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1978 J. Phys. A: Math. Gen. 11 545

(http://iopscience.iop.org/0305-4470/11/3/014)

J. Phys. A: Math. Gen., Vol. 11, No. 3, 1978. Printed in Great Britain. © 1978

The critical behaviour of two-dimensional isotropic spin systems

A J Guttmann
Department of Mathematics, University of Newcastle, New South Wales, 2308, Australia

Received 4 April 1977, in final form 8 August 1977

Abstract. The high-temperature susceptibility and internal energy series have been re-examined for four two-dimensional isotropic spin models on a triangular lattice. They are the planar classical Heisenberg (PCH), infinite spin $X-Y$, classical Heisenberg and step models. For all four models we find evidence of a phase transition. This evidence is good for the first two models, and weak for the last two. A method of series analysis is developed which permits us to rule out, with some degree of confidence, an algebraic singularity for either the susceptibility or the specific heat for all four models. For the PCH model we find the susceptibility fits the form suggested by Kosterlitz, while for the $X-Y$ model susceptibility a similar conclusion may be drawn, with a lesser degree of confidence.

1. Introduction

The nature of the critical point (if it exists) of two-dimensional planar models has recently been the subject of several experimental and theoretical attacks. Mermin and Wagner (1966) have proved that two-dimensional systems with finite-range interactions and with suitably symmetric order parameter have no spontaneous magnetisation at non-zero temperatures. This theorem excludes a conventional type of phase transition for the two-dimensional Heisenberg model, with a spherically symmetric interaction. A conventional phase transition is also exluded for spin systems with planar symmetry, including the planar classical Heisenberg (PCH) model, and the $X-Y$ model. The step model introduced by Guttmann *et al* (1972) and discussed in some detail by Guttmann and Joyce (1973) is also a spin system with planar symmetry, but the Mermin and Wagner proof does not apply, as the interaction function has discontinuous first and higher derivatives. As far as can be judged by series analysis, the nature of the phase transition for this model is similar to that of the PCH model (Guttmann and Joyce 1973), a conclusion that also follows from the usual universality type arguments.

Analysis of high-temperature susceptibility series by conventional methods has consistently indicated the presence of a non-regular point for all these planar models at some positive temperature. Thus for the two-dimensional Heisenberg model, Brown and Luttinger (1955) and Rushbrooke and Wood (1958) observed that conventional ratio analysis suggested a critical temperature some two-thirds that of the simple cubic lattice. Similar results were subsequently obtained by Stanley and Kaplan (1966).

For the PCH model, Stanley (1968) and Moore (1969) find numerical evidence of a conventional algebraic singularity. For the $S=\frac{1}{2}$, $X-Y$ model, Betts *et al* (1971) found evidence of an algebraic singularity, but with a critical exponent of approximately 1·5. This is a surprising result, as the corresponding Ising model critical exponent is 1·75, and we would expect the exponent for the $X-Y$ model—if it has an algebraic singularity—to be greater than that of the Ising model.

Other theoretical analyses include Berezinskii (1971), Doniach (1973), who gave plausible arguments for the existence of a finite non-zero critical temperature for two-dimensional spin systems of finite spin-space dimensionality, and Zittartz (1976) who showed that the PCH model undergoes a continuous phase transition, though the nature of the susceptibility divergence was not determined. None of the numerical work is entirely convincing, in that the ratio plots seemed to possess unremovable curvature, so that the more series coefficients were available, the larger was the value of the critical exponent. (This observation has been made by several people, including the present author and Yamaji and Kondo (1973).) Standard Padé analysis also indicated a slightly increasing trend of exponent with number of series coefficients.

The interpretation of this effect is rather difficult, as it could either be a 'small n' effect or indicative of a more complex type of singularity than the simple power law divergence normally assumed.

Recently Kosterlitz and Thouless (1973) proposed a new definition of order for two-dimensional systems called topological order. Such order is based on the overall system properties, rather than the more normal feature, the rate of decay of interactions. The existence of vortices is shown to be temperature dependent, so that at low temperatures the system contains no vortices. At high temperatures however, when the entropy term dominates the free energy, vortices will appear spontaneously. The critical temperature is that at which a single vortex is likely to occur, and corresponds to the free energy changing sign. The Hamiltonian is split into two parts, one representing the vortices, the other representing spin waves. In the approximation used, these two contributions are independent. The phase transition is produced by the vortex configurations alone. Kosterlitz (1974) finds for the correlation length ξ that

$$\begin{aligned} &\xi \sim \exp[b(T/T_c - 1)^{-\frac{1}{2}}] && T > T_c \\ &\xi = \infty && T < T_c \end{aligned} \tag{1.1}$$

with $b > 0$ and approximately equal to 1·5 for the square lattice PCH model, and for the susceptibility

$$\begin{aligned} &\chi \sim \xi^{2-\eta} && T > T_c \\ &\chi = \infty && T < T_c \end{aligned} \tag{1.2}$$

where the exponent η has the same value ($\frac{1}{4}$) as for the two-dimensional Ising model.

Above T_c the free energy is found to behave like

$$A \sim \xi^{-2} + \text{analytic parts.} \tag{1.3}$$

Thus $\chi \sim A \ \exp[c(T/T_c - 1)^{-1/2}]$ for $T > T_c$, which corresponds to a more rapid divergence than any algebraic singularity and is an essential singularity. The non-regular part of the free energy, and all derivatives, vanish at T_c.

A related type of behaviour was suggested by Yamaji and Kondo (1973) on the basis of a Green function calculation.

Recently Camp and Van Dyke (1975) have studied the susceptibilities of the PCH, $X-Y$ and CH models in two dimensions, and found evidence to support the Kosterlitz and Thouless form for the $X-Y$ model, with weaker support for this form for the PCH and CH models. They also found that the ratio plots in many cases had unremovable curvature, as referred to above.

In this paper we show how series analysis can be used to clearly distinguish between the conventional power law divergence and the essential singularity predicted by Kosterlitz. The series used are given by Moore (1969) for the CH and PCH model, Camp and Van Dyke (1975) for the infinite spin $X-Y$ model and Guttmann and Joyce (1973) for the step model.

The method of series analysis is discussed in the next section, while in § 3 we analyse the susceptibility series and attempt to analyse the free energy series. Section 4 is devoted to a discussion and conclusion.

2. Method of analysis

The conventional power law singularity normally assumed for the susceptibility of lattice models is

$$\chi \sim C^{+}(1-K/K_c)^{-\gamma}, \qquad K \to K_c^{-} \tag{2.1}$$

where $K = J/kT$. One standard method of estimating the critical exponent γ and critical point K_c is by forming Padé approximants (PA) to the logarithmic derivative of χ. Thus

$$\frac{\mathrm{d}}{\mathrm{d}K}\ln\chi = \frac{\chi'}{\chi} \sim \frac{\gamma/K_c}{1-K/K_c} \tag{2.2}$$

which has a pole at $K = K_c$ and a residue at $K = K_c$ of $-\gamma$. Consider now the logarithmic derivative of the logarithmic derivative,

$$\frac{\mathrm{d}}{\mathrm{d}K}\ln\frac{\chi'}{\chi} \sim \frac{1}{K_c - K}. \tag{2.3}$$

This has a pole at $K = K_c$ and a residue at the pole of -1.

Turning to the form of susceptibility predicted by Kosterlitz we have

$$\begin{aligned}\chi &\sim A\{\exp[b(1-K/K_c)^{-\gamma}]\}^{2-\eta},\\ &= A\exp[c(1-K/K_c)^{-\gamma}]\end{aligned} \tag{2.4}$$

so that

$$\frac{\mathrm{d}}{\mathrm{d}K}\ln\chi = \frac{\chi'}{\chi} = \frac{\gamma c}{K_c}(1-K/K_c)^{-(\gamma+1)} \tag{2.5}$$

which has an algebraic singularity at $K = K_c$. Thus one might expect that the PA to the logarithmic derivative would show steadily increasing estimates of γ.

An analogous situation is to form the PA to a series with an algebraic singularity, rather than to the logarithmic derivative of the series. As an example, table 1 shows the poles and residues of PA to the high-temperature susceptibility series $\chi(v)$ of the spin-$\frac{1}{2}$ Ising model on a triangular lattice. This function is known to have an algebraic singularity at $v = v_c = \tanh(J/kT_c) = 2-\sqrt{3} \approx 0{\cdot}2679492$. From table 1 it appears that there is evidence of a singularity in the vicinity of $v = v_c = 0{\cdot}265$, but the residues are increasing, in agreement with the expected behaviour. From (2.5), if we form the

Table 1. Poles and residues of Padé approximants to the high-temperature susceptibility of the triangular lattice Ising model.

N	$[N/N-1]$	$[N/N]$	$[N/N+1]$
4		0·2547 (−0·946)	0·3675 (0·375)
5	0·2597 (−1·370)	0·2603 (−1·453)	0·2612 (−1·593)
6	0·2577 (−1·197)*	0·3393 (0·268)	0·2644 (−2·627)
7	0·2638 (−2·338)	0·2642 (−2·516)	0·2643 (−2·577)
8	0·2651 (−3·130)	0·2652 (−3·151)	

* In this and all subsequent tables, an asterisk denotes a defective approximant, with a spurious pole.

logarithmic derivative again, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}K}\ln\frac{\chi'}{\chi}=\frac{\gamma+1}{K_c-K} \tag{2.6}$$

which has a simple pole at $K=K_c$ with residue $-(\gamma+1)$. Thus forming the PA to $\ln \mathrm{div}^2(\chi)$ should enable us to distinguish between an algebraic and an essential singularity. For the former, the residue at the pole is -1, while for the latter it is $-\gamma-1$. Provided that we do not have an essential singularity with a value of γ close to zero, it should be possible to distinguish between the two types of singularity.

For example, the high-temperature susceptibility of the spin-$\frac{1}{2}$ Ising model $\chi(v)$ on a triangular lattice is known to have an algebraic singularity at $v_c=\tanh(J/kT_c)=2-\sqrt{3}\approx 0{\cdot}2679492$. The last few diagonal and off-diagonal PA to $\mathrm{d}[\ln(\chi'(v)/\chi(v))]/\mathrm{d}v$ are shown in table 2. The sequences of poles and residues are apparently converging to the expected values of v_c for the position of the pole, and -1 for the residue, indicative of an algebraic singularity.

Table 2. Poles and residues of Padé approximants to $\ln \mathrm{div}^2\, \chi_0$ of the triangular lattice Ising model.

N	$[N/N-1]$	$[N/N]$	$[N/N+1]$
4	0·2709 (−1·066)	0·2698 (−1·044)*	0·2700 (−1·046)*
5	0·2674 (−0·984)	0·2678 (−0·994)	0·2679 (−0·998)
6	0·2680 (−1·005)	0·2680 (−1·001)	0·2680 (−1·001)
7	0·2680 (−1·001)	0·2680 (−1·001)*	

There are two points worthy of emphasis here. Firstly, forming the PA to the logarithmic derivative applied twice should enable us to test whether the singularity is of the conventional algebraic type or not. Secondly, if the sequence of poles and residues of the PA coverge well, and the residues converge to a value different from -1, this is evidence of an essential singularity of the type proposed by Kosterlitz (1974).

A related analysis was carried out by Camp and Van Dyke (1975), who formed the PA to $\ln \mathrm{div}(\ln \chi)$. This has the effect of converting the Kosterlitz form to a simple pole with a confluent singularity. The approach taken here eliminates the confluent singularity.

3. Analysis of series

In this section we will examine the high-temperature susceptibility series, and comment on the free energy series, on the triangular lattice of three models, the $X-Y$, CH and PCH models, to which the Mermin and Wagner (1966) proof applies, and to the step model (Guttmann *et al* 1972), which exhibits similar behaviour to the PCH model, though (as previously discussed) the Mermin and Wagner proof does not apply.

In table 3 the diagonal and off-diagonal PA to the logarithmic derivative (LD) of the susceptibility of the PCH model are shown. Apart from a different normalisation of K_c, this is identical to the table given by Camp and Van Dyke (1975). This erratic table, with half the entries defective, indicates the possibility of singular behaviour around $K_c = 0{\cdot}3$, with an ill-defined exponent. In table 4 we show the PA to LD^2 of the same series. This is rather better converged, with only one defective entry. A critical temperature of $K_c \approx 0{\cdot}34$ is indicated, with residue around $-1{\cdot}4$. Most significantly, the residue seems to be clearly less than -1, which demonstrates that the singularity is not of the usual algebraic type. The convergence of the residue and critical temperature suggests that this model has an essential singularity at the critical temperature of the form suggested by Kosterlitz. That is, we find

$$\chi \sim A \exp[c(1-K/K_c)^{-\gamma}] \tag{3.1}$$

with $K_c \approx 0{\cdot}34$ and $\gamma \approx 0{\cdot}4$ in surprisingly good agreement with the value of $\gamma = 0{\cdot}5$ suggested by Kosterlitz on the basis of heuristic arguments.

Table 3. Poles and residues of Padé approximants to ln div χ_0 of the triangular lattice PCH model.

N	$[N/N-1]$	$[N/N]$	$[N/N+1]$
2		0·309 (−2·40)	0·310 (−2·44)*
3	0·306 (−2·32)*	0·306 (−2·31)*	0·313 (−2·56)
4	0·306 (−2·32)*	—	0·328 (−3·70)
5	0·326 (−3·43)		

Table 4. Poles and residues of the Padé approximants to ln div^2 χ_0 of the triangular lattice PCH model.

N	$[N/N-1]$	$[N/N]$	$[N/N+1]$
2		0·318 (−1·10)*	0·359 (−1·59)
3	0·277 (−0·88)	0·329 (−1·22)	0·337 (−1·34)
4	0·344 (−1·49)	0·340 (−1·39)	

Turning now to the $X-Y$ model, we show in table 5 the LD Q to the triangular lattice susceptibility (in agreement with Camp and Van Dyke 1975), and in table 6 the LD^2 PA. In table 5 we see slightly erratic entries. There is evidence of a singularity around $K_c \approx 0{\cdot}9$, with an exponent seemingly in the range 3–4. In table 6 we see similarly erratic behaviour, though the entries appear somewhat better converged, with evidence of a singularity around $K_c = 0{\cdot}9$–$0{\cdot}95$, with ill-converged residue,

Table 5. Poles and residues of Padé approximants to ln div χ_0 of the triangular lattice $S=\infty$, $X-Y$ model.

N	$[N/N-1]$	$[N/N]$	$[N/N+1]$
2		—	—
3	0·858 (−3·13)	0·883 (−4·250)	0·873 (−3·65)
4	0·876 (−3·84)	0·967 (−29·6)*	0·863 (−3·21)
5	0·876 (−3·42)		

Table 6. Poles and residues of Padé approximants to ln div^2 χ_0 of the triangular lattice $S=\infty$. $X-Y$ model.

N	$[N/N-1]$	$[N/N]$	$[N/N+1]$
2		0·924 (−1·59)	0·926 (−1·61)
3	0·926 (−1·60)	0·924 (−1·59)*	0·949 (−1·75)*
4	0·933 (−1·65)*	0·911 (−1·51)	

possibly around −1·6, but one which shows no sign of settling down to −1, which would be the case if this function had an algebraic singularity.

Thus for the $X-Y$ model we conclude that there *is* evidence for a singularity, but that it is not of the conventional algebraic type. However the evidence supporting the Kosterlitz form is weaker than for the PCH model. (See however the note added in proof.)

In tables 7 and 8 we give the LD PA and LD^2 PA to the CH model susceptibility. Note that due to the spherical symmetry of this model, the vortex excitations characteristic of the Kosterlitz argument are not applicable. Table 7 contains very little useful information, except that it permits the observation that the CH model is not analysable by LD PA. Table 8 is slightly better and suggests the possible presence of a singularity around $K_c = 0·4$, with a residue too erratic to estimate.

Table 7. Poles and residues of Padé approximants to ln div χ_0 of the triangular lattice CH model.

N	$[N/N-1]$	$[N/N]$	$[N/N+1]$
2	—	0·375 (−6·07)*	0·376 (−6·32)*
3	—	0·333 (−3·30)*	—
4	—	—	
5	—		

Table 8. Poles and residues of Padé approximants to ln div^2 χ_0 of the triangular lattice CH model.

N	$[N/N-1]$	$[N/N]$	$[N/N+1]$
2	0·404 (−1·685)	0·406 (−1·716)*	0·393 (−1·592)*
3	0·365 (−1·332)*	0·422 (−1·844)	—
4	1·399 (−62·37)	—	

Our conclusion for this model is therefore similar to that for the $X-Y$ model. The singularity does not appear to be of conventional type, but there is insufficient evidence for an essential singularity of the form (2.5).

Our results for the step model are shown in tables 9 and 10. The LD PA are somewhat erratic, though some evidence of a singularity around $K_c = 0{\cdot}45$ is present. The LD^2 PA are no better, and if anything, slightly worse. No evidence of convergence is detectable. The large residues however, are consistent with the absence of a conventional algebraic singularity.

Table 9. Poles and residues of Padé approximants to ln div χ_0 of the triangular lattice step model.

N	$[N/N-1]$	$[N/N]$	$[N/N+1]$
2		0·441 (−1·86)	0·461 (−2·22)
3	0·457 (−2·13)	0·430 (−1·77)*	—
4	0·536 (−4·99)		

Table 10. Poles and residues of Padé approximants to ln $\text{div}^2\, \chi_0$ of the triangular lattice step model.

N	$[N/N-1]$	$[N/N]$	$[N/N+1]$
2		1·067 (−10·7)	0·777 (−4·37)
3	0·511 (−0·80)	0·719 (−3·35)	0·758 (−4·10)
4	1·233 (−68·0)		

Thus for no model do we find evidence of a conventional algebraic singularity. For the PCH model an essential singularity of the Kosterlitz type is indicated. For the infinite spin $X-Y$ model there is some evidence of an essential singularity. For the CH model there is slight evidence of an essential singularity, but the evidence is very weak. For the step model there is some evidence for a singularity, but no convincing evidence for either an essential or an algebraic singularity.

Analysing the free energy, or equivalently, the internal energy series is much more delicate than analysing the susceptibility, as any non-analytic part is likely to vanish at the critical temperature. That is, as $T \to T_c$, the analytic part, (probably) being non-vanishing will dominate the expansion rather than the non-analytic part.

Nevertheless, if the analytic part can be reasonably represented by a constant, the method of analysis we have applied to the susceptibility series still applies. We have therefore attempted an analysis of these series in an identical manner *mutatis mutandis* to that employed in the analysis of the susceptibility series. We confine ourselves to the same models on the triangular lattice.

For the $X-Y$ model, we find the series too short to analyse. Betts (1977) has pointed out that later terms in the series are incorrect, which increases the difficulties of analysis!

For the remaining three models, the LD PA (not shown) gave no evidence of converging. The LD^2 PA (not shown) appeared to converge for the CH and PCH models. However, in both cases the residues are close to zero. This is characteristic of an analytic function. Thus either there is no detectable non-analyticity in the free energy, or, more likely, it is masked by the dominant additive analytic term. This last possibility would be consistent with the Kosterlitz form.

4. Conclusion

We have investigated the question of the existence and nature of a phase transition for a number of two-dimensional lattice models whose order-parameter symmetries are inconsistent with a conventional phase transition.

For the PCH and $X-Y$ model high-temperature susceptibilities we find: (*a*) strong evidence of a phase transition at real, positive temperature; (*b*) that the nature of the singularity is not of the conventional algebraic type; and (*c*) for the PCH model, the form suggested by Kosterlitz is well supported, while for the $X-Y$ model this conclusion is weaker.

This part of our work duplicates to some extent the earlier work of Camp and Van Dyke (1975). With their method of analysis, they found quite strong evidence of an essential singularity of the Kosterlitz type for the infinite spin $X-Y$ models. Their results, taken in combination with those presented here, strengthen conclusion (*b*) above.

For the CH and step models we find: (*a*) weak evidence of a phase transition at real, positive temperatures; and (*b*) the available evidence points away from a conventional algebraic singularity.

Since this work was completed, Monte Carlo studies by Suzuki *et al* (1977) support our results in the case of the $X-Y$ model.

Acknowledgments

I would like to thank Professor Colin J Thompson both for helpful discussions and for his hospitality while visiting the Department of Mathematics, University of Melbourne, where this work was, in part, carried out.

Note added in proof. Following a suggestion by the referee we have estimated c and re-estimated K_c, defined by (3.1), by forming Padé approximants to $(f(x))^{1/\gamma}$, where $f(x)$ is the logarithmic derivative of the susceptibility series. For the PCH model, with $\gamma = 0{\cdot}4$ in (3.1) we obtain $K_c = 0{\cdot}340 \pm 0{\cdot}002$ and $c = 1{\cdot}34 \pm 0{\cdot}07$. With $\gamma = 0{\cdot}5$ (as suggested by Kosterlitz 1974) we find $K_c = 0{\cdot}345 \pm 0{\cdot}006$ and $c = 1{\cdot}5 \pm 0{\cdot}3$. That is, $\gamma = 0{\cdot}4$ as obtained from the LD^2 series, gives estimates of K_c and c which are better converged.

For the infinite spin $X-Y$ model, with $\gamma = 0{\cdot}5$ we obtain $K_c = 0{\cdot}91 \pm 0{\cdot}01$ and $c = 1{\cdot}25 \pm 0{\cdot}1$, while with $\gamma = 0{\cdot}4$ we find $K_c = 0{\cdot}90 \pm 0{\cdot}01$ and $c = 1{\cdot}04 \pm 0{\cdot}08$. Thus this calculation strengthens our tentative conclusion of an essential singularity of the Kosterlitz type for this model, but in this case $\gamma = 0{\cdot}5$ seems as likely as $\gamma = 0{\cdot}4$, the value estimated for the PCH model.

For the step model and CH model we find no apparent convergence of Padé approximants to $(f(x))^{1/\gamma}$. This is consistent with the ill-converged behaviour of Padé approximants to ln div $f(x)$, as discussed earlier.

References

Berezinskii V L 1971 *Sov. Phys.-JETP* **32** 493–500

Betts D D 1977 *Physica* B in the press

Betts D D, Elliott C J and Ditzian R V 1971 *Can. J. Phys.* **49** 1327–34

Brown H A and Luttinger J M 1955 *Phys. Rev.* **100** 685

Camp W J and Van Dyke J P 1975 *J. Phys. C: Solid St. Phys.* **8** 336–52

Doniach S 1973 *Phys. Rev. Lett.* **31** 1450–1

Guttmann A J and Joyce G S 1973 *J. Phys. C: Solid St. Phys.* **6** 2691–712

Guttmann A J, Joyce G S and Thompson C J 1972 *Phys. Lett.* **38A** 297–8

Kosterlitz J M 1974 *J. Phys. C: Solid St. Phys.* **7** 1046–60

Kosterlitz J M and Thouless D J 1973 *J. Phys. C: Solid St. Phys.* **6** 1181–203

Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133–6

Moore M A 1969 *Phys. Rev. Lett.* **23** 861–3

Rushbrooke G S and Wood P J 1958 *Molec. Phys.* **1** 257

Stanley H E 1968 *Phys. Rev. Lett.* **20** 589–92

Stanley H E and Kaplan T A 1966 *Phys. Rev. Lett* **17** 913–15

Suzuki M, Miyashita S, Kuroda A and Kawabata C 1977 *Phys. Lett.* **60A** 478–80.

Yamaji K and Kondo J 1973 *Phys. Lett.* **45A** 317–8

Zittartz J 1976 *Z. Phys.* B **23** 55–62