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Series analysis of the two-dimensional step model

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Abstract. An n-fit series analysis of the susceptibility of the two-dimensional step model is carried out. The work follows a similar analysis by Ferer and Velgakis of the planar and XY models. Due to the nature of the interaction function, it is expected that a vortex induced transition is not possible for the step model. This is confirmed by the n-fit analysis.

We use the usual notation and write the classical Heisenberg Hamiltonian as

$$H = -\sum_{\langle ij\rangle} \sum_{\alpha=1}^{N} J_\alpha S_i^{(\alpha)} S_j^{(\alpha)}$$

where $(J_1, \ldots, J_N)$ and $(S_i^{(1)}, \ldots, S_i^{(N)})$ are N-dimensional interaction and spin vectors (respectively) and the summation is over nearest-neighbour pairs $\langle ij\rangle$. Strictly speaking, $\mathbf{J}$ is an N-dimensional, second-order diagonal tensor, but we adopt the conventional notational simplification of treating it as an N-dimensional vector.

If we restrict to $N=2$, we can associate an angle θ_i and interaction function $C(\theta_i)$ with each vector $\boldsymbol{S}_i$ and can write

$$H = -J \sum_{\langle ij\rangle} C(\theta_i - \theta_j)$$

where now $J = J_1 = J_2$, corresponding to the isotropic case.

With this notation the planar classical Heisenberg model Hamiltonian is defined by $C(\theta) = \cos(\theta)$, and the step model by $C(\theta) = 1$ for $|\theta| \leq \frac{1}{2}\pi$, $C(\theta) = -1$ for $\frac{1}{2}\pi < |\theta| < \pi$ and $C(\theta + 2\pi) = C(\theta)$.

Unlike the planar and step models, the XY model has a three-dimensional spin vector $\boldsymbol{S}_i = (S_i^{(1)}, S_i^{(2)}, S_i^{(3)})$ but with the diagonal components of the interaction tensor given by $\boldsymbol{J} = (J^{(1)}, J^{(2)}, 0)$. The Hamiltonian for the isotropic XY model is

$$H = -J \sum_{\langle ij\rangle} S_i^{(1)} S_j^{(1)} + S_i^{(2)} S_j^{(2)},$$

where $J = J^{(1)} = J^{(2)}$.

In 1966 Mermin and Wagner proved that no long-range order (and hence no spontaneous magnetisation) could exist for certain two-dimensional models with a symmetric and continuous interaction function. In 1973 Kosterlitz and Thouless put forward a mechanism by which certain two-dimensional models can have a phase transition, but have no long-range order. Models in this category have a low-temperature phase occupied by bound vortex–antivortex pairs which destroy the long-range order. At the critical temperature these pairs begin to dissociate, and this leads to increasing disorder in the system.

The Mermin and Wagner proof means that the planar model cannot have a conventional phase transition. The planar model can however undergo an unconventional phase transition of the type formulated by Kosterlitz and Thouless (KT), as can the XY model. The Mermin and Wagner proof does not apply to the step model, so it may have a conventional phase transition. It is expected (Guttmann and Joyce 1973), however, to be in the same universality class as the planar and XY models. It is therefore of much interest to know whether the step model has a phase transition, and if so, of what type.

Guttmann (1978) investigated the critical behaviour of the planar, XY and step models on a triangular lattice using a method of Padé analysis which differentiated between algebraic and exponential (KT type) singularities. He studied the high-temperature susceptibility of these models and found good evidence in the case of the planar model, and weak evidence in the case of the XY model supporting a KT type phase transition. In the case of the step model, neither an algebraic nor an exponential singularity could be located.

Camp and Van Dyke (1975) also studied the susceptibility series of the two-dimensional planar and XY models using a Padé analysis. They also found support for a KT type transition for both these models. The support for the planar model was however only weak. They did not study the step model.

In neither of the above studies was it possible to confirm the susceptibility exponent $\nu = \frac{1}{2}$ as conjectured by Kosterlitz (1974).

In 1983, Ferer and Velgakis demonstrated that for certain types of singular behaviour, an n-fit analysis is more informative than a double logarithmic Padé analysis, as used by Guttmann (1978). In particular they found that whereas low order analytic or weakly divergent correction terms of a dominant KT type singularity can disrupt a double logarithmic Padé analysis, an n-fit analysis is much less affected. When they applied the n-fit analysis to the planar models, Ferer and Velgakis found good evidence to support a KT form for the dominant singularity of the susceptibility. The evidence is strongest for the XY model, and somewhat weaker for the planar model.

Using the same technique as Ferer and Velgakis, and assuming a KT form for the susceptibility we write

$$\chi_0 = A \exp[B(1 - K/K_c)^{-\nu}] \tag{1}$$

where $K = J/kT$.

Expanding $(1 - K/K_c)^{-\nu}$ by the binomial theorem, and using the theory of multinomials, we can, after some algebra, re-express (1) as

$$\chi_0 = \sum_{j=0}^{\infty} C_j K^j$$

where $C_j = C_j(A, B, \nu, K_c)$.

The four parameters A, B, ν and K_c in this expression can be 4-fitted to the known series expansion $\chi_0 = \Sigma_{i=0}^{n} d_j K^j$. We therefore have successive sets of four simultaneous equations in four unknowns of the form $C_i = d_i$ for $i = m-3$, $m-2$, $m-1$, m from which we find estimates A_m, B_m, ν_m and $K_{c,m}$ for $m \leq n$. In practice we can simplify these sets of four nonlinear equations into sets of two nonlinear equations in two unknowns. From these we can obtain ν_m and B_m. We can then calculate from the original equation $K_{c,m}$ and A_m, using a modification of the Powell hybrid method as implemented by the Numerical Algorithms Group (NAG), Mark 9, 1982 distribution. This library package is running on a VAX 11/780 computer.

Before applying this method to the step model, we repeated the analysis of Ferer and Velgakis on the correlation length and susceptibility series of the planar and XY models, using their coefficients. While in general the numerical results of our analysis agree with those of Ferer and Velgakis, the conclusions we draw from this analysis are more cautious. This is mainly due to the at best oscillatory (XY model) and at worst erratic (planar model) convergence of the estimates.

We are most interested in the planar model as this model most closely resembles the step model on thermodynamic grounds. For this model the results of the 4-fit analysis of the correlation length and susceptibility series is given in table 1. The corresponding table in Ferer and Velgakis is identical to this table except for a number of gaps which correspond to systems of equations for which they were unable to obtain a solution. This fuller table does, we think, show that the convergence is not oscillatory, as Ferer and Velgakis suggest, but somewhat erratic.

A number of general comments can be made about the analysis. The parameter $K_{c,n}$ varied little between the above results and trivial or 'ridiculous' solutions. The analysis was therefore insensitive to the choice of $K_{c,n}$. As already described, the estimates ν_n and B_n involved the numerical solution of a system of two nonlinear equations. A point was very quickly reached after which reducing the error bound any further had no effect on the choice of solution. The initial guesses ν_0 and B_0, however, had a dramatic effect on the analysis. The approach used was to let ν_0 take on values between 0.4 and 0.6, and change B_0 until a solution was located. For both the correlation length and the susceptibility it was found that the existence of a solution was heavily dependent upon the initial guess B_0. Straying too far from the 'correct' B_0 would lead to a breakdown in the numerical analysis procedure.

The analysis of the corresponding XY model series was far better behaved. There was however, still a pronounced but slow oscillation in the estimates which made extrapolation to large n difficult (see also Ferer and Velgakis). If we assume universality, then the results of the 4-fit analysis on the XY model together with the planar model does lead to good support for a KT type singularity, and furthermore, an exponent of $\nu = 0.5$ can be inferred from the sequence of estimates. If, however, we do not assume universality, then for the planar model alone, it would appear that the best we could say is that a KT type singularity is not inconsistent with the analysis.

We are now in a position to apply the n-fit analysis to the step model. The coefficients of the isothermal susceptibility on the square and triangular lattices are given in table 2.

Table 1. Planar model. 4-fit analysis of the correlation length and susceptibility series on the triangular lattice.

	ξ^2		$(\chi-1)/K$	
n	ν_n	$K_{c,n}$	ν_n	$K_{c,n}$
4	0.590	2.78	0.374	3.06
5	0.418	2.94	0.474	2.97
6	0.475	2.89	0.806	2.75
7	0.313	3.02	0.701	2.81
8	0.389	2.97	0.477	2.93
9	0.560	2.86	0.452	2.95
10	0.489	2.90	0.535	2.91
11	0.359	2.97	0.566	2.89

The 4-fit analysis of these series suggested quite srongly that no KT type transition is present. For most choices of the initial values ν_0 and B_0 no solution could be found. In those instances where a solution was found, the exponent ν persistently tended to zero. This was accompanied by the constant B also tending to zero, and the critical amplitude A tending to become very large. This suggests that the series cannot be fitted to a KT type exponential singularity.

Ferer and Velgakis found that better results could be acheived if a left-shifted series is used (i.e. subtract the constant and divide by K). In the case of the step model however, no improvement in behaviour between the original and left-shifted series could be found for either lattice.

As discussed earlier, when analysing a function of KT form, an n-fit analysis in most cases is less affected by analytic or weakly divergent confluent correction terms than a double logarithmic Padé analysis. However, since an n-fit analysis is essentially a variation of the ratio method, it will be less able to handle competing complex or non-physical singularities if they are present. Hence this method is not expected to be useful in a situation where there is more than one non-confluent singularity dominating low-order terms. If universality is to be satisified, then presumably this situation is the cause of the 'poor' behaviour of the 4-fit analysis when applied to the susceptibility of the spin $=\frac{1}{2}$ XY model. If the classical and quantum XY models are in the same universality class, complex singular behaviour must be disrupting the n-fit analysis of the quantum model. Camp and Van Dyke (1976) have studied the classical and quantum (three-dimensional) Heisenberg models using an n-fit analysis. They find that the analysis breaks down in the quantum case, and conjecture that particularly 'nasty' singularities must be at work for universality to be satisfied.

Is it possible that competing non-physical singularities are upsetting the n-fit analysis of the step model? We can test this theory somewhat by analysing the transformed susceptibility on the triangular lattice. Using Padé analysis, Guttmann and Joyce (1973) located on the negative real axis a competing singularity, and transformed it away by using an Euler transformation. The resulting series is given in Guttmann and

Table 2. Zero-field isothermal susceptibility coefficients $kT\chi_0(T)/Nm^2 = \Sigma_n d_n K^n$ for $K = J/k_B T$ on the square and triangular lattices.

n	Square lattice d_n	Triangular lattice d_n
0	1.000 000 00	1.000 000 00
1	4.000 000 00	6.000 000 00
2	6.000 000 00	15.000 0000
3	10.666 6667	44.000 0000
4	16.833 3333	112.750 000
5	23.733 3333	280.800 000
6	33.905 5556	666.591 667
7	44.380 9524	1532.973 81
8	57.068 1542	3424.240 92
9	71.013 7562	7476.85†
10	85.044 1729	
11	102.113 786	
12	117.764 703	

† This coefficient is not known exactly (see Guttmann and Joyce 1973), the central estimate is used here. The possible error is too small to affect the subsequent analysis.

Joyce. The 4-fit analysis of this series however, was no better behaved than the original series. In those few cases where solutions did exist, estimates were erratic, with ν_n and B_n tending to zero, and A_n very large. We should add however, that the triangular lattice series at order 9 is still rather short.

Based on this evidence we can conclude with some confidence that no KT type phase transition occurs for the two-dimensional step model.

Very recent work by Barber (1983) supports a stronger conclusion. Using a Migdal renormalisation group scheme Barber finds that the step model has no low-temperature phase. However, he does find evidence to suggest that a modified step model, which can be defined by the interaction function $C(\theta)=1$ for $|\theta|\leq\delta\pi$, $C(\theta)=-1$ for $\delta\pi<|\theta|<\pi$ and $C(\theta+2\pi)=C(\theta)$ where $\delta=\frac{1}{2}$ defines the step model, does have a phase transition for $\delta<\frac{1}{2}$. This model is now being investigated.

References

Barber M N 1983 *J. Phys. A: Math. Gen.* **16** 4053
Camp W J and Van Dyke J P 1975 *J. Phys. C: Solid State Phys.* **8** 335
—— 1976 *J. Phys. A: Math. Gen.* **9** 731
Ferer M and Velgakis M J 1983 *Phys Rev.* B **27** 314
Guttmann A J 1978 *J. Phys. A: Math. Gen.* **11** 545
Guttmann A J and Joyce G S 1973 *J. Phys. C: Solid State Phys.* **6** 2691
Kosterlitz J M 1974 *J. Phys. C: Solid State Phys.* **7** 1046
Kosterlitz J M and Thouless D J 1973 *J. Phys. C: Solid State Phys.* **6** 1181
Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133