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LETTER TO THE EDITOR

Linear defects in two-dimensional systems: a finite-size investigation

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Abstract. Finite-size scaling theory is employed to study non-universal and crossover critical behaviour in two-dimensional systems with linear defects. The finite-size method is shown to reproduce very accurately the non-universality as known to be present in the case of the Ising model. The calculations show that the non-universal behaviour of all the models investigated in the Ising universality class can be described approximately by a single universal curve.

Non-universal critical behaviour in two-dimensional systems is well known for systems with a two-component (Krinsky and Mukamel 1977) order parameter. Typical examples are the Baxter (1970) model and the Gaussian model (Wegner 1967). Recently, a new type of non-universality has been discovered (Bariev 1979, McCoy and Perk 1980) in the two-dimensional Ising model with a line defect, i.e. a line of enhanced nearest-neighbour couplings. Exact calculations have revealed that at the defect the local spontaneous magnetisation and the spin–spin correlation function are described by a magnetic defect exponent which depends continuously on the enhancement.

Scaling theory for defect planes has previously been discussed by Bariev (1979) and by Burkhardt and Eisenriegler (1981). For completeness, we reformulate their treatments.

Consider a d-dimensional lattice of generalised spins with (among others) a nearest-neighbour interaction K, as defined explicitly in individual cases below. There is a d^*-dimensional defect with enhanced coupling strength $(1+D)K$. The relative deviation from the critical temperature T_c is denoted by $\varepsilon = (T-T_c)/T_c$. We assume the presence of a bulk magnetic field h; h_1 is the magnetic field acting on the defect spins only. The singular part of the defect free energy per site f^*—defined as the difference of the total free energy with and without defects divided by the number of defect sites—satisfies a scaling relation. For small $|D|$ and for arbitrary scaling length L with $L^{y_T^*}|D|$ small, this relation reads

$$f^*(\varepsilon, h, h_1, D) = L^{-d^*} f^*(L^{y_T}\varepsilon, L^{y_h}h, L^{y_h^*}h_1, L^{y_T^*}D), \tag{1}$$

where the scaling indices y_T and y_h are the usual thermal and magnetic exponents, and y_T^* and y_h^* are related exponents: $y_T - d = y_T^* - d^*$ and $y_h - d = y_h^* - d^*$. These relations may be derived as follows. Consider a parameter in the d-dimensional Hamiltonian with exponent y. Denote by ω the critical dimension of the conjugate operator:

the corresponding correlation function at large separation r decays as $r^{-2\omega}$. Then $\omega + y = d$, a well known relation which follows from the fact that the second-order derivative of the bulk free energy can be expressed as a sum over space of a conjugate correlation function. If y^* is the scaling index of the parameter in the defect contribution to the Hamiltonian conjugate to the same correlation function, then one finds $\omega + y^* = d^*$, applying the same argument to the second-order derivative of the defect free energy. Eliminating ω one obtains $y - d = y^* - d^*$.

Beyond the crossover regime—i.e. for $|D|$ or $L^{y_T^*}|D|$ large—one has

$$f^*(\varepsilon, h, h_1, D) = L^{-d^*} f^*(L^{y_T}\varepsilon, L^{y_h}h, L^{y_{h_1}}h_1, D). \tag{2}$$

If the enhancement is irrelevant ($y_T^* < 0$), one expects $y_{h_1} = y_h^*$, whereas crossover to new values for y_{h_1} depending on the sign of D occurs for relevant enhancement ($y_T^* > 0$). Only if D is marginal ($y_T^* = 0$), may y_{h_1} continuously depend on D. Note that failure to scale D in equation (2) amounts to neglecting corrections to scaling and allowing only for D dependence in the critical amplitudes. Recall that the two-dimensional Ising model has a logarithmically divergent specific heat: $\alpha = 0$; that is, $\omega_T = d^* = 1$, $y_T^* = 0$. In other words, at $D = 0$ the enhancement is a marginal operator. From the exact results it follows that the marginality persists for $D \neq 0$. The exact expression for the magnetic defect exponent (Bariev 1979, McCoy and Perk 1980) is

$$y_{h_1} = 1 - \frac{1}{2\pi^2}[\cos^{-1}\tanh(2K_c^{\mathrm{I}}D)]^2 \tag{3}$$

for the two-dimensional Ising model on a square lattice with nearest-neighbour coupling K, with enhanced coupling $(1+D)K$ for spins within one single row of the lattice; $K_c^{\mathrm{I}} = \frac{1}{2}\ln(\sqrt{2}+1)$ is the critical point. For the defects considered below the enhancement D is defined in the same way.

In recent years finite-size scaling theory has been applied, in the form of phenomenological renormalisation, to a variety of exactly solved models (Nightingale 1976, 1977, 1979, Sneddon 1978, Kinzel and Schick 1981a). Also, models for which critical exponents can be deduced with the universality hypothesis have been investigated. Since, as these calculations have indicated, the theory works so well already for very small systems, it has become a powerful tool for the calculation of critical point exponents (e.g. Hamer and Barber 1981, Blöte *et al* 1981, Derrida 1981, Kinzel and Schick 1981a, b, Ràcz 1980, Roomany and Wyld 1980). Under these circumstances an investigation of finite-size scaling for defect phenomena is very interesting. The formulation of finite-size scaling in this case is quite analogous to the theory for surface effects (Fisher 1971) and may be obtained as follows.

Consider a system of finite extent. The finite size is characterised by a linear dimension n which is measured in units of the lattice spacing. The generalisation of equations (1) and (2) may then be obtained by introducing $1/n$ as an additional scaling field, with exponent 1. Below we invariably set the bulk parameters to their critical values. This being understood, they are henceforth omitted. For a finite system equation (2) generalises to

$$f^*(h_1, 1/n; D) = L^{-d^*} f^*(L^{y_{h_1}}h_1, L/n; D). \tag{4}$$

For the defect susceptibility $\chi_{11} \equiv \partial^2 f^*/\partial h_1^2$ one consequently finds

$$\chi_{11}(0, 1/n; D) = L^{2y_{h_1}-d^*}\chi_{11}(0, L/n; D) \sim n^{2y_{h_1}-d^*}. \tag{5}$$

In applying this relation to the analysis of two-dimensional systems with line defects, χ_{11} is obtained by numerical differentiation of the free energy. The latter in turn is computed with a transfer matrix technique. Fitting χ_{11} for systems of increasing size to equation (5) yields y_{h_1}. Note that χ_{11} follows directly from the total free energy so that f^* need not be calculated explicitly.

To investigate the validity of finite-size scaling for systems with defects, we first consider generalised Ising systems in the Ising universality class. The reduced Hamiltonian (which includes $-1/k_BT$ as a factor) reads

$$\mathcal{H} = K \sum_{(i,j)} s_i s_j + L \sum_{(k,l)'} s_k s_l + M \sum_{(m,n,p,q)} s_m s_n s_p s_q, \tag{6}$$

where $s_i = \pm 1$; the sums are over pairs of nearest-neighbour sites (i, j), pairs of next-nearest-neighbour sites $(k, l)'$, and quartets of sites (m, n, p, q) on the elementary squares of a simple square lattice.

For $L = M = 0$ one obtains the *Ising* model. If the condition $\cosh 4L = \exp(-4M)$ is satisfied, the system reduces to a special case of the *free-fermion* model solved exactly by Fan and Wu (1969). This model has a critical line: $\sinh 2K = \exp(-4L)$. Another special case we investigate is the *eight-neighbour* model $M = 0$.

To calculate the critical line of this model, for which no exact result is available, we employed phenomenological renormalisation (Nightingale 1976, 1979). From infinitely long strips, with periodical boundary conditions, of widths n and $n+1$ an estimate $K_c(n, 0)$ of the critical value of K is obtained. Table 1 shows the results for a series of increasing values of n for $\alpha \equiv L/K = 1$ and $\alpha = -1/4$. The extrapolated estimates $K_c\ (n, i)$ were obtained by fitting subsequent values of $K_c\ (n, i-1)$ to $K_c(n, i) = K_c(n, i-1) + an^{-b}$. For $i = 1$ we chose a fixed $b = 3$; for the Ising model

Table 1. Various estimates of the critical points of the eight-neighbour model for $\alpha = 1$, $-1/4$.

	$\alpha = 1$				$\alpha = -1/4$		
n	$K_c(n, 0)$ 0.19	$K_c(n, 1)$ 0.190	$K_c(n, 2)$ 0.190 19	$K_c(n, 3)$ 0.190 19	$K_c(n, 0)$ 0.6	$K_c(n, 1)$ 0.69	$K_c(n, 2)$ 0.69
2	508 389 47	—	—	—	280 8162	—	—
3	251 120 13	543 93	—	—	436 1817	—	—
4	137 387 29	368 16	388	—	635 0671	1776	—
5	088 308 42	277 84	—	190	773 0230	6888	—
6	062 809 50	240 10	126	978	855 5349	8158	—
7	048 443 68	220 79	178	263	902 2058	8139	—
8	039 741 19	210 35	220	271	928 3416	7852	6974
9	034 173 03	204 31	239	269	943 2783	7604	7159
10	030 449 01	200 63	251		952 1571	7442	7202
11	027 866 29	198 30	257		957 6943	7347	7215
12	026 019 90	196 75			961 3194	7294	7219
13	024 665 52	195 70			963 7994	7264	
14	023 649 85				965 5612	7247	
15					966 8526		

Note. In each column the values in question are obtained by appending the digits below to the number in the heading. The absence of a result indicates a breakdown of the power-law fit or a result outside the range allowed by the format.

($\alpha = 0$) this is an exact result (Derrida and Vannimenus 1980). Performing similar extrapolations with b as a free parameter also for $i = 1$ corroborates this assumption and yields fully consistent though slightly less accurate results. We conclude $K_c =$

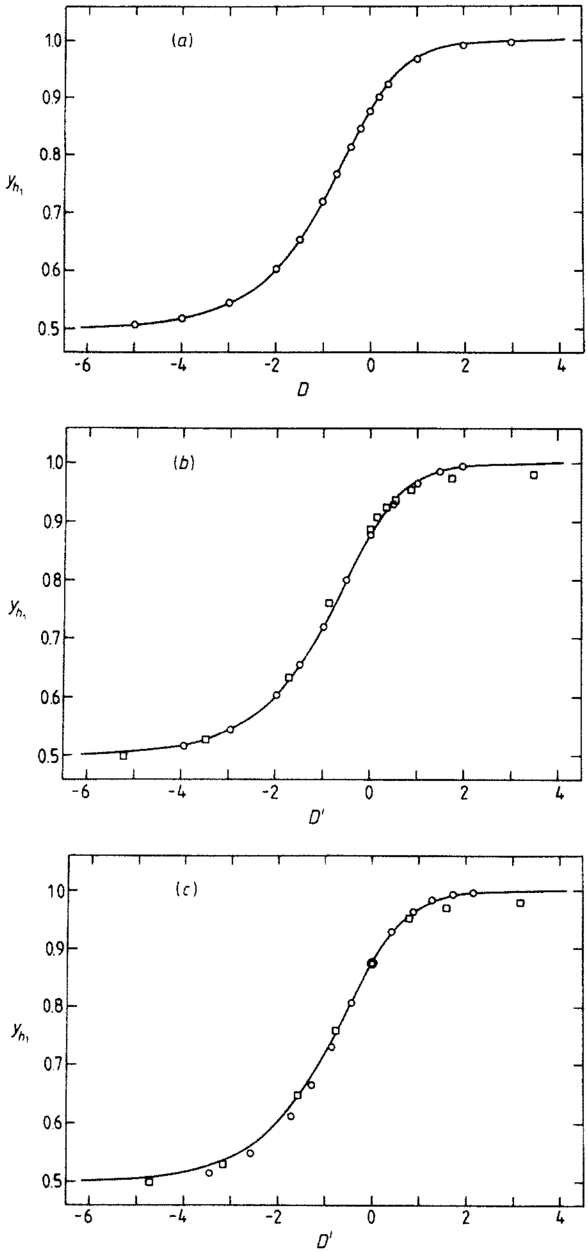

Figure 1. The magnetic defect exponent, calculated by fitting χ_{11} for subsequent n (up to 10) to equation (5) and extrapolated assuming power-law behaviour, for various values of the enhancement (data points) compared with y_{h_1} as given by the generalisation of equation (3) (full curves): (a) the Ising model; (b) the free-fermion model: $L = 1/5$ (circles), $-1/5$ (squares); (c) the eight-neighbour model: $\alpha = 1$ (circles), $-1/4$ (squares).

0.190 192 69 (5) for $\alpha = 1$ and $K_c = 0.697\,220$ (5) for $\alpha = -1/4$, where the number in parentheses is an estimate of the error in the last digit. Note that the value $K_c = 0.1902$ for $\alpha = 1$, obtained previously from series expansion (Dalton and Wood 1969), is consistent with our estimate.

Figure 1 shows our results for y_{h_1} as a function of D. For the Ising model the agreement with the exact result (3) is very good except for large D, where also the apparent convergence is less rapid. Also shown in figure 1 are the results for the free-fermion model ($L = -1/5$, $1/5$) and the eight-neighbour model ($\alpha = 1, -1/4$). Qualitatively, the behaviour of y_{h_1} is similar to the Ising case, in agreement with what is to be expected from universality and scaling. A surprising result is that y_{h_1} is described rather accurately by equation (3) with $D' = DK_c/K_c^{\mathrm{I}}$ substituted for D. It is consistent with our numerical results to attribute deviations from this generalisation of equation (3) to incomplete convergence. However, lacking a theoretical justification and in view of the limited present numerical accuracy it is impossible to make a definite statement.

Similar calculations were performed for the q-state Potts model. The reduced Hamiltonian of this model reads

$$\mathcal{H} = 2K \sum_{(i,j)} \delta_{s_i s_j},$$

where $s_i = 1, \ldots, q$, (i, j) runs through all pairs of nearest-neighbour sites of a simple square lattice. The critical point is $K_c = \frac{1}{2}\ln(\sqrt{q}+1)$ (Potts 1952). The model can be generalised (Kasteleyn and Fortuin 1969, Baxter 1973) to non-integral values of q. Also in the general case a transfer matrix may be formulated and a finite-size analysis can be performed (Blöte *et al* 1981). Two cases were investigated: $q = 1/2$ and $q = 3$. The values of y_T are believed to be 0.56 . . . and 6/5 respectively (den Nijs 1979 and, e.g., Blöte et al 1981). As explained above, this implies the enhancement to be irrelevant for $q = 1/2$ and relevant for $q = 3$. Figure 2 shows some results obtained for y_{h_1} in both cases. Convergence is rather poor, but it is clear that there is the tendency of y_{h_1} to be independent of D for $q = 1/2$ and of y_{h_1} to assume three different values for

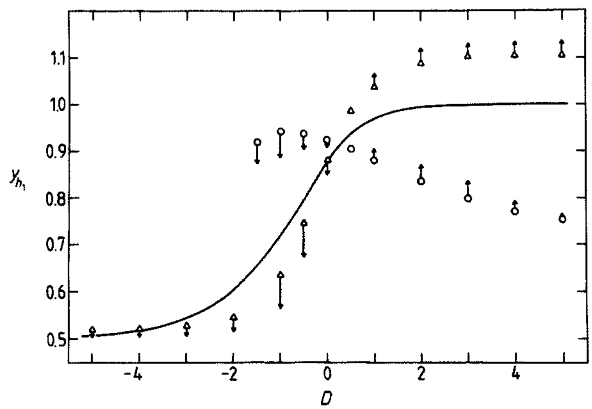

Figure 2. The magnetic defect exponent for the Potts model with $q = 1/2$ (circles) and $q = 3$ (triangles), calculated by fitting χ_{11} to equation (5) for subsequent values of n (up to 9); to compute χ_{11} a magnetic field was introduced giving defects spins with $s_i = 1$ a different statistical weight. The arrows indicate the trend of the estimates of y_{h_1} obtained for increasing n; their length is 10 times the difference of the estimates with largest n. The full curve is the result for $q = 2$ (the Ising model), included for comparison.

$q = 3$, depending on whether $D < 0$, $D = 0$, or $D > 0$. We note that from the conjectured values of the magnetic exponent of the Potts model (Nienhuis *et al* 1980, Blöte *et al* 1981) one obtains $y_{h_1} = 0.917\ldots$ for $q = 1/2$ and $y_{h_1} = 0.866\ldots$ for $q = 3$. For $q = 3$ and large D convergence seems to be to an unphysical value of $y_{h_1} > 1$, which corresponds to a negative, and therefore meaningless, critical dimension. We do not at present have an explanation of this result. However, if in a renormalisation group description the behaviour of the system for $D > 0$ is governed by a fixed point at infinite coupling, a breakdown of finite-size scaling for $n \times \infty$ systems is not unexpected. In fact, unphysically large results for critical exponents of the Potts model with $q > 4$ as obtained in a finite-size analysis (Blöte *et al* 1981) have been interpreted in terms of a zero-temperature fixed point (Blöte and Nightingale 1982).

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