Low temperature series for the Ising S=1 model with biquadratic interactions and the Potts model

1974 J. Phys. A: Math. Nucl. Gen. 7 L152

(http://iopscience.iop.org/0301-0015/7/15/002)

J. Phys. A: Math., Nucl. Gen., Vol. 7, No. 15, 1974. Printed in Great Britain. © 1974

LETTER TO THE EDITOR

Low temperature series for the Ising $S = 1$ model with biquadratic interactions and the Potts model

R Ditzian

Institute for Fundamental Studies, Department of Physics and Astronomy, University of Rochester, Rochester, New York 14627, USA

Received 18 June 1974, in final form 20 August 1974

Abstract. The low-temperature high-field polynomials for the free energy are given for the general Blume–Emery–Griffiths model on the FCC lattice.

The order parameters and susceptibilities are obtained for three values of the biquadratic interaction and a specific form of the external field Δ. One of the treated cases is the Potts model.

In a previous paper (Ditzian and Oitmaa 1974), the high-temperature behaviour of a subclass of the model of Blume *et al* (1971), including the Potts model, was investigated on the FCC lattice and tricritical behaviour was seen. In this letter we calculate the low-temperature series for the general Blume–Emery–Griffiths model and analyse them for a number of specific cases including the Potts model. A number of critical indices are obtained. The question of the order of the transition of the Potts model is not solved.

The model is

$$\mathscr{H} = -J\sum_{\langle ij\rangle} S_{iz}S_{jz} - J^Q \sum_{\langle ij\rangle} (S_{iz}^2-\tfrac{2}{3})(S_{jz}^2-\tfrac{2}{3}) - h\sum_i S_{iz} + \Delta\sum_i (S_{iz}^2-\tfrac{2}{3}),$$

where $S_z = -1, 0, 1$.

Using the method developed by Saul *et al* (1974) with a modification to include the biquadratic term and the tables of Sykes *et al* (1965), we calculated six polynomials of the low-temperature free energy. Defining $\Delta' = \Delta + \frac{2}{3}qJ^Q$,

$$-\beta f(\beta J, \beta J^Q, \beta\Delta', \beta h) = \tfrac{1}{2}q(J+J^Q) - \Delta' + h + \sum_{n=1}^{\infty} (u^{12}\mu)^n \sum_{m=0}^{n} \eta^m v^{12m} L_{nm}(u, v)$$

where $\mu = e^{-\beta h}$, $\eta = e^{\beta\Delta'}$, $u = e^{-\beta J}$ and $v = e^{-\beta J^Q}$. The L_{nm} are listed in the appendix. We looked at the case $\eta = v^8$ and three values of the ratio J^Q/J, namely: $v = u, u^2$ and u^3. The last is the Potts model. Following Saul *et al* (1974) in re-expressing the Hamiltonian in terms of two fermions with occupation numbers n_1 and n_2 satisfying $n_1^{(i)} + n_2^{(i)} \leqslant 1$ we obtain

$$Z(\beta J, \beta J^Q, \beta\Delta', \beta h)$$
$$= \exp[\beta N(\tfrac{1}{2}qJ + \tfrac{1}{2}qJ^Q - \Delta')] \sum_{\{n_1^i n_2^i\}} [(u^q v^q \eta\mu)^{\Sigma n_1^i}(u^q\mu)^{\Sigma n_2^i}$$
$$\times u^{-[\Sigma_{\langle ij\rangle}(n_1^i n_1^j + 2n_1^i n_2^j + 2n_2^i n_1^j + 4n_2^i n_2^j)]} v^{-(\Sigma_{\langle ij\rangle} n_1^i n_1^j)}].$$

Now the weight of each graph is

$$W(G) = (u^q v^q \mu\eta)^{N_1}(u^q\mu)^{2N_2}u^{-B(G)}v^{-C(G)}$$

where only the appearance of v differs from Saul *et al* (1974):

$$B(G) = b_{11}(G)+2b_{12}(G)+4b_{22}(G)$$

and $C(G) = b_{11}$, b_{ij} is the number of ij bonds in the graph G. The order parameters $M = \langle S_z \rangle$ and $Q = \langle S_z^2 - \frac{2}{3} \rangle$, and the initial susceptibilities

$$\chi_M = -\frac{\partial f}{\partial h^2}\bigg|_{\substack{h=0\\ \Delta'=8JQ}} \quad \text{and} \quad \chi_Q = -\frac{\partial^2 f}{\partial \Delta'^2}\bigg|_{\substack{\Delta'=8JQ\\ h=0}}$$

are given by

$$M = \sum_{n=1}^{\infty} nu^{12n} \sum_{m=0}^{n} v^{8m}L_{nm}(u, v)$$

$$Q = \beta \sum_{n=1}^{\infty} u^{12n} \sum_{m=1}^{n} mv^{8m}L_{nm}(u, v)$$

$$\chi_M = \beta^2 \sum_{n=1}^{\infty} n^2u^{12n} \sum_{m=0}^{n} v^{8m}L_{nm}(u, v)$$

$$\chi_Q = \beta^2 \sum_{n=1}^{\infty} u^{12n} \sum_{m=1}^{n} m^2v^{8m}L_{nm}(u, v).$$

We had some checks on the series. The series for $v = 1$ should reduce to the Ising $S = 1$ series and the magnetization and susceptibility in fact check out. To my knowledge, Q and χ_Q had not been calculated before for the Ising model, analysis gave $\beta_Q = 0{\cdot}6 \pm 0{\cdot}05$ which agrees with the expected $\beta_Q = 2\beta_M$. The susceptibility χ_Q has no singularities.

The free energy reduces to that for the Blume–Capel model of Saul *et al* (1974) when $(\eta v^{12})^m \to \eta^m$ and in the $L_{nm}(u, v)$ the variable v is set equal to 1.

The series are long but have gaps. We chose to look in the first instance at $v = u^n$ and the higher the n the less information could we use, so that this is not the best way to look at the $n = 3$ Potts model.

The convergence of the Padé approximants to $(\mathrm{d}/\mathrm{d}x) \ln f(x)$ was not good for locating the critical point so this information we took from the high-temperature series in Ditzian and Oitmaa (1974). While for well converged series decapitation before or after taking $(\mathrm{d}/\mathrm{d}x) \ln f(x)$ makes no difference, in this case we saw a remarkable effect. For instance the series for Q in the Potts model when partially beheaded (starting from u^{12} omitting the initial constant) seems to indicate, in a not well converged way, a divergence, rather than a falling to zero. Taking powers of series and looking for the correct critical point can also be misleading as only a small number of Padé approximants gave a reasonable estimate and this number did not vary much with choice of powers.

The series for the magnetization were the better behaved ones. The results are:

	$v = u$	$v = u^2$	$v = u^3$
β_M	$0{\cdot}33 \pm 0{\cdot}03$	$0{\cdot}21 \pm 0{\cdot}04$	$0{\cdot}21 \pm 0{\cdot}06$
β_Q	$0{\cdot}27 \pm 0{\cdot}05$	$0{\cdot}27 \pm 0{\cdot}05$	

For the Potts model $M = 3Q$ as only one order parameter exists. We see that the Ising behaviour is still holding for $u = v$ so that we are still not in the cross-over region.

The magnetic susceptibility is affected by the cross-over region earlier. Already at $u = v, \gamma$ seems to be between 1·30 to 1·80, $\gamma_Q \sim 0{\cdot}32 \pm 0{\cdot}05$, while at $u^2 = v, \chi_M$ is wild and γ_Q seems to be $0{\cdot}20 \pm 0{\cdot}10$.

In the Potts model both susceptibilities gave unconverged estimates for the indices. During the writing of this letter, papers by Straley (1974) and by Enting (1974) on the Potts model in three dimensions arrived. Using the special symmetry of the Potts model they obtain longer series.

To better locate the tricritical point we propose to first analyse the series for the magnetization for various numerical values of v while locating the appropriate critical point from the high-temperature series and second to do a free-energy matching.

Acknowledgments

The author wishes to thank Professor Montroll for his support. Research partially supported by the NSF Grant (GU-4040). Thanks are due to Dr I Enting who found some mistakes in the polynomials.

Appendix. Free-energy low-temperature polynomials $L_{ij}(u, v)$

$$L_{11} = 1$$

$$L_{20} = 1$$

$$L_{22} = -\frac{13}{2}+\frac{6}{uv}$$

$$L_{31} = -13+\frac{12}{u^2}$$

$$L_{33} = \frac{211}{3}-\frac{120}{uv}+\frac{42}{u^2v^2}+\frac{8}{u^3v^3}$$

$$L_{40} = -\frac{13}{2}+\frac{6}{u^4}$$

$$L_{42} = 211-\frac{120}{uv}-\frac{240}{u^2}+\frac{84}{u^3v}+\frac{42}{u^4}+\frac{24}{u^5v}$$

$$L_{44} = -944\tfrac{1}{4}+\frac{2322}{uv}-\frac{1653}{u^2v^2}+\frac{126}{u^3v^3}+\frac{123}{u^4v^4}+\frac{24}{u^5v^5}+\frac{2}{u^6v^6}$$

$$L_{51} = 211-\frac{240}{u^2}-\frac{78}{u^4}+\frac{84}{u^6}+\frac{24}{u^8}$$

$$L_{53} = -3777+\frac{4644}{uv}+\frac{4644}{u^2}-\frac{1122}{u^2v^2}-\frac{4368}{u^3v}-\frac{1122}{u^4}+\frac{696}{u^4v^2}+\frac{120}{u^5v^3}-\frac{36}{u^5v}+\frac{44}{u^6}+\frac{252}{u^6v^2}$$
$$+\frac{120}{u^7v}+\frac{48}{u^7v^3}+\frac{48}{u^8v^2}+\frac{8}{u^9v^3}-\frac{200}{u^3v^3}$$

$$L_{55} = 14303\tfrac{1}{5} - \frac{45792}{uv} + \frac{49290}{u^2v^2} - \frac{16296}{u^3v^3} - \frac{2871}{u^4v^4} + \frac{792}{u^5v^5} + \frac{448}{u^6v^6} + \frac{96}{u^7v^7} + \frac{30}{u^8v^8}$$

$$L_{60} = \frac{211}{3} - \frac{120}{u^4} + \frac{42}{u^8} + \frac{8}{u^{12}}$$

$$L_{62} = -5665\tfrac{1}{2} + \frac{2322}{uv} + \frac{9288}{u^2} - \frac{2244}{u^3v} - \frac{2046}{u^4} - \frac{1248}{u^5v} - \frac{1680}{u^6} + \frac{804}{u^7v} - \frac{180}{u^8} + \frac{276}{u^9v} + \frac{240}{u^{10}} + \frac{96}{u^{11}v} + \frac{24}{u^{12}} + \frac{12}{u^{13}v}$$

$$L_{64} = 71516 - \frac{137376}{uv} - \frac{91584}{u^2} + \frac{74574}{u^2v^2} - \frac{2236}{u^3v^3} + \frac{146592}{u^3v} + \frac{25284}{u^4} - \frac{62160}{u^4v^2} - \frac{3882}{u^4v^4} - \frac{720}{u^5v^5} - \frac{924}{u^5v^3} - \frac{15636}{u^5v} + \frac{2184}{u^6v^4} - \frac{56}{u^6v^6} - \frac{1448}{u^6} - \frac{6594}{u^6v^2} + \frac{24}{u^8v^6} + \frac{936}{u^8v^4} + \frac{552}{u^8v^2} + \frac{9}{v^8} + \frac{144}{u^9v^5} + \frac{712}{u^9v^3} + \frac{96}{u^9v} + \frac{240}{u^{10}v^2} + \frac{24}{u^{10}v^6} + \frac{216}{u^{10}v^4} + \frac{96}{u^{11}v^3} + \frac{72}{u^{11}v^5} + \frac{54}{u^{12}v^4} + \frac{408}{u^7v^5} + \frac{1848}{u^7v^3} - \frac{2964}{u^7v}$$

$$L_{66} = -234103\tfrac{1}{6} + \frac{922152}{uv} - \frac{1329240}{u^2v^2} + \frac{771272}{u^3v^3} - \frac{64224}{u^4v^4} - \frac{65070}{u^5v^5} - \frac{6904}{u^6v^6} + \frac{3930}{u^7v^7} + \frac{1212}{u^8v^8} + \frac{776}{u^9v^9} + \frac{168}{u^{10}v^{10}} + \frac{30}{u^{11}v^{11}} + \frac{1}{u^{12}v^{12}}.$$

References

Blume M, Emery J and Griffiths R B 1971 *Phys. Rev.* A **4** 1071
Ditzian R and Oitmaa I 1974 *J. Phys.* A: *Math., Nucl. Gen.* **7** L61
Enting I G 1974 *J. Phys.* A: *Math., Nucl. Gen.* **7** 1617–26
Saul D M, Wortis M and Stauffer D 1974 *Phys. Rev.* B **9** 4964
Straley J P 1974 *J. Phys.* A: *Math., Nucl. Gen.* **7** in the press
Sykes M F, Essam J W and Gaunt D S 1965 *J. Math. Phys.* **6** 283