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Critical behaviour of the four-dimensional $n = 0$ model with a free surface

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Abstract. A study has been made of the layer and local susceptibilities of the four-dimensional $n = 0$ (self-avoiding walk) model. A renormalisation group calculation for general n gives $\chi_1(t) \sim At^{-1/2}|\ln t|^{(n+2)/2(n+8)}$ and $\chi_{11}(t) \sim B + Ct^{1/2}|\ln t|^{-(n+2)/2(n+8)}$ where $t = (T - T_c)/T_c$. Series expansions to 11th order have been generated for these quantities for $n = 0$, and analysis allows estimates of A, B and C to be made. These are then shown to be qualitatively similar to known exact amplitudes for the analogous spherical model.

1. Introduction

In an earlier paper (Barber *et al* 1978) the critical behaviour of the layer and local susceptibilities of the two- and three-dimensional n-vector model in the $n=0$ (self-avoiding walk) limit was studied. Using exact series expansions, estimates of the critical exponents were obtained both by standard methods (Gaunt and Guttmann 1974) and by 'tailor made' methods appropriate to the particular problem. In this study of the four-dimensional model, we have obtained exact series expansions, and additionally have calculated the critical exponents using renormalisation group arguments, which are expected to be exact in four dimensions. Given the critical exponents, series analysis is used to provide estimates of the critical amplitudes. (The critical temperature was obtained in an earlier paper (Guttmann 1978).)

The Hamiltonian for the model is

$$H = -J \sum_{\langle i,j\rangle} \sum_{\alpha=1}^{n} \mu_{i,\alpha}^{(n)} \mu_{j,\alpha}^{(n)} - mH_1 \sum_{i=1}^{N} \mu_{i,1}^{(n)} - mH_1' \sum_{i=1}^{n'}{}' \mu_{i,1}^{(n)}.$$

The above Hamiltonian applies to a system of n component spins $\mu_{i,\alpha}^{(n)}$ $(\alpha = 1, 2, \ldots, n)$ on a d-dimensional semi-infinite hypercubic lattice of N spins, with $n' = O(N^{(d-1)/d})$ spins in the $(d-1)$-dimensional surface hyperplane. The first summation is over nearest neighbour pairs. The magnetic field H_1 couples to the '1' component of each spin, while a surface field, H_1', couples to the '1' component of each surface spin. The layer susceptibility is defined by $\chi_1 = -\partial^2 F/\partial H \partial H_1$ and the local susceptibility is defined by $\chi_{11} = -\partial^2 F/\partial H_1^2$. Near the critical temperature, parametrised by the variable $t = (T - T_c)/T_c$, one has $\chi_1 \sim t^{-\gamma_1}$, $\chi_{11} \sim t^{-\gamma_{11}}$. In four dimensions, $\gamma_1 = \frac{1}{2} = -\gamma_{11}$ which follows from mean field theory, but as expected at the critical dimension, the appearance of ultraviolet divergences signals the presence of confluent logarithmic terms. In fact, as we show in the next section, $\chi_1 \sim At^{-1/2}|\ln t|^{(n+2)/2(n+8)}$ and $\chi_{11} \sim$

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$B+Ct^{1/2}|\ln t|^{-(n+2)/2(n+8)}$, which may be compared to the bulk result $\chi\sim Dt^{-1}|\ln t|^{(n+2)/(n+8)}$. In the third section we discuss the generation and analysis of exact series expansions, which permit the estimates of the amplitudes A, B and C to be made.

2. Renormalisation group calculations

In the momentum representation the Hamiltonian for the system is

$$H=\tfrac{1}{2}\int \mathrm{d}^d q(m^2+q^2)\phi_i(\boldsymbol{q})\phi_i(\nu\boldsymbol{q})$$
$$+(g_0/4!)\tfrac{1}{8}\sum_{\epsilon_i=\pm1}\epsilon_1\epsilon_2\epsilon_3\epsilon_4\int\Big(\prod_i \mathrm{d}^d q_i\Big)\phi_i(\boldsymbol{q}_1)\phi_i(\boldsymbol{q}_2)\phi_j(\boldsymbol{q}_3)\phi_j(\boldsymbol{q}_4)$$
$$\times\delta^{d-1}(\boldsymbol{p}_1+\boldsymbol{p}_2+\boldsymbol{p}_3+\boldsymbol{p}_4)\delta\Big(\sum_i\epsilon_i k_i\Big)$$

where $\boldsymbol{q}=(\boldsymbol{p},k)$, $\boldsymbol{p}$ being a $(d-1)$-dimensional vector, $\nu\boldsymbol{q}=(-\boldsymbol{p},k)$ and the Fourier expansion functions are

$$\psi_q(\boldsymbol{X})=\sqrt{2}\exp(\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{\rho})\sin(kz+\Phi).$$

We will particularise to the case where the spin interaction strength in the surface is the same as in the bulk, so that $\Phi=k$ (see Lubensky and Rubin 1975a). The position variable $\boldsymbol{X}=(\boldsymbol{\rho},z)$ and the $d-1$ components of $\boldsymbol{\rho}$ extend from plus to minus infinity and $0\leqslant z<\infty$.

To calculate the susceptibilities in four dimensions we need to solve the Callen–Symanzik equation for the two-point vertex function defined as the inverse of the two-point Green's function, that is,

$$2\int \mathrm{d}k\,\Gamma_{\mathrm{p}}^{(2)}(k_1,k_2)G_{\mathrm{p}}^{(2)}(k_2,k_3)=\delta(k_1-k_3)-\delta(k_1+k_3).$$

That there is only one correlation length involved is manifest by the Wilson functions being proportional to $\delta(k_1-k_2)-\delta(k_1+k_2)$. For instance in the minimal subtraction scheme, only terms in $\Gamma_{\mathrm{p}}^{(2)}(k_1,k_2)$ that are proportional to $\delta(k_1-k_2)-\delta(k_1+k_2)$ have poles in $\epsilon=4-d$. Consequently we can immediately write down the Callen–Symanzik equation (Brézin *et al* 1976) for the renormalised two-point vertex function,

$$\left[\mu\frac{\partial}{\partial\mu}+w(g)\frac{\partial}{\partial g}-\eta(g)-\left(\frac{1}{\nu(g)}-2\right)t\frac{\partial}{\partial t}\right]\Gamma_{\mathrm{p}}^{\mathrm{R}}(k_1,k_2,t,g,\mu)(\delta(k_1-k_2)-\delta(k_1+k_2))$$
$$=0$$

where t, g and μ are the renormalised mass squared, the coupling constant and the momentum scale parameter respectively, and

$$w(g)=\tfrac{1}{6}(n+8)g^2$$
$$\eta(g)=\tfrac{1}{72}(n+2)g^2$$
$$1/\nu(g)-2=-\tfrac{1}{6}(n+2)g$$

are given by Brézin *et al* (1976).

The Callen–Symanzik equation is solved using the standard method of characteristics. Defining $g(\lambda)$ and $t(\lambda)$ via

$$\frac{\mathrm{d}g(\lambda)}{\mathrm{d}\ln\lambda}=W(g)$$

and

$$\frac{\mathrm{d}\ln t(\lambda)}{\mathrm{d}\ln\lambda}=-\left(\frac{1}{\nu(g(\lambda))}-2\right)$$

we obtain

$$\Gamma^{\mathrm{R}}_{\mathrm{p}}(k_1,k_2,t,g,\mu)=Z(\lambda)\Gamma^{\mathrm{R}}_{\mathrm{p}}(k_1,k_2,t(\lambda),g(\lambda),\lambda\mu)$$

with

$$\ln Z(\lambda)=-\int_g^{g(\lambda)}\frac{\eta(g')}{W(g')}\mathrm{d}g'.$$

Solving the above equations with the initial conditions $g(1)=g$, $t(1)=t$ in the small-g region gives

$$Z=\exp\left(-\frac{n+2}{12(n+8)}g(\lambda)\right)\approx 1$$

$$g(\lambda)\sim|\ln\lambda|^{-1}$$

$$t\sim(\lambda\mu)^2(g(\lambda))^{-(n+2)/(n+8)}\sim(\lambda\mu)^2|\ln\lambda|^{(n+2)/(n+8)}$$

where we have put $t(\lambda)=(\lambda\mu)^2$.

Using $Z\approx 1$ and dimensional analysis gives

$$\Gamma^{\mathrm{R}}_{\mathrm{p}}(k_1,k_2,t,g,\mu)=\mu\lambda\,\Gamma^{\mathrm{R}}_{\mathrm{p}/\lambda\mu}(k_1/\lambda\mu,k_2/\lambda\mu,t(\lambda)/\lambda\mu,g(\lambda),1)$$

which we invert to find an equation for $G^{\mathrm{R}}_{\mathrm{p}}(k_1,k_2)$ that is subsequently inverse Fourier transformed to an equation for $G^{\mathrm{R}}_0(z_1,z_2)$, namely

$$G^{\mathrm{R}}_0(z_1,z_2,t,g,\mu)=t^{-1/2}g^{-(n+2)/2(n+8)}G^{\mathrm{R}}_0(\lambda\mu z_1,\lambda\mu z_2,g(\lambda),1).$$

Into this we can substitute the mean field function

$$\begin{aligned}G^2_0&(z_1,z_2,t,g,\mu)\\&=-\tfrac{1}{2}\{[(1-\lambda_1\,.\,\lambda\mu)/(1+\lambda_1\,.\,\lambda\mu)]\exp(-\lambda\mu|z_1+z_2|)-\exp(-\lambda\mu|z_1-z_2|)\}\\&=G_0(z_1,z_2)\end{aligned}$$

given by Lubensky and Rubin (1975b) (λ_1 is the extrapolation length).

It is now a simple matter to find the scaling relations for the susceptibilities

$$\chi=\lim_{z_1\to\infty}\sum_{z_2\geqslant 0}G_0(z_1,z_2)$$

$$\chi_1=\sum_{z_2\geqslant 0}G_0(0,z_2)$$

$$\chi_{11}=G_0(0,0).$$

Substituting for $\lambda\mu$ and $g(\lambda)$ in terms of t gives

$$\chi \sim t^{-1}|\ln t|^{(n+2)/(n+8)}$$

$$\chi_1 \sim t^{-1/2}|\ln t|^{(n+2)/2(n+8)}$$

$$\chi_{11} \sim t^{1/2}|\ln t|^{-(n+2)/2(n+8)}.$$

A check on the above results is obtained by writing the mean field Green's function in terms of the correlation length $\xi = t^{-1/2}$ (equation 4.6 of Lubensky and Rubin (1975b)) and then substituting in the corrected value of

$$\xi = t^{-1/2}|\ln t|^{(n+2)/2(n+8)}$$

which then yields expressions for χ_1 and χ_{11} in agreement with those obtained above.

Further, in the limit as $n \to \infty$, the results agree with those obtained by Barber (1974) for the spherical model.

3. Series calculations

As shown in Barber *et al* (1978), the graphs contributing to the layer susceptibility χ_1 in the $n = 0$ case are just self-avoiding walks with one end attached to the surface—called TASAWS, an acronym for terminally attached self-avoiding walks. For the local susceptibility χ_{11} the appropriate graphs in the $n = 0$ case are self-avoiding walks which both start and finish on the surface.

Series expansions for χ_1 and χ_{11} have been obtained by enumerating the above class of walks on a four-dimensional lattice, taking account of appropriate symmetries. Coefficients up to and including v^{11} in the reduced high-temperature isothermal susceptibility series $k_BT\chi_1/m^2 = \Sigma_{n\geq 0}\, a_n v^n$ and $k_BT\chi_{11}/m^2 = \Sigma_{n\geq 0}\, b_n v^n$ were obtained. As a by-product of this calculation the mean-square-end-to-end distance of TASAWS was also obtained, though no subsequent analysis of this series has been attempted. These series are shown in table 1.

Table 1. Series expansion coefficients of the local susceptibility χ_1, the layer susceptibility χ_{11} and the mean-square-end-to-end distances of TASAWS for the four-dimensional n-vector model with $n = 0$.

n	Local susceptibility χ_1	Layer susceptibility χ_{11}	Mean-square-end-to-end-distance of TASAWS $\langle R_n^2 \rangle$
0	1	1	—
1	7	6	1·000 000 000 00
2	43	30	2·325 581 395 30
3	271	156	3·686 346 863 50
4	1 705	816	5·154 252 199 40
5	10 927	4 500	6·618 376 498 60
6	70 159	25 176	8·162 202 996 10
7	454 975	146 028	9·706 834 441 50
8	2 954 977	853 776	11·314 225 457 60
9	19 303 531	5 105 652	12·925 302 578 10
10	126 259 225	30 653 760	14·585 664 532 60
11	828 984 223	186 886 296	16·250 057 068 90

The critical value of the expansion variable for the bulk system was obtained in an earlier study (Guttmann 1978) and is $1/v_c = 6{\cdot}7720 \pm 0{\cdot}0005$. As shown in Barber *et al* (1978), the surface and layer susceptibilities also diverge at the same critical temperature as the bulk system.

Though the renormalisation group analysis yields estimates of the exponents multiplying the confluent logarithmic terms, we thought it worthwhile to see if these could be extracted from the series. The method used was that described in Guttmann (1978). Unfortunately, the results were quite disappointing, in that a wide range of values of the confluent logarithmic exponent seemed to be possible. It is at least reassuring to note that this wide range included the exact values obtained from RG analysis. We only mention these calculations for the sake of completeness, and to suggest that these series constitute an excellent benchmark for any new method of analysis for confluent logarithms that may be proposed.

In order to analyse the series for critical amplitudes, given the critical exponents and critical temperatures, we first transformed the series using the transformation $v \to x/(2-x/x_c)$. This leaves v_c as a fixed point of the transformation, but maps $-v_c$ to infinity, thus removing the effect of the non-physical (antiferromagnetic) singularity at $v = -v_c$. Such a singularity is expected to be present in hypercubic lattices of any dimensionality $d > 1$. Given the new series $\chi_1^*(x) = \chi_1(v)$, we divided out by the singular part, $(v_c/v)^{1/8}(1-v/v_c)^{-1/2}|\ln(1-v/v_c)|^{1/8}$. The factor $(v_c/v)^{1/8}$ is introduced to remove the branch point at the origin, but does not affect the estimate of the amplitude. The resultant series is then an expansion for the amplitude. That is, given $k_BT\chi_1(v)/m^2 \sim B(v)(1-v/v_c)^{-1/2}|\ln(1-v/v_c)|^{1/8}$ we formed the series $k_BT\chi_1^*(x)(x/x_c)^{1/8}(1-x/x_c)^{1/2}|\ln(1-x/x_c)|^{-1/8}/m^2 \sim 2^{-1/2}B(x)$, where the factor $2^{-1/2}$ arises from the transformation. The amplitude $2^{-1/2}B(x_c)$ was estimated by forming diagonal and off-diagonal Padé approximants to the series, and evaluating these at $x = x_c = v_c$.

Convergence was moderately good, enabling the estimate $2^{-1/2}B(x_c) = 2{\cdot}8 \pm 0{\cdot}2$ to be made. A similar analysis was then performed for $\chi_{11}(v)$, though modification had to be made to take account of the fact that the singularity is cusp like. That is, since $k_BT\chi_{11}(v)/m^2 \sim C(v) + D(v)(1-v/v_c)^{1/2}|\ln(1-v/v_c)|^{-1/8}$, near $v = v_c$ the analytic part $C(v)$ will dominate. Therefore division by the vanishing singular part $(1-v/v_c)^{1/2}|\ln(1-v/v_c)|^{-1/8}$ would introduce a diverging singular part. To overcome this, the term $C(v)$ must first be removed, and this was done by evaluating Padé approximants to $\chi_{11}(v)$ at $v = v_c$. These were quite well converged, enabling the estimate $kT\chi_{11}(v_c)/m^2 = 6{\cdot}10 \pm 0{\cdot}10$ to be made. Subtracting this value from the original series then results in a series in which the singular part factors, and so can be removed by division as was done in the analysis of $\chi_1(v)$.

Repeating the transformation and division operations performed in the analysis of $\chi_1(v)$ leads to a series for the amplitude $2^{1/2}D(v)$. Evaluating Padé approximants to this series at $v = v_c$ gives reasonably well converged approximants, enabling the estimate $D(v_c) = -10{\cdot}1 \pm 0{\cdot}9$ to be made. Thus near T_c we can write

$$kT\chi_1(v)/m^2 \sim 4{\cdot}0(1-v/v_c)^{-1/2}|\ln(1-v/v_c)|^{1/8}$$

and

$$kT\chi_{11}(v)/m^2 \sim 6{\cdot}1 - 10{\cdot}1(1-v/v_c)^{1/2}|\ln(1-v/v_c)|^{-1/8}.$$

For the analogous four-dimensional spherical model with a free surface, Barber (1974) has evaluated the corresponding amplitudes exactly, and finds

$$J\chi_1(K)/m^2 \sim 0{\cdot}02813(K_c-K)^{-1/2}|\ln(K_c-K)|^{1/2}$$

$$J\chi_{11}(K)/m^2 \sim 0{\cdot}5 - 17{\cdot}772(K_c-K)^{1/2}|\ln(K_c-K)|^{-1/2}$$

where $K = J/kT$.

Recasting our results for the $n = 0$ case into a directly comparable form, we obtain

$$J\chi_1(K)/m^2 \sim 0{\cdot}23(K_c-K)^{-1/2}|\ln(K_c-K)|^{1/8}$$

and

$$J\chi_{11}(K)/m^2 \sim 0{\cdot}90 - 3{\cdot}9(K_c-K)^{1/2}|\ln(K_c-K)|^{-1/8}.$$

Corresponding amplitudes are of similar sign, and can be compared in magnitude in the following sense. For the spherical model the product of the amplitudes of the singular parts of χ_1 and χ_{11} is exactly $-\frac{1}{2}$, which is just the value of $-J\chi_{11}(K_c)/m^2$. This is not just numerology, but follows from equations (60) and (62) in Barber. That is, these observations can be made without knowing the values of the amplitudes. The corresponding amplitudes in the $n = 0$ case give $-0{\cdot}90$ for the products of the amplitudes of the singular parts, which is in precise agreement with the value of $-J\chi_{11}(K_c)/m^2$ for this model. Whether this is a feature of all four-dimensional n-vector models remains to be seen.

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