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Conformal invariance, finite-size scaling and surface magnetic exponent of the Potts model in two dimensions

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Abstract. The analysis of renormalisation group equations for the q-state Potts model in two dimensions is generalised to include the presence of a surface field H_S besides the bulk one, H_B. Combined with conformal invariance results, this allows prediction of a surface susceptibility behaviour $\partial^2 f/\partial H_S\,\partial H_B \sim L^{-1/8}(1-c'\ln L)^{15/16}$ for a $q=4$ system of size L at the critical temperature.

This prediction is checked by a Monte Carlo based finite-size scaling analysis, which also nicely reproduces the exact and conjectured magnetic surface exponents for $q=2$ and 3, respectively. For the Baxter-Wu model similar methods give results consistent with the $q=4$ behaviour without logarithmic corrections ($c'=0$).

1. Introduction

Surface critical phenomena received considerable attention in the recent literature (Binder 1983). For two-dimensional systems the 'surface' is one-dimensional (e.g. the linear boundary of a semi-infinite system) and the only surface critical phenomena occurring are those associated with the ordinary transition, i.e. in a magnetic context, with the simultaneous ordering of bulk and surface spins below the bulk critical temperature.

All the exponents of boundary quantities, for example, the surface magnetisation, are known once given the scaling dimension y'_H according to which the surface ordering field H_s has to scale in the homogeneous singular surface free energy near criticality§.

For the two-dimensional Ising model the exponent y'_H is known to be $\frac{1}{2}$ on the basis of exact calculations (McCoy and Wu 1967). For the q-state Potts model, which is a non-trivial generalisation of the Ising case ($q=2$), y'_H remained essentially unknown until the assumption of conformal invariance at criticality allowed most recently to conjecture both bulk (Belavin *et al* 1984a, b, Friedan *et al* 1984) and surface exponents (Cardy 1984).

For bulk critical properties of the two-dimensional q-state Potts model a large amount of exact or conjectured results were already available before the most recent developments based on conformal invariance. This body of knowledge was indeed very important for the correct application and confirmation of conformal invariance results. With respect to surface critical properties, the conformal invariance approach

§ Differences of the exchange coupling at the surface with respect to the bulk one can be shown to be always irrelevant with scaling dimension $y'_T=-1$ (Burkhardt and Cardy 1986).

played a more autonomous and important role, since it allowed to conjecture for the first time the values of surface exponents of Potts as well as of other types of two-dimensional systems (Cardy 1984).

First attempts to verify numerically these predictions for the Potts model were made by Droz *et al* (1985), von Gehlen and Rittenberg (1986), and von Gehlen *et al* (1986), with transfer matrix based finite-size scaling calculations.

In the case of the $q=3$ Potts model these calculations essentially confirmed the value of y'_H predicted on the basis of conformal invariance. For the $q=4$ model the situation appeared very different, with more poorly convergent results, which at first sight could indicate a possible disagreement with conformal invariance.

In the case of the $q=4$ Potts model a major difficulty for extracting numerically the correct bulk exponents is well known to be the presence of logarithmic corrections. Such corrections, which originate from the existence of a marginal scaling field in the renormalisation group (RG) equations for the model (Nauenberg and Scalapino 1980, Cardy *et al* 1980), must be taken into account in order to extract bulk exponents with a satisfactory degree of accuracy from finite-size scaling data (Blöte and Nightingale 1982).

In § 3 of this paper we present an extension, including the surface magnetic field, of the previous bulk RG equations analysis (Cardy *et al* 1980) for the Potts model around $q=4$. Combined with suitable information from conformal invariance, to be summarised in § 2, the new analysis allows us to predict the precise form of logarithmic corrections for quantities such as the boundary susceptibility of a finite system at criticality which is actually obtained by our numerical test calculations presented in § 4.

Such calculations, based on Monte Carlo methods, are a first successful step towards an accurate numerical test of y'_H for the $q=4$ Potts model. Similar calculations have been carried out here for the Ising, $q=3$ Potts, and Baxter–Wu models in two dimensions, as well.

Section 5 is devoted to some concluding remarks and to the discussion of further consequences of the results of § 3.

2. Magnetic surface exponent and conformal invariance

In order to formulate a scaling theory of both bulk and surface critical phenomena in the q-state Potts model, let us consider, for later convenience, the free energy per spin of a finite square system of side L. For the singular part of this free energy near criticality and at large L we expect

$$f(\phi, h, h_s, 1/L) = l^{-d} f(l^{y_T}\phi, l^{y_H} h, l^{y'_H} h_s, l/L) \tag{2.1}$$

where d is the dimensionality of the lattice (2 in our case) and l is a rescaling factor. ϕ and h are the temperature and magnetic bulk scaling fields, respectively. Near criticality ϕ and h will be proportional to $K-K_c$ and H_B, respectively, K being the nearest-neighbour reduced bulk coupling with critical value K_c and H_B a symmetry-breaking field, also acting in the bulk. The surface scaling field h_s depends on both bulk and surface couplings and is proportional to the symmetry-breaking fields H_s, acting on the surface spins only.

The exponent y_T and y_H are the familiar bulk temperature and magnetic exponents, respectively; y'_H is the surface magnetic exponent. Irrelevant bulk and surface scaling fields are not included in equation (2.1), as they do not affect the dominant singular behaviour. The quantity $1/L$ plays the role of scaling field with scaling dimension $y = 1$.

In the limit of L going to infinity the free energy in equation (2.1) will split into a bulk part, f_B, and a surface part, f_S, according to

$$f \underset{L\to\infty}{\simeq} f_B + \frac{1}{L} f_S + O\left(\frac{1}{L}\right). \tag{2.2}$$

f_B depends only on the bulk scaling fields, whereas f_S depends on both bulk and surface scaling fields. An equation similar to (2.2) is also satisfied by the regular part of the free energy per site. Because of the assumed regularity, equation (2.2) in this case implies that, for example, a derivative of this function with respect to both H_B and H_S should simply go to zero as $1/L$ in the thermodynamic limit.

This property of the regular contribution to the boundary susceptibility of the finite system will turn out to be very important for our numerical investigation of the four-state Potts model in § 4.

Within the field theoretic approach to second-order phase transitions, the principle of conformal invariance has proved extremely powerful as far as two-dimensional systems are concerned (Belavin *et al* 1984a, b, Friedan *et al* 1984). Critical exponents within various universality classes appear to be determined in terms of a single dimensionless number, c, the central charge of the Virasoro algebra (Virasoro 1970), or conformal anomaly. When the value of this charge is less than one, reflection positivity (unitarity) further constrains the values of c to be quantised (Friedan *et al* 1984) according to

$$c = 1 - \frac{6}{m(m+1)} \qquad m = 3, 4, \ldots. \tag{2.3}$$

The critical q-state Potts model has been shown to correspond to $m = 3$ for $q = 2$ (Ising), $m = 5$ for $q = 3$ and $m = \infty$ for $q = 4$ (Kadanoff 1984, Dotsenko and Fateev 1985). Introducing the scaling dimensions $x = d - y = 2 - y$ and $x' = d - 1 - y' = 1 - y'$ for bulk and surface operators, respectively, on the basis of a formula due to Kac (1979) one derives (Cardy 1984)

$$x_T = (m+3)/2m \tag{2.4a}$$

$$x_H = (m+3)(m-1)/8m(m+1) \tag{2.4b}$$

$$x'_H = (m-1)/(m+1). \tag{2.4c}$$

For example, (2.4c) yields $y'_H = \frac{1}{2}, \frac{1}{3}$ and 0 for the $q = 2, 3$ and 4 Potts models, respectively. For m odd between 5 and ∞, formulae (2.4) apply to unitary Potts models with non-integer q, given by (Kadanoff 1984, Cardy 1986)

$$\sqrt{q} = 2\cos(\pi/(m+1)). \tag{2.5}$$

The values of q given by equation (2.5) accumulate at $q = 4$. Equations (2.4a), (2.4b) and (2.5) are consistent with the den Nijs (1979) conjecture for y_T and with a similar conjecture for y_H (Nienhuis *et al* 1980, Pearson 1980). Since equations (2.4) are also consistent with

$$x'_H = 4x_H/x_T \tag{2.6}$$

it is reasonable to conjecture that this last relation can be used to infer the q dependence of x'_H by substituting the q-dependent expressions of x_H and x_T resulting from the above-mentioned conjectures. This should be most plausible in the neighbourhood of $q=4$, where the points of equation (2.5) accumulate. To leading order in $\varepsilon=q-q_c$, we have in particular (Nienhuis *et al* 1980, Pearson 1980)

$$y_H=\tfrac{15}{8}-(1/16\pi)(-\varepsilon)^{1/2}+O(-\varepsilon) \qquad \varepsilon<0 \tag{2.7}$$

and (den Nijs 1979)

$$y_T=\tfrac{3}{2}-(3/4\pi)(-\varepsilon)^{1/2}+O(-\varepsilon). \tag{2.8}$$

Using (2.6) this gives

$$y'_H=(1/\pi)(-\varepsilon)^{1/2}+O(-\varepsilon). \tag{2.9}$$

This result will be crucial for the analysis to be carried out in the next section.

We should like to make one further remark here. If we extend the Potts model to a Potts lattice gas, the system for $q<4$ possesses both a critical and a tricritical point, which coalesce at $q=4$ (Nienhuis *et al* 1979).

In conformal theory, tricritical points are described by central charges with m even, which modifies the relations (2.4) but not (2.6) (Friedan *et al* 1984). Using appropriate conjectures for the tricritical y_T and y_H (Nienhuis *et al* 1979) we thus find

$$y'_H=-(1/\pi)(-\varepsilon)^{1/2}+O(-\varepsilon). \tag{2.10}$$

While for the critical points of the Potts model the surface field is relevant and marginal for $q=4$ it is irrelevant for the tricritical points.

Finally, it is rather natural to use the relation (2.6) for all q and thus to make a conjecture for the surface magnetic exponent for arbitrary q. In terms of the usual Potts variable u which is

$$u=(2/\pi)\cos^{-1}\sqrt{q}/2 \tag{2.11}$$

we have the very simple conjecture

$$y'_h=u. \tag{2.12}$$

This implies for percolation $(q\to 1)$, $y'_h=\frac{2}{3}$. This result, which was also found by Cardy (1984), is in agreement with an approximate calculation based on series expansion methods (De Bell and Essam 1980). It is interesting because percolation is a non-unitary theory and so far conformal invariance has given few results for such theories. The result $y'_h=\frac{2}{3}$ is now being verified with Monte Carlo calculations; the results will be published elsewhere.

3. Scaling theory of bulk and surface properties at the $q=4$ Potts multicritical point

The scaling formulation discussed at the beginning of the previous section should in general be sufficient for setting up a successful finite-size scaling strategy for determining y'_H. As we will see in the next section, the strategy we follow here amounts to computing the boundary susceptibility

$$\chi_{BS}=\left.\frac{\partial^2 f}{\partial H_S\,\partial H_B}\right|_{H_S=H_B=0,\,K=K_c} \tag{3.1}$$

for systems of different sizes L at the bulk critical temperature. On the basis of equation (2.1) and the assumed properties of the scaling fields, one expects

$$\chi_{BS} \underset{L\to\infty}{\sim} L^x \tag{3.2}$$

with

$$x = -d + y_H + y'_H. \tag{3.3}$$

For the two-dimensional nearest-neighbour q-state Potts model $K_c = \ln(1+\sqrt{q})$ is known from self-duality, so the problem of determining y'_H essentially reduces to fitting, with the power law behaviour (3.2), a sufficiently asymptotic set of determinations of χ_{BS}.

Previous experience with the bulk scaling properties of the four-state Potts model, however, lets us suspect that in this case, to reach a sufficient degree of asymptoticity for the above fit can be practically impossible due to the possible presence of logarithmic corrections to the power law behaviour (3.2).

The analysis to be carried out below will, in particular, allow us to predict the form of the logarithmic corrections for the boundary susceptibility of a $q=4$ finite system at criticality, thus opening the way to the numerical determination of y'_H, to be discussed in the next section.

Logarithmic corrections of the bulk critical behaviour of the $q=4$ Potts model can be explained in terms of the presence of a marginal scaling field in the renormalisation group equations for the model (Nauenberg and Scalapino 1980, Cardy *et al* 1980). It is known that such marginal fields can lead to logarithmic corrections as well as to essential singularities (Wegner 1976). For the $q=4$ Potts model the marginal field, called the dilution field, is related to the chemical potential of vacancies in the lattice gas generalisation of the model, originally considered within the RG context by Nienhuis *et al* (1979).

Here we want to generalise the work of Cardy *et al* (1980) to the presence of a surface scaling field, namely the h_s already introduced in § 2.

Indicating by ψ the dilution field, the RG equations we obtain in the neighbourhood of $q = q_c = 4$ have the form

$$\mathrm{d}\phi/\mathrm{d}x = (y_T + b\psi)\phi \tag{3.4a}$$

$$\mathrm{d}h/\mathrm{d}x = (y_H + c\psi)h \tag{3.4b}$$

$$\mathrm{d}\psi/\mathrm{d}x = a(\psi^2 + \varepsilon) \tag{3.4c}$$

$$\mathrm{d}h_s/\mathrm{d}x = e\psi h_s \tag{3.4d}$$

$$\mathrm{d}L/\mathrm{d}x = -L \tag{3.4e}$$

to leading order in ε.

The first three equations are the same as those already obtained by Cardy *et al* (1980), who showed that the constants a, b and c are universal and equal to $1/\pi$, $3/4\pi$ and $1/16\pi$, respectively, on the basis of exact or conjectured results for the q-state Potts model. y_T and y_H are the $q=4$ bulk exponents, equal to $\frac{3}{2}$ and $\frac{15}{8}$ respectively, and x denotes the logarithm of the RG rescaling l.

The form of equations (3.4a)–(3.4c) follows from the assumption of analyticity in q and from other general projecties of the RG transformation, which are expected to be valid also on the basis of experience with approximate treatments.

The real space renormalisation group approach to surface critical phenomena (Burkhardt and Eisenriegler 1977) has shown that surface couplings cannot affect the transformation laws of bulk couplings. Once we assume the existence of a symmetry-breaking surface scaling field at the surface, equation (3.4*d*) is the only possibility for its evolution compatible with the symmetries and the general rules reviewed by Cardy *et al* (1980).

We still have to determine e. This can be done on the basis of the results of § 2. The fixed points of (3.4) are $\phi = h = h_s = 0$ and $\psi^*(\varepsilon) = \pm(-\varepsilon)^{1/2}(q \leq q_c)$. Working out the linearisation of the transformation (3.4) at the fixed point, we obtain a surface magnetic exponent $y'_H = \pm e(-\varepsilon)^{1/2}$, where the positive and negative signs apply to critical and tricritical fixed points, respectively. Identification with (2.9) and (2.10) immediately gives $e = 1/\pi$.

With inclusion of the marginal dilution field ψ, equation (2.1) now becomes

$$f(\phi(0), \psi(0), h(0), h_s(0), L) = e^{-xd} f(\phi(x), \psi(x), h(x), h_s(x), Le^{-x}) \tag{3.5}$$

where the fields on the RHS can be obtained by simple integration of (3.4). More explicitly, putting $e^x = L$ and

$$Z = [1 - (\psi(0)/\pi) \ln L]^{-1} \tag{3.6}$$

for $q = 4$ we find

$$f(\phi(0), \psi(0), h(0), h_s(0), L) = L^{-d} f(L^{y_T} Z^{3/4} \phi(0), Z\psi(0), L^{y_H} Z^{1/16} h(0), Z^{-1} h_s(0), 1). \tag{3.7}$$

The surface susceptibility given by equation (3.1) will thus behave as

$$\chi_{SB}(L) \simeq L^{-1/8} Z^{-15/16} A(Z\psi(0)) \tag{3.8}$$

where $A(t) = f(0, t, 0, 0, 1)$ is analytic.

The leading behaviour is thus

$$\chi_{BS}(L) \simeq L^{-1/8} [1 - (\psi(0)/\pi) \ln L]^{15/16} \tag{3.9}$$

where $\psi(0)$ is the as yet unknown value of the dilution scaling field for the model under consideration, in our case the undiluted nearest-neighbour critical $q = 4$ Potts model.

4. Numerical results for Potts and Baxter–Wu models

As anticipated above, we follow here the strategy of computing χ_{BS} for blocks of different sizes L, by the Monte Carlo technique. A transfer matrix calculation of the same quantity for infinite strips ($L \times \infty$), would give the advantage of essentially exact calculations.

Here, however, in view of the difficulties with the four-state Potts model, we prefer to give up some precision in the determinations of χ_{BS} in favour of the possibility of testing sizes ($L \leq 24$), which are inaccessible by the transfer matrix approach. At the same time we try to reduce as much as possible the fluctuations by performing very long runs (up to 10^6 MC steps per spin).

We consider Potts models on square lattices with reduced Hamiltonians

$$H = K \sum_{\langle ij \rangle} \delta_{s_i, s_j} \tag{4.1}$$

where $s_i = 0, 1, \ldots, q$ and the sum is over nearest neighbours in a square $L \times L$ box Λ. It turns out to be convenient to choose periodic boundary conditions in one direction (this makes our blocks closer to the $L \times \infty$ strips considered in the transfer matrix approach). The sides perpendicular to the other direction are left as free boundaries, so the spins there properly constitute the surfaces $\partial\Lambda$ of our blocks.

The boundary susceptibility is computed as

$$\chi_{\mathrm{SB}} = \frac{q}{L^2} \sum_{\substack{i \in \Lambda \\ j \in \partial\Lambda}} (\langle \delta_{s_i,0} \delta_{s_j,0} \rangle - \langle \delta_{s_i,0} \rangle \langle \delta_{s_j,0} \rangle). \tag{4.2}$$

For the Ising case ($q = 2$) we calculated (4.2) for $L = 6, 8, 10, \ldots, 20$, with runs of about 5×10^5 MC steps per spin. In this case verification of equation (3.2) is very straightforward, and a simple least-squares fit with a straight line for $\ln \chi_{\mathrm{BS}}$ as a function of $\ln L$ gives $x = 0.38 \pm 0.01$ which is in excellent agreement with the exact result $x = -2 + 1.875 + 0.5 = 0.375$.

The situation is considerably less easy for the $q = 3$ case. We calculated χ_{BS} for $L = 4, 6, \ldots, 24$ with runs of up to 10^6 MC steps per spin. The slope x as determined by a simple fit turned out to be $x = 0.23 \pm 0.03$. The value expected on the basis of conformal invariance is $x = -2 + \frac{28}{15} + \frac{1}{3} = 0.20$. A more satisfactory agreement can be obtained by making use of a strategy of analysis of Monte Carlo data recently used with remarkable success in some problems concerning random fractals (Stella *et al* 1986). The idea is to consider the various $\chi_{\mathrm{BS}}(L)$ as approximate coefficients of a series. It is then possible to estimate the asymptotic behaviour of the coefficients by applying Padé approximants to compute the residue at $t = 1$ of the logarithmic derivative of

$$g(t) = \sum_{L=2,4,\ldots} \chi_{\mathrm{BS}}(L) t^L$$

which should be equal to $1 + x$. This kind of analysis, which is typical of work with exact enumerations, is not too sensitive to fluctuations of individual data and yields reasonably consistent Padé tables for $1 + x$. What we lose due to these fluctuations is rather well balanced by the possibility of testing a more asymptotic range of L than allowed by exact calculations.

On the basis of the Padé analysis we could estimate $x = 0.21 \pm 0.01$. This is a rather nice confirmation of the predictions of conformal invariance for $q = 3$. For the $q = 4$ Potts model, previous attempts to verify $y'_H = 0$ and thus $x = -0.125$ without taking into account logarithmic corrections have failed. Droz *et al* (1985) found $y'_H \simeq 0.23$. Von Gehlen *et al* (1986), working with a quantum version of the Potts model in $d = 1$, found $y'_H \simeq 0.12$. An approximate real space calculation yielded $y'_H = 0.31$ (Lipowski 1982). If we simply try to fit our data, which are for $L = 4, 6, 8, \ldots, 24$ with up to 10^6 MC steps per spin, by (3.2), we find $x \simeq 0.11$. Finite-size data thus seem to indicate an increase of χ_{BS} with L, whereas the expected value of x is -0.125. A Padé analysis of the same data gives a considerably lower value for x ($x \simeq 0$), but there is still no indication of a χ approaching zero for $L \to \infty$. According to our discussion in § 2 this failure has not to be put down to the survival of some regular contribution to χ_{BS}, since we know that this contribution goes to zero rapidly as $1/L$. The effect is clearly due to the logarithmic correction reported in equation (3.9)†.

To fit our data on the basis of equation (3.9) we need an estimate of $\psi(0)$. To this end we performed independent calculations of the specific heat of our finite systems at criticality. For this specific heat one can indeed predict (Nauenberg and Scalapino 1980)

$$C(L) \simeq L[1-(\psi(0)/\pi)\ln L]^{-3/2}. \tag{4.3}$$

A simple logarithmic plot of $C(L)$ gives an exponent $\alpha/\nu \simeq \frac{2}{3}$ instead of the correct value $\alpha/\nu = 1$, as implied by equation (4.3), a problem similar to the one we have for χ_{BS}. We obtained an estimate $\psi(0) \simeq -1.59$ by plotting $(C(L)/L)^{-2/3}$ as a function of $\ln L$. Using this value of $\psi(0)$ we plotted $\ln(\chi_{BS}^{(L)} L^{1/8})$ as a function of $\ln[1-(\psi(0)/\pi)\ln L]$ and found a slope $\simeq 1.02$, whereas the theoretical slope should be $\frac{15}{16} = 0.9375$.

A more direct test of y'_H comes from our Padé estimate of x for the series of coefficients $\chi_{BS}^{(L)}/[1-(\psi(0)/\pi)\ln L]^{15/16}$. In this case we estimate $x = -0.13 \pm 0.02$, which is in good qualitative agreement with the conformal invariance prediction $x = -0.125$.

We also performed finite-size scaling calculations for the Baxter–Wu model (Baxter and Wu 1973) which, as far as bulk properties are concerned, is known to be in the same universality class as the $q = 4$ Potts model but with $\psi(0) = 0$ in the scheme outlined above. For this model, e.g., there are no logarithmic corrections for the specific heat, so we should be able to fit directly the behaviour $\chi_{BS}^{(L)} \sim L^{-1/8}$. This indeed seems to be the case, since preliminary finite-size data for $L = 4, 6, \ldots, 24$ allowed a Padé estimate $x = -0.15 \pm 0.05$, which is qualitatively consistent with our expectance.

5. Concluding remarks

In this paper we have shown how an extension of the analysis of RG equations for the q-state Potts lattice gas near $q = q_c = 4$ allows us to determine precisely the form of logarithmic corrections to the scaling behaviour of quantities involving response to the surface scaling field H_s. The boundary susceptibility, χ_{BS}, has the nice feature of possessing regular contributions which go to zero as $1/L$ for $L \to \infty$. This highly simplifies the task of numerically determining y'_H for $q = 4$. An important ingredient, which is at the basis of the success of our numerical tests, is the somewhat unconventional Padé analysis of the approximate MC results.

Besides opening the way to the first successful verifications of the predictions of conformal invariance for the surface properties of the $q = 4$ Potts model, the analysis of RG equations performed in § 3 allows us to make at least one other interesting prediction, which should hopefully be confirmed by exact calculations.

We know that for the Potts model with $q > 4$ the transition is of first order, with a latent heat $L \sim \exp(-\pi^2/2\sqrt{\varepsilon})$ having an essential singularity in ε for $\varepsilon \to 0+$ (Baxter 1973). Knowledge of this result indeed allows us to put $a = 1/\pi$ in the bulk scaling field equation (3.4c) (Nauenberg and Scalapino 1980). Following steps similar to those

† We notice also that the unlikely possibility of $A(0) = 0$, which would modify (3.9), seems to be clearly ruled out, since in such a case the leading corrections would act in the sense of a more rapid apparent convergence to zero.

required to derive the latent heat result from equation (3.4), we can find how the discontinuity of the surface spontaneous magnetisation behaves for $q \geqslant 4$.

Considering directly the singular part f_s of the surface free energy for $L=\infty$, we can write

$$\Delta M_S(\psi(0)) \sim \frac{\partial}{\partial h_s(0)} f_S(\phi(0), \psi(0), h(0)=0, h_s(0)=0)\Big|_{\phi(0)=0-}^{\phi(0)=0+}$$

$$= \exp[-(d-1)x] \frac{\partial h_s(x)}{\partial h_s(0)} \frac{\partial}{\partial h_s(x)} f_S(\phi(x), \psi(0), 0, h_s(x))\Big|_{\phi(x)=0-}^{\phi(x)=0+} \quad (5.1)$$

where ΔM_s is the discontinuity of the surface magnetisation at the transition point (notice that $h_S \sim H_S$ for $H_S \to 0$). It is then immediate to rearrange (5.1) as

$$\Delta M_S(\psi(0)) \sim \exp\left(\int_{\psi(0)}^{\psi(x)} \frac{(1-d+e\psi)}{a(\psi^2+\varepsilon)} \mathrm{d}\psi\right)$$

$$\times \frac{\partial}{\partial h_s(x)} f_s(\phi(x), \psi(x), 0, h_s(x))\Big|_{\phi=0-}^{\phi=0+}. \quad (5.2)$$

Evaluation of the elementary integral in (5.2), together with the assumption that a discontinuity exists for the surface magnetisation for $q > q_c = 4$ leads us to predict for a pure system ($\psi < 0$), an essential singularity:

$$\Delta M_s \underset{q \to q_c^+}{\sim} \exp(-\pi^2/\sqrt{\varepsilon})[1+\mathrm{O}(\varepsilon)] \quad (5.3)$$

in which the coefficient in the exponential is $(\pi/a)(d-1)$. This is to be compared with the discontinuity in the bulk magnetisation $\Delta M \sim \exp(-\pi^2/8\sqrt{\varepsilon})$, as found by Cardy *et al* (1980).

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