Liverpool Preprint: LTH 355

Critical Behaviour of the Two Dimensional Step Model

A.C. Irving and R. Kenna[1]

DAMTP, University of Liverpool L69 3BX, England

August 1995

Abstract

We use finite–size scaling of Lee–Yang partition function zeroes to study the critical behaviour of the two dimensional step or sgn $O(2)$ model. We present evidence that, like the closely related XY–model, this has a phase transition from a disordered high temperature phase to a low temperature massless phase where the model remains critical. The critical parameters (including logarithmic corrections) are compatible with those of the XY–model indicating that both models belong to the same universality class.

[1]Supported by EU Human Capital and Mobility Scheme Project No. CHBI–CT94–1125

1 Introduction

In a recent paper [1], we demonstrated the power of finite–size scaling applied to Lee–Yang zeroes [2] in uncovering logarithmic corrections to scaling in the two–dimensional XY– or $O(2)$ spin model. In this paper we apply the same techniques to the closely related 'step model' [3, 4], also known [5, 6] as the sgn $O(2)$ model. The question of criticality of this model has, until now, been unresolved despite several analyses based on high temperature series (see [6] for a review) and on numerical simulation [7, 8]. The interest in the model arises from its possible membership of the XY–model universality class which exhibits the Kosterlitz–Thouless [KT] phase transition [9]. Like the XY–model, the step model has a configuration space which is globally and continuously symmetric. Unlike the XY–model, however, the interaction function is discontinuous and the Mermin–Wagner theorem [10] does not apply. Nonetheless, it is expected that if a phase transition exists in the step model, it should not be to a phase with long range order [4, 8, 11].

Sánchez–Velasco and Wills [8] presented evidence of critical behaviour starting at $\beta_c = 1/T_c = 0.91 \pm 0.04$. This was based on finite–size scaling [FSS] of the spin susceptibility. Since the associated critical index $\eta(T_c)$ was significantly greater than that measured for the XY–model, it was concluded that the step and XY models are not in the same universality class. In this paper we present evidence that the step model is *not* critical at that temperature. However it *is* critical at lower temperatures with a critical index $\eta(T_c)$ compatible with the XY value. The accuracy afforded by the Lee–Yang zeroes study is a crucial part of the analysis.

2 The step model and the XY–model

Consider the partition function

$$Z(\beta, h) = \sum_{\{\vec{s}_x\}} e^{-\beta H + h\hat{n}\cdot\vec{M}} , \tag{1}$$

where the Boltzmann factor is $\beta = 1/kT$, $\hat{n}$ is a unit vector defining the direction of the external magnetic field and h is a scalar parameter representing its strength. The summation is over all configurations open to the system and $\vec{s}_x$ is a unit length two-component spin at each site x in the cubic lattice $\Lambda \equiv L^d$ ($d = 2$). The magnetisation for a given configuration is

$$\vec{M} = \sum_{x\in\Lambda} \vec{s}_x .$$

In the case of the XY–model, the interaction hamiltonian is

$$H_{XY} = -\sum_{x\in\Lambda}\sum_{\mu=1}^{d} \vec{s}_x \cdot \vec{s}_{x+\mu} ,$$

while for the step model it is

$$H_{\rm step} = -\sum_{x\in\Lambda}\sum_{\mu=1}^{d} {\rm sgn}(\vec{s}_x \cdot \vec{s}_{x+\mu}) .$$

Thus the continuous (cosine) dependence of the interaction energy in the usual XY–model is replaced by a discrete step function dependence.

The leading infinite volume critical behaviour of the 2D XY–model is characterized by exponential divergences (essential singularities) in the thermodynamic functions [9]. In terms of the reduced temperature $t \equiv 1 - \beta/\beta_c \to 0^+$ the (leading) infinite volume scaling behaviour of the correlation length and the zero-field magnetic susceptibility is (respectively) [9]

$$\xi_\infty(t) \sim e^{at^{-\nu}}, \tag{2}$$

$$\chi_\infty(t) \sim \xi_\infty^{2-\eta}, \tag{3}$$

where $\nu = 1/2$ and $\eta = 1/4$. The XY–model remains critical for all $\beta > \beta_c$.

In [1] we showed that for the 2D XY–model this behaviour and the corresponding behaviour of the Yang–Lee edge, $z_{\rm YL}$, is in fact modified by logarithmic corrections:

$$\chi_\infty(t) \sim \xi_\infty^{2-\eta} t^r, \tag{4}$$

$$z_{\rm YL}(t) \sim \xi_\infty^{\lambda} t^p, \tag{5}$$

where

$$\lambda = -\frac{1}{2}(d + 2 - \eta) = -\frac{15}{8} \tag{6}$$

and the parameters r and p $(= -r/2)$ are logarithmic correction indices [1]. The corresponding FSS behaviour for the susceptibility and the first zero z_1 $(= z_{YL})$ at $t = 0$ is [1]

$$\chi_L(0) \sim L^{2-\eta}(\ln L)^{-\frac{r}{\nu}}, \tag{7}$$

$$z_1(0) \sim L^{\lambda}(\ln L)^{r}. \tag{8}$$

For the 2D XY–model the numerical value of r was found to be small but non-zero (-0.023 ± 0.010) [1].

The objects of the present analaysis were to establish

1. if the scaling behaviour of the very precisely determined Yang–Lee edge would unequivocably determine whether the step model had a critical phase
2. if so, whether the phase transition is in the same universality class as the XY–model.

3 Method and results

The methods used are those described in [1]. A single cluster algorithm [12] is used to generate a large number of measurements (100K for each lattice size L and temperature $1/\beta$) of the energy H and the magnetisation $\vec{M}$ at zero external magnetic field. Such data were obtained for lattice sizes $L = 32$, 48, 64, 128 and 256 covering the β range 0.86 to 1.40 with varying degrees of spacing. Multi–histogram techniques [13, 14] were used to combine data at different values of β and so obtain detailed β dependence. In the neighborhood of possible critical points we used sufficiently fine spacing (typically 0.025) to ensure adequate overlap between histograms for a given size of lattice.

The partition function for a complex magnetic field ($h = h_r + ih_i$, $h_r, h_i \in \mathbb{R}$) can be written in terms of a real and an imaginary part [1, 15, 16] as

$$Z(\beta, h_r + ih_i) = \mathrm{Re}Z(\beta, h_r + ih_i) + i\mathrm{Im}Z(\beta, h_r + ih_i)\,, \tag{9}$$

where

$$\mathrm{Re}Z(\beta, h_r + ih_i) = Z(\beta, h_r)\langle\cos(h_i M)\rangle_{\beta,h_r}\,, \tag{10}$$

$$\mathrm{Im}Z(\beta, h_r + ih_i) = Z(\beta, h_r)\langle\sin(h_i M)\rangle_{\beta,h_r}\,. \tag{11}$$

Here the subscripts indicate that the expectation values are taken at (inverse) temperature β and in a (real) external field h_r. If the Lee–Yang theorem [2] holds for this model then the zeroes are on the imaginary h–axis where $\mathrm{Im}Z$ vanishes. Then the Lee–Yang zeroes are simply the zeroes in h_i of

$$\mathrm{Re}Z(\beta, ih_i) \propto \langle\cos(h_i M)\rangle_{\beta,0}\,. \tag{12}$$

Thus the zeroes are easily found and at no stage is a simulation involving a complex action involved.

The analysis began with a rough search for the leading critical behaviour predicted by (8). An independent test was also made using the (less accurate) susceptibility data and (7). Both methods indicated critical behaviour setting in for $\beta \gtrsim 1.2$. In Fig. 1 we show a typical log–log plot of z_1 the Yang–Lee edge versus L. This is at a typical candidate value of the critical temperature ($\beta = 1.22$). The errors are considerably smaller than the symbols. For example, at $\beta = 1.22$ we found $z_1 = 0.0024136(7)$ and $0.00017902(6)$ at $L = 32$ and 128 respectively. The slope of Fig. 1 gives the effective leading index λ_{eff} ignoring corrections. At $\beta = 1.22$ this is $\lambda_{\mathrm{eff}} = -1.8761(2)$ where the chi-squared per degree of freedom (χ^2/dof) for the linear fit shown is 0.85. In Fig. 2(a) we display the result of such fits as a function of β. The effective exponent λ_{eff} is just the slope of the log–log linear fit which should obtain if critical behaviour is present (ignoring logarithmic corrections). The corresponding χ^2/dof for the linear fit is also shown. Acceptable values are only found for β in excess of around 1.2. To quantify this statement we demand

$$\chi^2/\mathrm{dof} \leq 2.0 \tag{13}$$

which means $\beta_c \gtrsim 1.185$. We note that the corresponding values of λ_{eff} ($\lesssim -1.872(2)$) include that ($-15/8 = -1.875$) corresponding to the KT prediction.

The evidence for critical behaviour is the existence of a range of acceptable chi-squared values for a linear fit. In view of the similarity of λ_{eff} to the expected KT value, we now proceed to test the further hypothesis that the step model is in fact in the same universality class as the XY–model. We *assume* the behaviour (8) with a particular value of λ (given by (6)). This should be valid at $\beta = \beta_c$. The expected leading behaviour is removed and linear fits to

$$\ln\left(z_1 L^{15/8}\right) \quad \mathrm{vs.} \quad \ln\ln L \tag{14}$$

performed. The results are shown in Fig. 3. Since the value $\lambda = -15/8$ ($\eta = 1/4$) is only expected at β_c these results can be used to identify the possible values of critical temperature and to test for the presence of logarithmic corrections as in the XY–model [1].

Applying the same criterion (13) as for the leading behaviour, we search for a range of β_c values giving an acceptable fit. We find

$$1.195 \leq \beta_c \leq 1.295 \quad \text{and correspondingly,} \quad 0.009 \geq r \geq -0.034\,. \tag{15}$$

The range of acceptable r values includes that found [1] for the XY–model (-0.023 ± 0.010) and that corresponding to no logarithmic corrections ($r = 0$). As in our previous work [1], this range excludes the prediction $r = -1/16$ coming from an approximate renormalisation group treatment of the XY–model [9]. Thus we conclude that the present data are compatible with the step model being in the same universality class as the XY–model. We do not, however, exclude other possibilities.

The susceptibility data are consistent with the above analysis. If one assumes the KT value of $\eta(\beta_c) = 1/4$, one can construct a so-called Roomany–Wyld beta function approximant [17] from the finite–size data and use its zero to locate β_c [1]. These approximants, based on pairs of lattice size L, L', converge very rapidly [17]. We estimate $\beta_c = 1.22 \pm 0.02$. This last analysis of course neglects possible logarithmic corrections to scaling.

We have also studied the specific heat. As for the XY–model, the step model data show a broad peak with no obvious relationship to the position of the leading critical point. The finite–size dependence is not dramatic and is likely to be of little value in further elucidating the criticial behaviour. A related question is to what extent one can make use of the Fisher zeroes [15, 18], i.e. zeroes of the partition function in the complex β plane at zero external magnetic field h. For both this and the XY–model, these are much harder to locate than the Lee–Yang zeroes and are consequently less accurately determined.

4 Conclusions

The use of finite–size scaling applied to Lee–Yang zeroes has allowed us to present detailed evidence of critical behaviour in the two-dimensional step (sgn $O(2)$ spin) model. The data are consistent with this model being in the same universality class as the XY– ($O(2)$ spin) model. That is, it undergoes a Kosterlitz–Thouless type transition with susceptibility index $\eta(\beta_c) = 1/4$ and we determine that β_c lies in the range $1.195 \leq \beta_c \leq 1.295$. With the available statistics, we found the logarithmic correction exponent to lie in the range $-0.034 \leq r \leq 0.009$. This should be compared with our measurement for the XY correction exponent [1], $-0.033 \leq r \leq -0.013$ with which it is compatable. The step model results are however also compatable with no logarithmic corrections ($r = 0$ corresponds to $\beta_c = 1.21$ and $\chi^2/\text{dof} = 0.92$).

The Mermin–Wagner theorem [10] does not apply directly to the step model because of the discontinuous nature of the interaction hamiltonian. However, it has long been believed [4, 8] that if a phase transition does exist, it will not involve a phase with long range order. The evidence presented here supports this view.

This raises a question as to the nature of the mechanism driving the phase transition in the step model. The KT phase transition of the XY–model is understood to be driven by the binding/unbinding of topological solutions (vortices). However, the energetics of vortex formation are very different in the step model [11, 6, 8]. Since vortices with effectively zero excitation energy can be created at all non-zero temperatures, the usual KT argument does not naturally lead one to expect such a phase transition in the step model.

If this is indeed the case, some other driving mechanism must be responsible for any phase transition. It would then be remarkable if — as the evidence presented here indicates – both models belong to the one universality class.

References

[1] R. Kenna and A. C. Irving, Phys. Lett. B **351**, 273 (1995).

[2] C. N. Yang and T. D. Lee, Phys. Rev. **87** 404 (1952); ibid. 410.

[3] A. J. Guttmann, G. S. Joyce and C. J. Thompson, Phys. Lett. A **38**, 297 (1972).

[4] A. J. Guttmann and G. S. Joyce, J. Phys. C **6**, 2691 (1973).

[5] I-H. Lee and R. E. Shrock, Phys. Rev. B **36**, 3712 (1987).

[6] I-H. Lee and R. E. Shrock, J. Phys. A **21**, 2111 (1988).

[7] A. Nymeyer and A. C. Irving, J. Phys. A **19**, 1745 (1986).

[8] E. Sánchez-Velasco and P. Wills, Phys. Rev. B **37**, 406 (1988).

[9] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973); J. M. Kosterlitz J. Phys. C **7**, 1046 (1974).

[10] N.D. Mermin and H. Wagner, Phys. Rev. Lett. **17** 1133 (1966).

[11] A. J. Guttmann and A. Nymeyer, J. Phys. A **11** 1131 (1978).

[12] U. Wolff, Phys. Rev. Lett. **62** 361 (1989).

[13] A.M. Ferrenberg and R.H. Swendsen, Phys. Rev. Lett. **61** 2635 (1988); Computers in Physics, Sep/Oct 1989.

[14] K. Kajantie, L. Kärkkäinen and K. Rummukainen Nucl. Phys. B **357** 693 (1991).

[15] R. Kenna and C. B. Lang, Phys. Lett. B **264** 396 (1991); Nucl. Phys. B (Proc. Suppl.) **30** 697 (1993); Nucl. Phys. B **393** 461 (1993); Err. ibid. B **411** (1994) 340.

[16] R. Kenna and C. B. Lang, Phys. Rev. E **49** 5012 (1994).

[17] M.P. Nightingale, Physica A **83** (1976) 561; H. Roomany and H.W. Wyld, Phys. Rev. D **21** (1980) 3341.

[18] M.E. Fisher, in Critical Phenomena, Proc. 51th Enrico Fermi Summer School, Varena, ed. M.S. Green (Academic Press, NY, 1972).

Figure 1: Scaling behaviour of the Yang–Lee edge at a typical critical β value ($\beta = 1.22$).

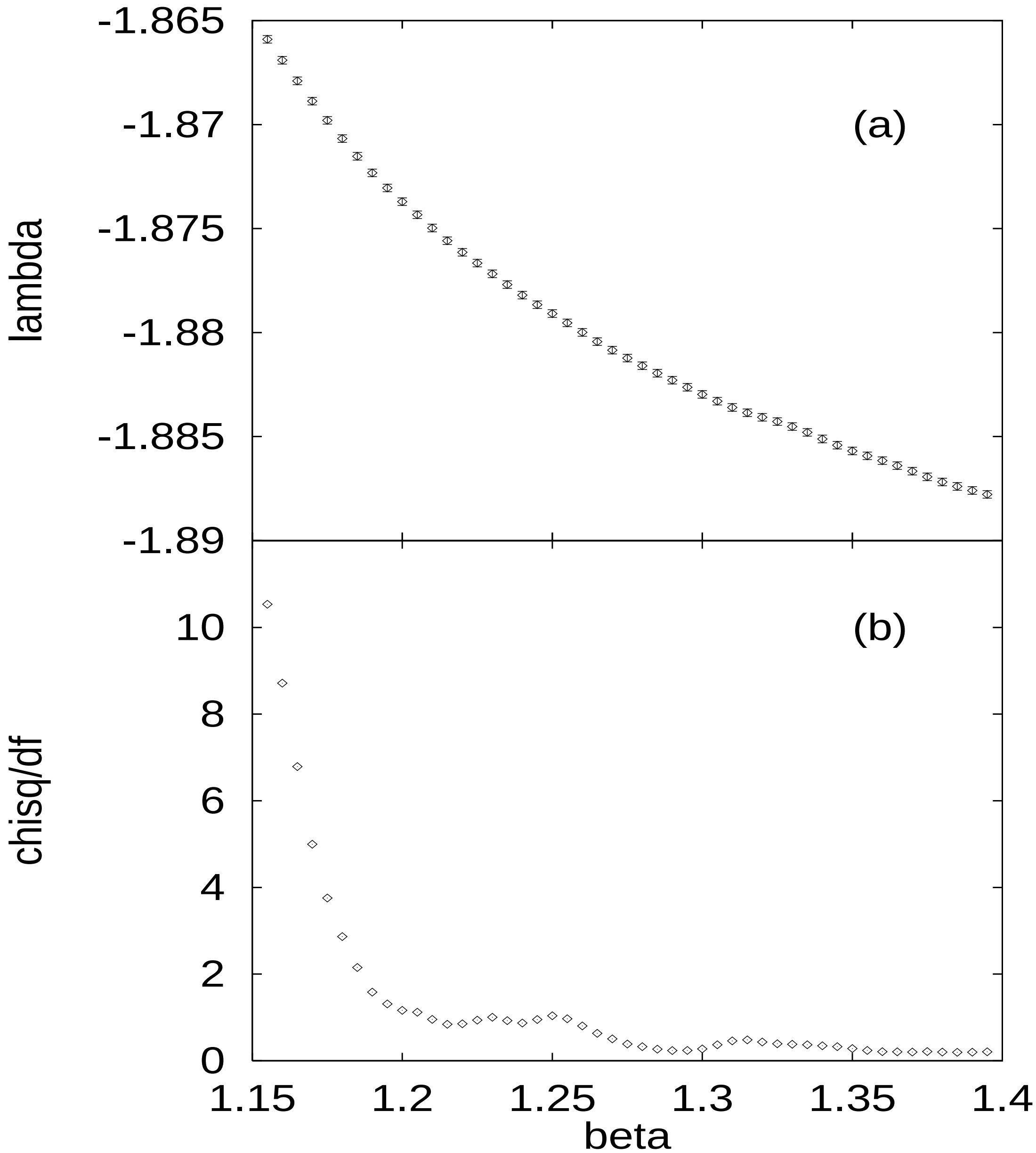

Figure 2: Test of expected leading critical behaviour: (a) the effective exponent λ_{eff} (slope of a straight line fit) and (b) the corresponding χ^2/dof versus β.

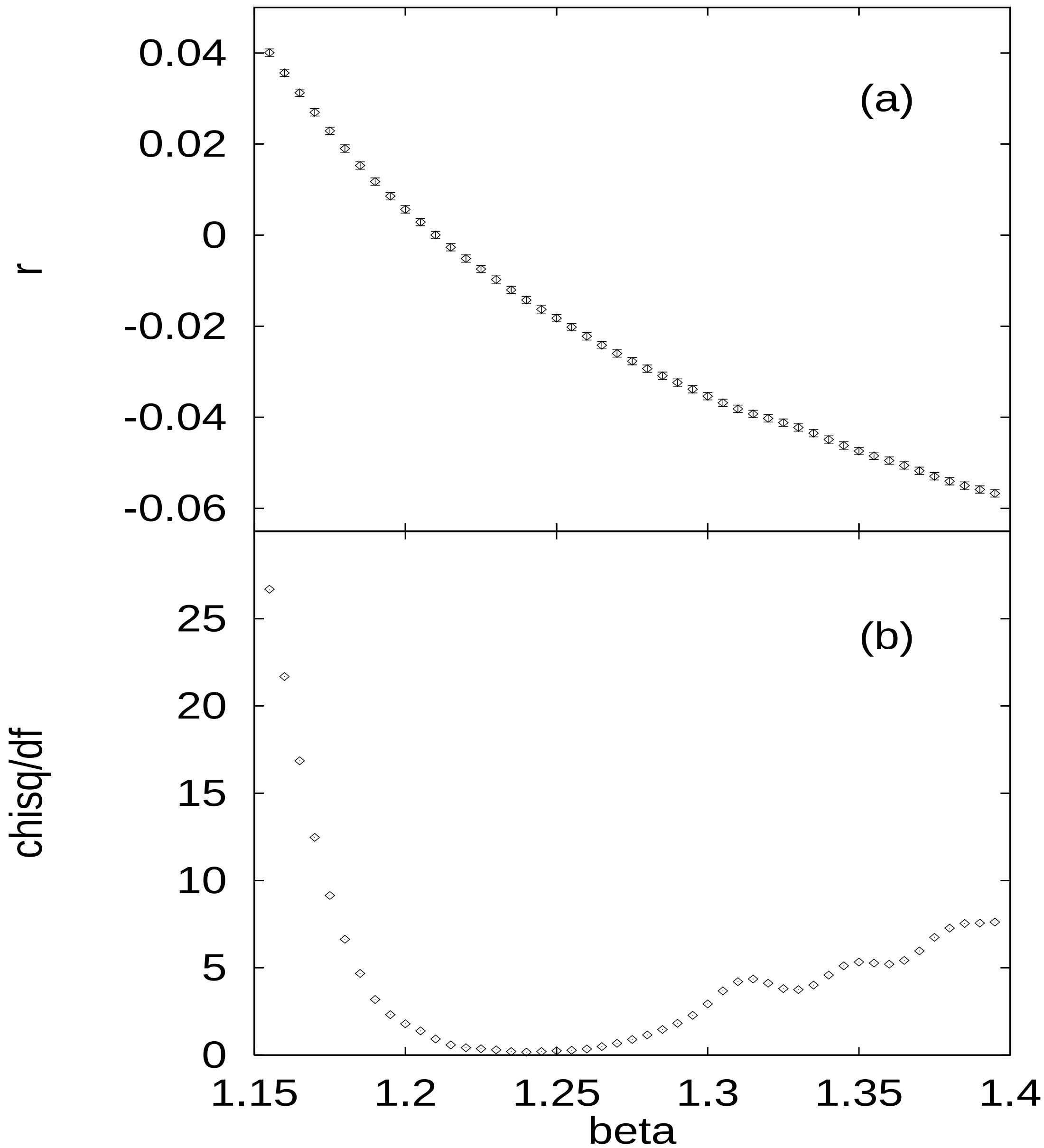

Figure 3: Logarithmic corrections: (a) the logarithmic correction exponent r to the Yang–Lee edge is shown as a function of the assumed critical coupling β_c and (b) the corresponding χ^2/dof.