L_\beta^{d-2y_h} \frac{\partial^2 f_{0\beta}}{\partial h_\beta^2}. \end{aligned} \tag{2.11}$$

The universality of $s(X_1, X_2)$, $m(X_1, X_2)$ and $\chi(X_1, X_2)$ has been studied numerically in the 2D Ising universality class, with $y_t = 1$ and $y_h = \frac{15}{8}$, on the following systems:
(i) $S = \frac{1}{2}$ Ising model on the square lattice,
(ii) $S = 1$ Ising model on the square lattice,
(iii) hard square lattice gas.
The reference system is then the spin-$\frac{1}{2}$ Ising model.

In the 2D Potts $q = 3$ universality class, with $y_t = \frac{6}{5}$ and $y_h = \frac{28}{15}$, we have studied the three-state Potts model on the square lattice, which is taken as a reference, and the hard hexagon lattice gas.

The transfer matrix (figure 1) is always taken in the diagonal direction on the square lattice in order to achieve a better convergence with strip width.

The critical points of the different models are given in table 1. We have used the known exact results for the $S = \frac{1}{2}$ Ising model (Kramers and Wannier 1941), the

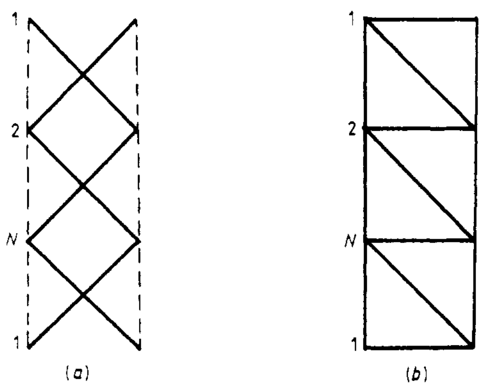

Figure 1. Transfer matrix for (a) the square lattice and (b) the triangular lattice for strip width $N = 3$.

Table 1. Models and lattices considered in this paper and their critical couplings.

Model	Ising $S=\frac{1}{2}$	Ising $S=1$	Hard squares	Potts $q=3$	Hard hexagons
Lattice	Square	Square	Square	Square	Triangular
K_c, z_c	$\frac{1}{2}\ln(1+\surd 2)$	0.590 48	3.7962	$\ln(1+\surd 3)$	$\frac{1}{2}(11+5\surd 5)$

Table 2. Extrapolated values of the ratio $c_{1\beta}/c_{1\alpha}$ and $c_{2\beta}/c_{2\alpha}$ deduced from data on strips of increasing width in the Ising universality class. The Ising $S=\frac{1}{2}$ model on the square lattice is the reference.

Model	Ising $S=\frac{1}{2}$	Ising $S=1$	Hard squares
$c_{1\beta}/c_{1\alpha}$	1	0.912 62	0.125 07
$c_{2\beta}/c_{2\alpha}$	1	0.902 80	0.445 95

three-state Potts model (Wu 1982) and the hard hexagon lattice gas (Baxter 1980). The approximate values for the $S=1$ Ising model and the hard square lattice gas were taken from Adler and Enting (1984) and Baxter *et al* (1980).

The unit length used to measure l and L is such that the surface per site is the surface unit. In the calculations we use the more convenient definition $t=K-K_c$ $(K=J/k_BT)$ for the temperature variable and the field h is chosen in such a way that the order parameter is equal to one (zero) when the system is completely ordered (disordered). For the hard square lattice gas the variables t and h are chosen as

$$\begin{aligned} &z_1=z_2=z_c\exp(t) && (h=0) \\ &z_1=z_c\exp(h) \qquad z_2=z_c\exp(-h) && (t=0) \end{aligned} \tag{2.12}$$

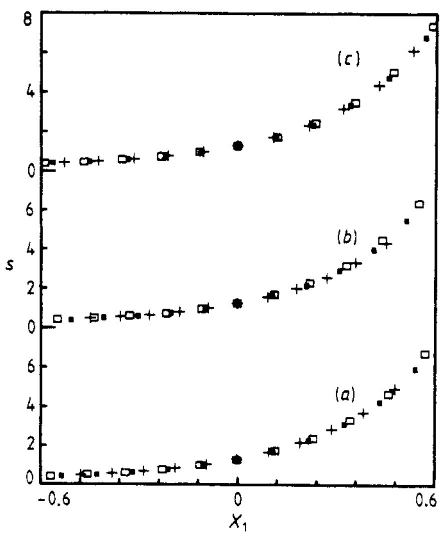

Figure 2. The universal correlation length function $s(X_1)$ for different strip widths: (a) the Ising $S=\frac{1}{2}$ model, (b) the hard squares model and (c) the Ising $S=1$ model. For (a), (b) +, $N=4$; ■, $N=6$; □, $N=8$. For (c) +, $N=3$; ■, $N=4$; □, $N=5$.

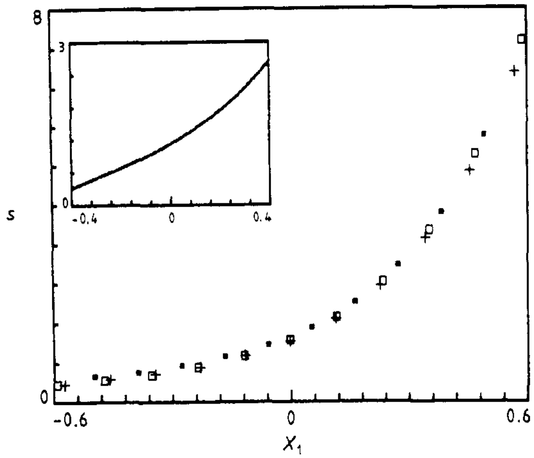

Figure 3. $s(X_1)$ for the wider strips in the Ising universality class: (+) Ising $S=\frac{1}{2}$ ($N=8$), (■) hard squares ($N=8$), (□) Ising $s=1$ ($N=5$). The curve for the 1D Ising model is given in the insert for comparison.

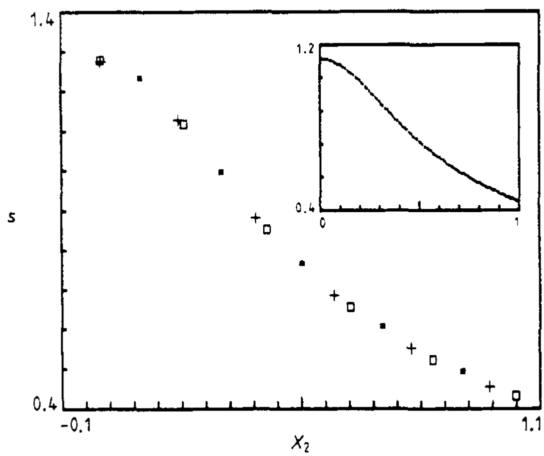

Figure 4. As in figure 3 for $s(X_2)$.

and for the hard hexagon lattice gas

$$\begin{aligned} &z_1 = z_2 = z_3 = z_c \exp(t) && (h=0) \\ &z_1 = z_c \exp(h) \qquad z_2 = z_3 = z_c \exp(-h/2) && (t=0) \end{aligned} \tag{2.13}$$

where z_i is the fugacity on the ith sublattice and z_c is the critical fugacity.

3. Numerical results and discussion

Table 2 gives the ratio $c_{1\beta}/c_{1\alpha}$ and $c_{2\beta}/c_{2\alpha}$ extrapolated for the Ising universality class from results on strips with increasing width and table 3 gives the Potts $q=3$ results.

The correlation length results $s(X_1)$ are presented in figure 2 for the three models in the Ising universality class for different lattice widths. The results obtained for the

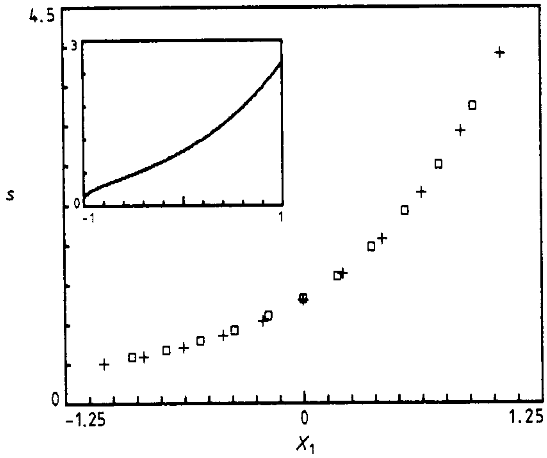

Figure 5. $s(X_1)$ in the Potts $q=3$ universality class: (+) Potts $q=3$ ($N=5$), (□) hard hexagons ($N=12$). The same curve for the 1D Potts $q=3$ model is shown in the insert.

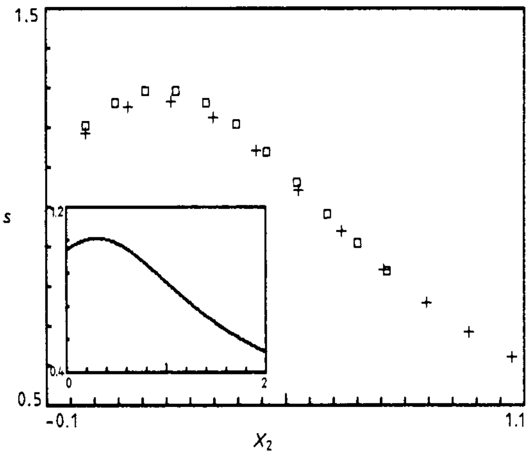

Figure 6. $s(X_2)$ in the Potts $q=3$ universality class.

three models on the wider strips are reproduced in figure 3. The correlation length of the 1D Ising model is given in the insert.

Figure 4 gives $s(X_2)$ on the wider strips in the Ising universality class. $s(X_1)$ and $s(X_2)$ for the Potts $q=3$ universality class are shown in figures 5 and 6.

Similar curves for the order parameter $m(X_2)$ are given in figure 7 for the Ising universality class and in figure 8 for the Potts $q=3$ universality class ($m(X_1, 0)$ vanishes on a strip).

The susceptibility results are presented in figures 9-12.

Although we limited ourselves to small widths, especially for the $S=1$ Ising and the three-state Potts models, the Privman-Fisher conjecture is confirmed by our numerical results. These results were tested for the Ising $S=\frac{1}{2}$ model on the square lattice for which the exact values of Λ_0 and Λ_1 are known at any temperature(Onsager 1944). Using these values we computed the function $s(X_1)$ for strips of width up to 10 000 and verified that it is exactly superimposable on the curve of figure 3.

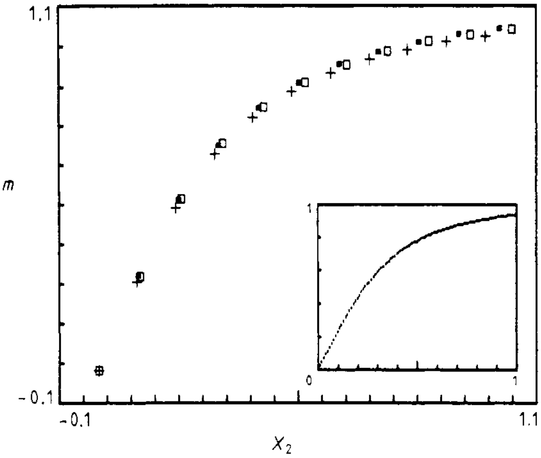

Figure 7. $m(X_2)$ in the Ising universality class.

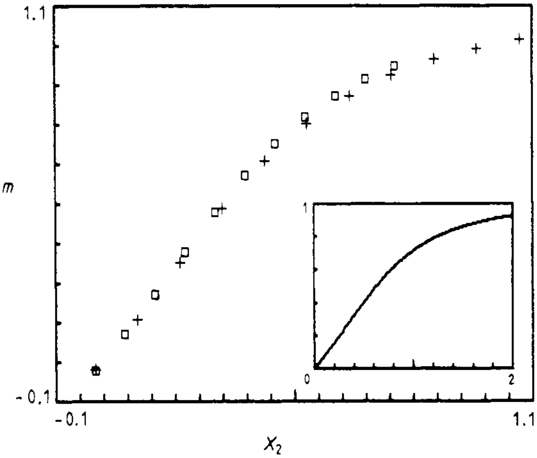

Figure 8. $m(x_2)$ in the Potts $q = 3$ universality class.

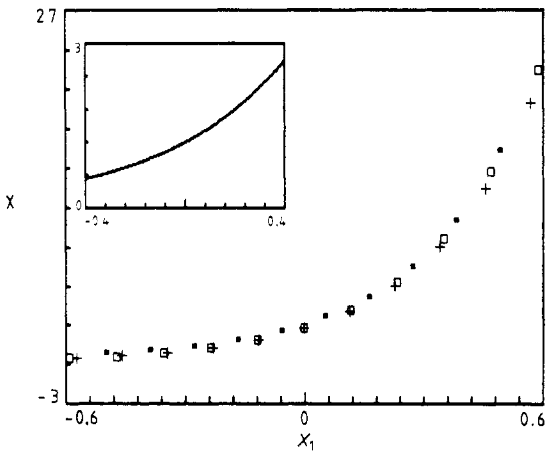

Figure 9. $\chi(X_1)$ in the Ising universality class.

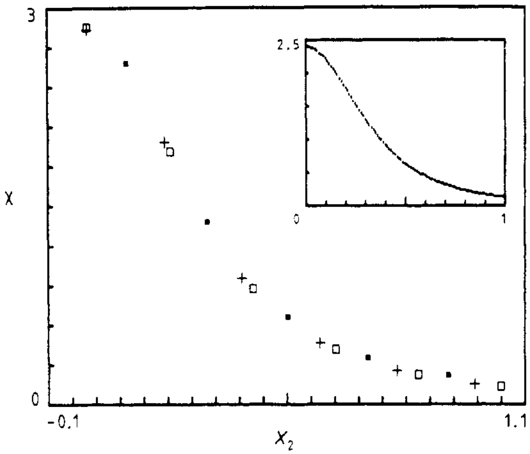

Figure 10. $\chi(X_2)$ in the Ising universality class.

Table 3. As in table 2 for the Potts $q=3$ universality class. The reference is the three-state Potts model on the square lattice.

Model	Potts $q=3$	Hard hexagons
$c_{1\beta}/c_{1\alpha}$	1	0.165 19
$c_{2\beta}/c_{2\alpha}$	1	0.338 34

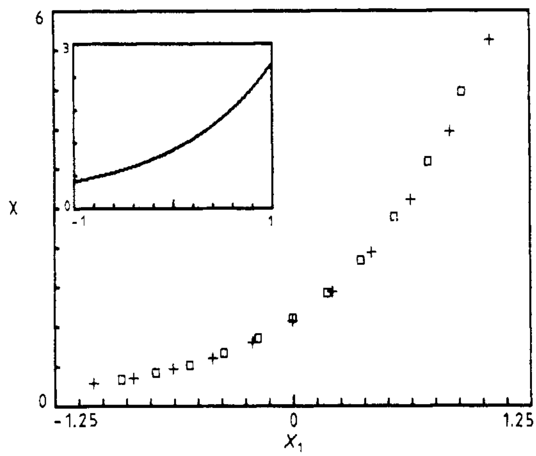

Figure 11. $\chi(X_1)$ in the Potts $q=3$ universality class.

Finally we observe that the universal functions behave like their one-dimensional counterparts, a result which is not unexpected, since in a single step change of the length scale by a factor $b=L$, a strip of width L is transformed into a linear chain.

Note added. In a recent work Burkhardt and Guim (1986) have deduced the exact form of the universal scaling functions of the spin-spin and energy-energy correlation lengths of the spin-$\frac{1}{2}$ Ising model for different types of boundary conditions from the correspondence between the two-dimensional Ising model and the one-dimensional quantum Ising model in a transverse field.

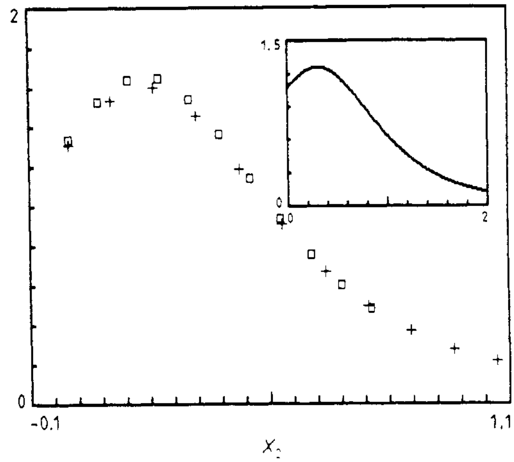

Figure 12. $\chi(X_2)$ in the Potts $q = 3$ universality class.

References

Adler J and Enting I G 1984 *J. Phys. A: Math. Gen.* **17** 2233
Affleck I 1986 *Phys. Rev. Lett.* **56** 746
Baxter R J 1980 *J. Phys. A: Math. Gen.* **13** L61
Baxter R J, Enting I G and Tsang S K 1980 *J. Stat. Phys.* **22** 465
Blöte H W J, Cardy J C and Nightingale M P 1986 *Phys. Rev. Lett.* **56** 742
Burkhardt T W and Guim I 1986 *Universal scaling form of the correlation length in Ising strips. Preprint* Temple University
Cardy J C 1984 *J. Phys. A: Math. Gen.* **17** L385
Derrida B and de Seze J 1982 *J. Physique* **43** 475
Kramers H A and Wannier G H 1941 *Phys. Rev.* **60** 252
Luck J M 1982 *J. Phys. A: Math. Gen.* **15** L169
Nightingale M P and Blöte H W 1983 *J. Phys. A: Math. Gen.* **16** L657
Onsager L 1944 *Phys. Rev.* **65** 117
Penson K A and Kolb M 1984 *Phys. Rev.* B **29** 2854
Pichard J L and Sarma G 1981 *J. Phys. C: Solid State Phys.* **14** L617
Privman V and Fisher M E 1984 *Phys. Rev.* B **30** 322
Turban L and Debierre J M 1986a *J. Phys. A: Math. Gen.* **19** 1033
—— 1986b *J. Phys. A: Math. Gen.* **19** L411
Wu F Y 1982 *Rev. Mod. Phys.* **54** 235