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1977 J. Phys. A: Math. Gen. 10 65

(http://iopscience.iop.org/0305-4470/10/1/016)

J. Phys. A: Math. Gen., Vol. 10, No. 1, 1977. Printed in Great Britain. © 1977

# Potts model specific heat critical exponents

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Received 10 June 1976

**Abstract.** A series expansion for the free energy of the $q$-state Potts model on a square lattice is used to estimate the specific heat critical exponents. The analysis is based on a series transformation which was suggested by the known solution of the two-state Potts (Ising) model, and which makes optimum use of the duality theorem. The transformed series is quite smooth. Neville tables yield the estimates $\alpha(2) = 0{\cdot}0001 \pm 0{\cdot}0003$ for the two-state model, $\alpha(3) = 0{\cdot}296 \pm 0{\cdot}002$ for the three-state model, and $\alpha(4) = 0{\cdot}45 \pm 0{\cdot}02$ for the four-state model. Our value for $\alpha(3)$ differs considerably from one reported by Straley and Fisher, and substantially improves compliance with the Rushbrooke inequality.

We report numerical estimates for the specific heat critical exponents $\alpha(q)$ of the $q$-state Potts model on a square lattice. For $q = 2$ we obtain $\alpha(2) = 0{\cdot}0001 \pm 0{\cdot}0003$; this is consistent with the correct value $\alpha(2) = 0$. For $q = 3$ we obtain $\alpha(3) = 0{\cdot}296 \pm 0{\cdot}002$; this differs considerably from the value $0{\cdot}05 \pm 0{\cdot}10$ reported by Straley and Fisher (1973). For $q = 4$, we obtain $\alpha(4) = 0{\cdot}45 \pm 0{\cdot}02$; there are no other results with which this may be compared. In the terminology of Mittag and Stephen (1971), we are concerned here with the Potts model, and not the Potts *vector* model. These models differ for $q = 4$.

The zero field series for the free energy of the $q$-state Potts model on a square lattice was investigated first by Kihara *et al* (1954). In the notation of Straley and Fisher, the free energy $F$ per lattice site is a function of the low temperature variable $x$; $x = \exp(-\epsilon_1/kT)$ and $-F/kT = A(x)$. Kihara *et al* (in a slightly different form) calculated the series expansion of $A(x)$ up to $x^{16}$. Straley and Fisher checked the series up to $x^{13}$, and by means of an independent expansion in a high temperature variable $t$, we checked the series up to $x^{14}$. In the following, we also include the $x^{15}$ and $x^{16}$ terms.

The free energy series, and the derived specific heat series, are quite irregular; the standard ratio method of analysis does not work well. Straley and Fisher obtained $\alpha(3)$ by means of Pade approximants.

We found it possible to smooth the free energy series substantially by means of a series transformation using a change of variable. Our procedure was motivated by the duality theorem for the $q$-state Potts model, and by what is known about the two-state Potts (or Ising) model. The resulting series is remarkably smooth, and Neville tables provide the estimates given above.

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The duality theorem (Potts 1952, Kihara *et al* 1954, Mittag and Stephen 1971) provides two equivalent forms for the free energy, involving the low temperature variable $x$ and the high temperature variable $t$, related by the dual transformation

$$t=\frac{1-x}{1+(q-1)x}; \qquad x=\frac{1-t}{1+(q-1)t}.$$

The two forms of the free energy are:

$$-F/kT=A(x)=-\ln\{[1+(q-1)t]^2/q\}+A(t).$$

Then the quantity $B(x)$ defined by

$$B(x)=A(x)-\ln[1+(q-1)x^2]$$

is invariant to the above dual transformation, $B(x)=B(t)$. Any phase transition must be associated with a singularity of $B(x)$. The physical singularity is self-dual, and occurs at the point $x_0$, $x_0=t(x_0)=(1+\sqrt{q})^{-1}$. Our method of series analysis depends on this separation of the free energy into a term which is duality invariant and contains the physical singularity, and a remainder which is uninteresting.

The exact expression for the free energy of the Ising model may be written in just this form. The function $B(x)$ is an integral,

$$B(x)=\frac{1}{2}\left(\frac{1}{2\pi}\right)^2\int_0^{2\pi}\int_0^{2\pi} \mathrm{d}\theta_1\,\mathrm{d}\theta_2 \ln[1-z(\cos\theta_1+\cos\theta_2)]$$

and $z$ is a function of $x$,

$$z=2x(1-x^2)/(1+x^2)^2.$$

This may also be written in a form which exhibits its invariance to the dual transformation,

$$z=2xt(x)/[1-xt(x)]^2.$$

Thus $B(x)$ is a function of the variable $xt(x)$.

The exact form of $B(x)$ for the $q$-state Potts model is not known. However, the series expansion of $A(x)$ is known, and this provides the series expansion of $B(x)$. Further (by analogy with the Ising model) we expect that $B(x)$ is more appropriately expressed as a function of the new variable $y=xt(x)$ so that each term in the expansion is manifestly invariant to the dual transformation. This change in variable leads to the series

$$B(x)=B^*(z)=\sum b_n z^n, \qquad z=y/x_0t(x_0).$$

The singularity of $B^*(z)$ occurs at $z=1$. Coefficients $b_n$ for the two-, three-, and four-state models are given in table 1.

The determination of the critical exponent is based on the following observations. First, we suppose that $B^*(z)$ has the branch point behaviour $B^*(z)\sim(1-z)^\rho$. Near the transition temperature $T_0$, $1-z$ is proportional to the square of the temperature deviation, $1-z\sim(T-T_0)^2$. This is a consequence of the definition of $y$. Then, near the

**Table 1.** Coefficients of the series expansion of $B^*(z)$. The tabulated quantity is $-10^3\, b_n$.

| $n$ \ $q$ | 2 | 3 | 4 |
|---|---|---|---|
| 0 | 0 | 0 | 0 |
| 1 | 0 | 0 | 0 |
| 2 | 29·43725152 | 35·89838486 | 37·03703704 |
| 3 | 20·20253553 | 28·85682970 | 32·92181070 |
| 4 | 12·56500077 | 19·97475755 | 24·46273434 |
| 5 | 8·325899679 | 13·98483331 | 17·88345273 |
| 6 | 5·875550571 | 10·19306826 | 13·37307434 |
| 7 | 4·359129225 | 7·731926891 | 10·30907790 |
| 8 | 3·360518850 | 6·065617199 | 8·179142146 |
| 9 | 2·669141007 | 4·890015806 | 6·652059127 |
| 10 | 2·170959556 | 4·030385783 | 5·523356303 |
| 11 | 1·800217077 | 3·382594241 | 4·665993495 |
| 12 | 1·516900497 | 2·881987283 | 3·999117346 |
| 13 | 1·295544029 | 2·486832308 | 3·469739948 |
| 14 | 1·119318614 | 2·169240652 | 3·042098452 |
| 15 | 0·9767425006 | 1·910001205 | 2·691383338 |
| 16 | 0·8597652257 | 1·695526641 | 2·399950858 |

transition temperature, the specific heat $C(T)$ has the $T$ dependence

$$C(T) \sim (T - T_0)^{2\rho-2}$$

so that the specific heat exponent is $\alpha = 2 - 2\rho$. Because this analysis is invariant to the dual transformation, the high and low temperature exponents are identical.

Now we turn to the standard ratio method of analysis of the series $B^*(z)$. First, we construct the sequence

$$g_n = n(b_n/b_{n-1} - 1).$$

If the series behaves as assumed, then the exponent $\rho$ is given by the limit

$$\rho = -\lim_{n\to\infty} (1 + g_n).$$

When the sequence $g_n$ is plotted against $1/n$, the resulting curves are quite smooth. Visual inspection gives the estimates $\alpha \sim 0$ for $q = 2$, and $\alpha \sim 0{\cdot}3$ for $q = 3$.

These estimates can be sharpened by constructing Neville tables (Jasnow and Wortis 1968). We define $g_n^0 = g_n$, and construct the sequences

$$g_n^r = (n/r)g_n^{r-1} - [(n-r)/r]g_{n-1}^{r-1}.$$

Table 2 shows the results for $q = 2$, 3 and 4, and for $r = 0$–3. (Note that all $g_n^r$ are negative; the sign has been suppressed.) Because of the rapid accumulation of numerical uncertainty due to roundoff, these numbers were all computed originally to eight decimal places. Numerical tests of the effect of roundoff in the eighth place suggest that the numbers displayed in table 2 are accurate to four decimal places. The next column, $g_n^4$, has lower accuracy and does not provide any useful information.

**Table 2.** Neville tables $-g_n^r$ for $q = 2$, 3 and 4.

| $n$ \ $r$ | 0 | 1 | 2 | 3 |
|---|---|---|---|---|
| $q=2$ | | | | |
| 10 | 1·8664 | 1·9999 | 1·9870 | 2·0463 |
| 11 | 1·8785 | 1·9991 | 1·9955 | 2·0182 |
| 12 | 1·8885 | 1·9990 | 1·9984 | 2·0070 |
| 13 | 1·8970 | 1·9990 | 1·9993 | 2·0023 |
| 14 | 1·9043 | 1·9991 | 1·9996 | 2·0008 |
| 15 | 1·9107 | 1·9992 | 1·9997 | 2·0003 |
| 16 | 1·9162 | 1·9993 | 1·9998 | 2·0001 |
| $q=3$ | | | | |
| 10 | 1·7579 | 1·8804 | 1·7767 | 1·9252 |
| 11 | 1·7680 | 1·8687 | 1·8161 | 1·9211 |
| 12 | 1·7759 | 1·8633 | 1·8366 | 1·8980 |
| 13 | 1·7825 | 1·8606 | 1·8460 | 1·8773 |
| 14 | 1·7879 | 1·8591 | 1·8498 | 1·8640 |
| 15 | 1·7926 | 1·8580 | 1·8512 | 1·8567 |
| 16 | 1·7966 | 1·8572 | 1·8515 | 1·8530 |
| $q=4$ | | | | |
| 10 | 1·6968 | 1·8477 | 1·6226 | 1·7589 |
| 11 | 1·7075 | 1·8145 | 1·6788 | 1·8288 |
| 12 | 1·7151 | 1·7986 | 1·7193 | 1·8409 |
| 13 | 1·7209 | 1·7903 | 1·7442 | 1·8272 |
| 14 | 1·7255 | 1·7856 | 1·7579 | 1·8080 |
| 15 | 1·7293 | 1·7829 | 1·7647 | 1·7919 |
| 16 | 1·7325 | 1·7810 | 1·7677 | 1·7807 |

The sequences $g_n^r$ are quite smooth. If we assume that the trends seen for $n = 10$–16 are maintained for larger $n$, then we can place upper and lower bounds on the limiting values,

$$-2{\cdot}0001 < g_\infty < -1{\cdot}9998 \quad (q=2)$$

$$-1{\cdot}8530 < g_\infty < -1{\cdot}8515 \quad (q=3)$$

$$-1{\cdot}7810 < g_\infty < -1{\cdot}7677 \quad (q=4).$$

This leads to the estimates of $\alpha(q)$ given at the beginning of this article.

Straley and Fisher obtained also the critical exponents $\beta$ and $\gamma'$ for the three-state Potts model, and combined them to test compliance with the Rushbrooke inequality $\alpha' + 2\beta + \gamma' \geqslant 2$. Their exponent sum was $1{\cdot}76 \pm 0{\cdot}21$, which violates the inequality. When their value of $\alpha'$ is replaced by ours, the sum becomes $2{\cdot}00 \pm 0{\cdot}12$, which is consistent with the inequality.

## Acknowledgments

We are grateful to C Domb, M E Fisher, and J P Straley for their comments on earlier versions of the manuscript. A portion of this work was supported by the Air Force Office of Scientific Research through the National Research Council.

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