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Critical behaviour at an edge for the SAW and Ising model

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Abstract. We have studied the behaviour of two- and three-dimensional self avoiding walks confined to a wedge of wedge angle α. Series have been obtained and analysed for the (angular dependent) critical exponents characterising various edge susceptibilities. In terms of a general scaling form for the edge free energy, $f_e \sim t^{(d-2)\nu}\psi_e(ht^{-y_0\nu}, h_1 t^{-y_1\nu}, h_2 t^{-y_2\nu})$, we find for the two-dimensional case the following scaling indices: $y_0 = 91/48$, $y_1 = 3/8$, $y_2(\alpha) = -5\pi/8\alpha$. We argue that these results are exact, from which follow all exponents for the bulk, surface and edge problem. In three dimensions we obtain $y_0 \approx 2.488$, $y_1 = 0.65 \pm 0.02$, $y_2(\alpha) = a + b\pi/\alpha$ where $a = 0.51 \pm 0.04$, $b = -0.847 \pm 0.017$, which, for y_2, is precisely of the functional form given by mean-field theory, $y_2(\alpha) = \frac{1}{2} - \pi/2$. We argue that $a = \frac{1}{2}$ for all three-dimensional O(N) models.

This simple angular dependence of y_2 is different from that suggested by Cardy's one-loop ε-expansion.

For the square lattice, we have also studied the case in which the wedge is rotated through an angle of $\pi/4$, and find that the various exponents are unchanged.

For the three-dimensional Ising model in a wedge, analogy with our SAW results, plus mean-field results in conjunction with RG and series work yield $y_0 \approx 2.485$, $y_1 = 0.71 \pm 0.02$ and $y_2 = a + b\pi/\alpha$ with $a = \frac{1}{2}$ and $b = -0.79 \pm 0.02$.

1. Introduction

We consider the critical behaviour of the N-vector model confined to a wedge geometry. That is, the model is confined to the wedge formed by the intersection of two non-parallel $(d-1)$-dimensional planar surfaces in a d-dimensional hypercubic lattice, with cartesian coordinate system labelled $\{x_\delta | \delta = 1, 2, \ldots, d\}$. The two surfaces intersect on a $(d-2)$-dimensional line perpendicular to x_1 and x_2, with wedge angle α.

The Hamiltonian of the model is

$$\mathscr{H} = -K \sum_{\langle ij \rangle} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j - L_0 \sum_i \sigma_i^{(1)} - L_1 \sum_i{}' \sigma_i^{(1)} - L_2 \sum_i{}'' \sigma_i^{(1)} \tag{1.1}$$

where $\boldsymbol{\sigma}_i$ is a N-dimensional spin with components $(\sigma_i^{(\beta)}, \beta = 1, 2, \ldots, N)$ and L_0, L_1 and L_2 are bulk, surface and edge fields respectively, and are all parallel to $\sigma_i^{(1)}$. The first sum is over nearest-neighbour pairs, the second is over all spins, the third is over all surface spins in one of the $(d-1)$-dimensional surface planes, and the fourth is over all edge spins. The edge magnetisation is

$$m_2(K; L_0, L_1, L_2) = \langle \sigma_i^{(1)}(x_1 = x_2 = 0) \rangle, \tag{1.2}$$

that is, the expectation value of an edge spin. The derivative of m_2 with respect to the three fields yield three susceptibilities, namely,

$$\chi_2(K)=\lim_{L_0\to 0}\partial m_2(K;L_0,L_1,L_2)/\partial L_0\sim t^{-\gamma_2}$$
$$\chi_{21}(K)=\lim_{L_1\to 0}\partial m_2(K;L_0,L_1,L_2)/\partial L_1\sim t^{-\gamma_{21}} \qquad (1.3)$$
$$\chi_{22}(K)=\lim_{L_2\to 0}\partial m_2(K;L_0,L_1,L_2)/\partial L_2\sim t^{-\gamma_{22}}.$$

These three edge susceptibilities are a natural generalisation of the surface susceptibilities, χ_1 and χ_{11} introduced by Binder and Hohenberg (1972), and, as shown by Cardy (1983), can be related to bulk exponents by a pair of scaling laws.

Following Cardy's notation, we write the free energy in the form

$$F=Vf_b+Af_s+Lf_e+\ldots \qquad (1.4)$$

where V is the d-dimensional 'volume' of the system, A is the $(d-1)$-dimensional 'area' of a surface and L is the $(d-2)$-dimensional 'length' of the edge formed by the intersection of the two surfaces defining the wedge. The free energies f_b, f_s and f_e denote the bulk, surface and edge free energies per spin respectively, and can be written in terms of bulk, surface and edge magnetic fields and temperatures as:

$$f_b\sim t^{2-\alpha}\psi_b(ht^{-y_0\nu})$$
$$f_s\sim t^{2-\alpha_s}\psi_s(ht^{-y_0\nu},h_1t^{-y_1\nu}) \qquad (1.5)$$
$$f_e\sim t^{2-\alpha_e}\psi_e(ht^{-y_0\nu},h_1t^{-y_1\nu},h_2t^{-y_2\nu})$$

where t is the reduced temperature $(T-T_c)/T_c$; y_0, y_1 and y_2 are the bulk, surface and edge scaling indices, and $(2-\alpha)=d\nu$, $(2-\alpha_s)=(d-1)\nu$ and $(2-\alpha_e)=(d-2)\nu$. All susceptibilities follow by taking the appropriate derivatives of (1.5), and we find

$$\chi=\partial^2f_b/\partial h^2\sim t^{-\gamma}, \qquad \gamma=\nu(2y_0-d) \qquad (1.6a)$$
$$\chi_1=\partial^2f_b/\partial h\,\partial h_1\sim t^{-\gamma_1}, \qquad \gamma_1=\nu(y_0+y_1-d+1) \qquad (1.6b)$$
$$\chi_{11}=\partial^2f_s/\partial h_1^2\sim t^{-\gamma_{11}}, \qquad \gamma_{11}=\nu(2y_1-d+1) \qquad (1.6c)$$
$$\chi_2=\partial^2f_e/\partial h\,\partial h_2\sim t^{-\gamma_2}, \qquad \gamma_2=\nu(y_0+y_2+2-d) \qquad (1.6d)$$
$$\chi_{21}=\partial^2f_e/\partial h_1\,\partial h_2\sim t^{-\gamma_{21}}, \qquad \gamma_{21}=\nu(y_1+y_2+2-d) \qquad (1.6e)$$
$$\chi_{22}=\partial^2f_e/\partial h_2^2\sim t^{-\gamma_{22}}, \qquad \gamma_{22}=\nu(2y_2+2-d) \qquad (1.6f)$$

where the mean-field or Gaussian fixed point values can be obtained by setting $\nu=\frac{1}{2}$, $\gamma=1$, $d=4$, $\gamma_1=\frac{1}{2}$, $\gamma_2=-\pi/\alpha$. The surface scaling law of Barber (1973), $2\gamma_1-\gamma_{11}=\gamma+\nu$ follows immediately from this formulation, as do two new edge scaling laws:

$$2\gamma_2-\gamma_{22}=\gamma+2\nu, \qquad 2\gamma_{21}-\gamma_{22}=\gamma_{11}+\nu. \qquad (1.7)$$

To connect susceptibility exponents to correlation function exponents, we extend the treatment of Binder and Hohenberg (1972) to the wedge geometry.

Consider the correlation function $C(r'=0;\boldsymbol{\rho},x_1,x_2)$ between a spin at the edge ($\boldsymbol{r}'=0$, corresponding to $\boldsymbol{\rho}'=x_1'=x_2'=0$) and a spin at a distance $(\boldsymbol{\rho},x_1,x_2)$, where $\boldsymbol{\rho}$ is a $(d-2)$-dimensional vector with components $x_3,x_4,\ldots,x_d$.

The correlation function will depend on the orientation of the vector $(\boldsymbol{\rho},x_1,x_2)$ even near T_c. Denote the magnitude of the vector by r, its orientation within the

(x_1, x_2) plane by θ (clearly $0 \leq \theta \leq \alpha$) and its orientation within the surface plane by ϕ, measured with respect to the edge. Thus we write $C_1(\boldsymbol{\rho}, x_1, x_2) = C_1(r, \theta, \phi) = C(\boldsymbol{\rho}'=0,\ x_1'=0,\ x_2'=0;\ \rho,\ x_1,\ x_2)$. For fixed $T > T_c$, we define the *true* correlation length $\xi_{\theta,\phi}$ by $x_1' = 0$

$$C_1(r, \theta, \phi) \underset{r\to\infty}{\sim} f(r, \theta, \phi) \exp[-r/\xi_{\theta,\phi}(t)], \qquad t > 0 \tag{1.8}$$

where f decays more slowly than the exponential term. For $T = T_c$ the correlations decay with the usual power-law behaviour

$$C_1(r, \theta, \phi) \underset{r\to\infty}{\sim} A(\theta, \phi)/r^{d-2+\eta_{\theta,\phi}}, \qquad t = 0 \tag{1.9}$$

which leads to the special cases $\eta_2 = \eta(\theta > 0,\ \phi > 0)$, $\eta_{21}(\theta = 0,\ \phi > 0)$ and $\eta_{22}(\theta = 0,\ \phi = 0)$. Clearly $\eta_2 < \eta_{21} < \eta_{22}$ as there are more paths for η_2 than for η_{21}, and more paths for η_{21} than for η_{22}.

In terms of the previously defined correlation length, we have

$$\begin{aligned}
\chi_2 &= \sum_{\rho} \sum_{x_1=0}^{\infty} {\sum_{x_2=0}^{\infty}}' C_1(\boldsymbol{r}' = 0; \boldsymbol{\rho}, x_1, x_2) \\
\chi_{21} &= \sum_{\rho} {\sum_{x_2=0}^{\infty}}' C_1(\boldsymbol{r}' = 0; \boldsymbol{\rho}, x_1 = 0, x_2) \\
\chi_{22} &= {\sum_{\rho}}' C_1(\boldsymbol{r}' = 0; \boldsymbol{\rho}, x_1 = 0, x_2 = 0)
\end{aligned} \tag{1.10}$$

where the prime on the summation indicates the additional constraint $\theta \leq \alpha$.

In the limit $N \to 0$ of the N-vector Hamiltonian, following Sarma's argument (Daoud *et al* 1975) we find that χ_2 is the generating function for self avoiding walks in the wedge that are terminally attached to the edge, χ_{21} is the generating function for walks in the sector terminally attached to the edge and with their last vertex in the surface plane $x_1 = 0$, while χ_{22} is the generating function for walks that start and finish on the edge. (There is a slight problem here for the $d = 2$ system as the 'edge' becomes a point, and the SAW's become polygons. For this reason we will only discuss χ_{22} for $d > 2$.)

Replacing sums in (1.10) by integrals and using (1.8) and (1.9) we find

$$\chi \sim t^{-\gamma_2} = \int_0^{\alpha} \sin\theta\, d\theta \int_0^{\pi} d\phi \int_0^{\infty} r^{d-1}\, dr\, g(\theta, \phi) r^{2-d-\eta_{\min}} \Gamma[r/\xi_{\theta,\phi}(t), \theta, \phi] \tag{1.11}$$

where we have combined the correlation function behaviour for $t > 0$ and $t = 0$ to get the general form used above. Substituting $x = r/\xi$ yields

$$\chi_2 \sim t^{-\gamma_2} \sim \xi^{2-\eta_{\min}} \int dx\, d\theta\, d\phi\, h(x, \theta, \phi), \qquad \text{and } \xi \sim t^{-\nu} \tag{1.12}$$

where $\eta_{\min} = \min(\eta_2, \eta_{12}, \eta_{22}) = \eta_2$. Hence

$$\gamma_2 = \nu(2 - \eta_2). \tag{1.13}$$

Similarly, we see that

$$\chi_{21} \sim t^{-\gamma_{21}} = \int_0^{\alpha} \sin\theta\, d\theta \int_0^{\pi} d\phi \int_0^{\infty} r^{d-2}\, dr\, g(\theta, \phi) r^{2-d-\eta_{\min}} \Gamma(r/\xi, \theta, \phi) \tag{1.14}$$

where now $\eta_{\min} = \min(\eta_{12}, \eta_{22}) = \eta_{12}$. Hence we find

$$\gamma_{12} = \nu(1-\eta_{12}) \tag{1.15}$$

and similarly

$$\gamma_{22} = -\nu\eta_{22}. \tag{1.16}$$

Combining (1.14), (1.15) and (1.16) with (1.7), we obtain

$$\eta = 2\eta_2 - \eta_{22} \qquad \text{and} \qquad \eta_{22} = 2\eta_{21} - \eta_{11}. \tag{1.17}$$

This provides an alternative derivation for Cardy's result

$$\eta_{p,q} = \tfrac{1}{2}(\eta_{p,p} + \eta_{q,q}); \qquad p, q = 0, 1, 2 \qquad \text{where } \eta_{0,0} = \eta. \tag{1.18}$$

Cardy calculated these quantities to first order in $\varepsilon = 4-d$, and obtained

$$\eta_2 = \lambda - [(5\lambda^2+1)(N+2)/12\lambda(N+8)]\varepsilon + O(\varepsilon^2) \tag{1.19}$$

$$\eta_{22} = 2\lambda - [(5\lambda^2+1)(N+2)/6\lambda(N+8)]\varepsilon + O(\varepsilon^2) \tag{1.20}$$

with $\lambda = \pi/\alpha$. Previous one-loop results include

$$\eta = O(\varepsilon^2), \qquad \eta_1 = 1 - [(N+2)/2(N+8)]\varepsilon + O(\varepsilon^2),$$
$$\eta_{11} = 2 - [(N+2)/(N+8)]\varepsilon + O(\varepsilon^2) \tag{1.21}$$

and

$$\nu = \tfrac{1}{2} + [(N+2)/4(N+8)]\varepsilon + O(\varepsilon^2), \tag{1.22}$$

for which we can derive the following expansions:

$$\gamma_2 = 1 - \frac{\lambda}{2} - \frac{(N+2)}{(N+8)} \frac{(\lambda^2 - 12\lambda - 1)}{24\lambda} \varepsilon \tag{1.23}$$

$$\gamma_{12} = -\frac{\lambda}{2} - \frac{(N+2)}{(N+8)} \frac{1}{4} \left(\frac{\lambda^2 - 6\lambda - 1}{6\lambda} \right) \varepsilon \tag{1.24}$$

$$\gamma_{22} = -\lambda - \frac{(N+2)}{(N+8)} \frac{1}{2} \left(\frac{\lambda^2 - 1}{6\lambda} \right) \varepsilon. \tag{1.25}$$

For the scaling index y_2 Cardy gives

$$y_2 = \frac{d}{2} - \lambda - 1 + \left(\frac{5\lambda^2 + 1}{12\lambda} \frac{(N+2)}{(N+8)} \right) \varepsilon \tag{1.26}$$

which displays a complicated dependence on wedge angle which is not supported by our series analysis.

After much of this work was completed we heard of the work of Barber *et al* (1984), who have studied the two-dimensional Ising model in wedge and conical geometries. In our notation they find $y_2 = -\pi/2\alpha$ for the wedge geometry, a strikingly simple result.

In this paper we have generated and analysed the susceptibility series for the $N = 0$ (SAW) case, for both the square and simple cubic lattices. For the square lattice we have also generated and analysed some mean square end-to-end distance series.

We find in two dimensions that $y_2 = -5\pi/8\alpha$, a strikingly similar result to that found by Barber *et al* (1984) for the two-dimensional Ising model, and in three dimensions $y_2 = a + b\pi/\alpha$, where $a = 0.51 \pm 0.046$ and $b = -0.85 \pm 0.015$.

The generation of the series is discussed in the next section, while § 3 describes the analysis. The final section comprises a discussion and conclusion, in which we extend our results to the three-dimensional Ising model.

2. Enumeration of series coefficients

In order to determine the series coefficients, we have used a variant of the dimerisation technique previously used for neighbour avoiding walks (Torrie and Whittington 1975). In order to determine say, all $(m+n)$-step walks terminally attached to the edge and confined to the wedge, we first enumerate all such m-step terminally attached walks, and all n-step (unconstrained) SAW's. We then consider the set of $(m+n)$-step walks constructed by concatenating all m-step terminally attached walks with all n-step unconstrained SAW's, the common vertex being the non-terminally attached vertex of the m-step walk. The $(m+n)$-step walks so constructed include all $(m+n)$-step terminally attached walks, in addition to walks which must be discarded because either (a) they are not self avoiding or (b) they occupy regions of space outside the confining wedge.

By judicious bit-mapping of forbidden regions, the test for rejection reduces to a logical AND operation. In this manner we have obtained a variety of series, for both the square and simple cubic lattices.

We adopt the notational convention of denoting the various susceptibilities by C rather than χ, to indicate that they are in fact chain generating functions. The various subscripts have the same meaning as the subscripts on χ defined in the previous section.

Thus we denote the generating function for terminally attached walks confined to a wedge of angle α, with the terminal attachment taking place at the edge, by

$$C_2(\alpha, z) = \sum_{n\geq 0} c_n^{(2)}(\alpha) z^n \qquad (2.1)$$

where $c_n^{(2)}(\alpha)$ is the cardinality of such n-step walks. A similar notation is used for $C_{21}(\alpha, z)$ and $C_{22}(\alpha, z)$. Subsequently we may drop the explicit dependence on α or z for notational simplicity if no confusion can occur.

For the square lattice we have obtained expansions for $C_2(\alpha, z)$ and $C_{21}(\alpha, z)$ for $\alpha = \frac{1}{2}\pi$ and $\alpha = \frac{1}{4}\pi$. Series for $\alpha = \pi$ have been given previously in Barber *et al* (1978)—hereafter referred to as B1. We also give these expansions for $\alpha = \frac{1}{2}\pi$ in the case where the coordinate system has been rotated by $\frac{1}{4}\pi$ with respect to the lattice major axes. Mean square end-to-end distances for walks enumerated by $C_2(\alpha, z)$ have also been determined.

For the simple cubic lattice we have obtained expansions for $C_2(\alpha, z)$, $C_{21}(\alpha, z)$ and $C_{22}(\alpha, z)$, for $\alpha = \pi$, $\frac{1}{2}\pi$ and $\frac{1}{4}\pi$.

The square lattice series are listed in tables 1(*a*) and 1(*b*), and the simple cubic lattice series are given in table 2. This work corrects an error in the fourteenth coefficient of $C_{21}(\pi, z)$ in B1.

3. Analysis of series

Prior to analysing the series for the square and simple cubic lattices, we first wish to establish the connective constant. For the surface problem (which is just the wedge problem with $\alpha = \pi$), Whittington (1975) has shown that the connective constant

Table 1(*a*). Square lattice series coefficients, wedge angle $= \pi/2$.

	Lattice rotated by $\pi/4$				
n	c_n^2	c_n^{21}	c_n^2	$\rho_n c_n^2$	c_n^{21}
1	1	0	2	2	1
2	3	1	4	12	1
3	5	0	10	50	2
4	15	3	24	188	4
5	29	0	60	652	9
6	83	12	146	2140	18
7	179	0	366	6766	41
8	495	56	912	20 868	89
9	1125	0	2302	63 118	207
10	3063	281	5800	188 004	467
11	7179	0	14 722	553 074	1101
12	19 401	1495	37 368	1610 776	2552
13	46 363	0	95 304	4651 784	6092
14	124 673	8245	243 168	13 338 744	14 377
15	302 271	0	622 518	38 014 494	34 678
16	809 921	46 827	1594 622	107 767 964	82 959
17	1984 959	0	4094 768	304 100 432	201 800
18	5304 947	271 884	10 521 384	854 624 852	487 904
19	13 110 907	0	27 085 436	2393 093 804	1195 213
20	34 972 559	1607 277	69 768 478	6679 440 288	2914 427
21	87 014 349	0	179 982 688	18 589 013 256	7181 988
22	231 756 983	9641 935	464 564 220	51 597 951 784	17 635 162
23	579 803 757	0	1200 563 864		43 679 583
24	1542 417 375	58 555 291			107 879 951
25					268 378 064
26					666 121 087

remains unchanged from its bulk value by bounding the number of terminally attached walks by the number of polygons. A similar, but slightly more tortuous construction allows us to draw the same conclusion for $\alpha = \frac{1}{2}\pi$, but Hammersley and Whittington (1985) have produced an elegant proof that holds for arbitrary $\alpha > 0$, for all the generating functions considered here. Thus in analysing the wedge data we have used the bulk connective constants. For the square lattice we have used the mean of the most recent series analysis (Guttmann 1984), real-space RG (Derrida 1981) and Monte Carlo (Berretti and Sokal 1984) estimates, which give for the connective constant $\mu \approx 2.63815 \pm 0.00015$. For computational ease we have used the mnemonic $\mu = (11+\sqrt{5})^{1/2} - 1 = 2.63814\ldots$. For the simple cubic lattice we have re-analysed the bulk SAW generating function $C(x)$ using the RG estimate (Le Guillou and Zinn-Justin 1980) of the exponent $\gamma = 1.1615$. Padé approximants to $[C(x)]^{1/\gamma}$ have well-converged poles at $x_c = 1/\mu = 0.213494$, a change of 0.01% from the estimate used in a previous analysis (B1) for the analogous free surface problem.

In support of the scaling form (1.5), we next show that the mean square end-to-end distance exponent ν remains unchanged from its bulk value in the wedge geometry. We do this by computing $\langle R_n^2\rangle_{\text{bulk}}/\langle R_n^2(\theta)\rangle$ For $\theta = \frac{1}{2}\pi$ and $\theta = \frac{1}{4}\pi$ and for square lattice data. (The case $\theta = \pi$ has been studied previously by Whittington (1975) and by Guttmann *et al* (1978) for $\theta = \frac{1}{2}\pi$ but with a series four terms shorter.) Denoting the

Table 1(*b*). Square lattice series coefficients, wedge angle = $\pi/4$.

n	c_n^2	$\rho_n c_n^2$	c_n^{21}
1	1	1	1
2	2	6	1
3	3	19	1
4	8	68	2
5	14	190	4
6	36	610	8
7	70	1618	15
8	177	4870	31
9	372	12 776	66
10	942	37 270	142
11	2056	97 264	306
12	5222	277 858	678
13	11 736	723 856	1512
14	29 878	2039 120	3410
15	68 576	5309 076	7750
16	175 038	14 805 780	17 786
17	408 328	38 549 984	41 067
18	1044 533	106 693 682	95 514
19	2468 261	277 890 081	223 295
20	6326 688	764 597 138	525 203
21	15 107 015	1992 327 855	1240 734
22	38 791 865	5456 154 914	2945 383
23	93 432 564		7019 239
24	240 296 399		16 795 983
25	583 001 850		40 325 120
26			97 153 672
27			234 753 693
28			568 950 192

exponents by ν_b and ν_θ respectively, we have that

$$r_n = \langle R_n^2 \rangle_{\text{bulk}} / \langle R_n^2(\theta) \rangle \sim A n^{2(\nu_b - \nu_\theta)}. \tag{3.1}$$

Linear and quadratic alternate extrapolants, defined by

$$\begin{cases} \phi_n = \log(r_n/r_{n-2})/\log[n/(n-2)] & (3.2a) \\ s_n = \frac{1}{2}[n\phi_n - (n-2)r_{n-2}] & (3.2b) \end{cases}$$

$$t_n = [n^2 s_n - (n-2)^2 s_{n-2}]/(4n-4) \tag{3.3}$$

should then provide estimators of $2(\nu_b - \nu_\theta)$. For $\theta = \frac{1}{2}\pi$ we find $\nu_\theta - \nu_b < 0.025$, and for $\theta = \frac{1}{4}\pi$, $\nu_\theta - \nu_b < 0.03$. In both cases the sequences of estimates $\{s_n\}$ and $\{t_n\}$ are steadily decreasing, and support the conclusion that $\nu_\theta = \nu_b$ for $\theta > 0$.

Our series analysis uses the methods of our earlier work (B1), in which we first transform the series using an Euler transformation $z = 2x/(1+\mu x)$ which maps the non-physical singularity in the generating function at $x = -1/\mu$ to infinity, while the physical singularity is a fixed point of the transformation. If $\tilde{c}_n$ are the coefficients of the transformed generating function $\tilde{C}(z)$, so that $\tilde{C}(z) = \sum \tilde{c}_n z^n \sim \tilde{A}(1-\mu x)^{-\lambda}$, then the exponent λ can be estimated from $\lambda_n = 1 + n(\tilde{c}_n/\mu\tilde{c}_{n-1} - 1)$. Better converged estimates of λ can be obtained by Neville table extrapolation of the sequence $\{\lambda_n\}$ against $1/n$ in the usual manner (Gaunt and Guttmann 1974).

Table 2. Simple cubic lattice series coefficients.

n	$c_n^2(\pi)$	$c_n^{21}(\pi)$	$c_n^{22}(\pi)$
1	5	4	2
2	21	12	2
3	93	40	8
4	409	136	20
5	1853	528	88
6	8333	2032	264
7	37 965	8344	1200
8	172 265	33 576	3864
9	787 557	140 912	17 812
10	3593 465	582 088	61 044
11	16 477 845	2482 240	282 808
12	75 481 105	10 451 064	1012 932
13	346 960 613	45 101 536	4707 048
14	1593 924 045	192 562 328	17 417 356
15	7341 070 889	838 630 216	81 117 028
16			307 858 040
17			1436 163 312

n	$c_n^2(\pi/2)$	$c_n^{21}(\pi/2)$	$c_n^{22}(\pi/2)$	$c_n^2(\pi/4)$	$c_n^{21}(\pi/4)$	$c_n^{22}(\pi/4)$
1	4	3	2	3	3	2
2	14	7	2	8	7	2
3	56	22	6	27	19	4
4	226	70	14	92	52	8
5	958	261	54	336	160	22
6	4052	950	150	1264	524	50
7	17 508	3741	622	4906	1847	162
8	75 634	14 363	1882	19 307	6651	442
9	330 804	58 039	7978	77 346	24 630	1590
10	1448 830	230 777	25 898	312 972	92 132	4718
11	6397 288	951 321	111 298	1282 188	351 686	17 350
12	28 293 338	3877 714	379 798	5296 014	1356 640	54 134
13	125 845 174	16 230 430	1649 502	22 073 614	5314 070	204 324
14	560 617 586	67 368 995	5845 638	92 599 312	20 994 170	669 172
15	2507 890 716	285 373 770	25 600 082	391 122 480	83 886 700	2588 952
16			93 459 726		337 513 782	8805 572
17			412 071 226			34 687 814
18			1540 777 002			121 539 150
19						485 928 042

In this way, in B1, we obtained $\gamma_1 = 0.945 \pm 0.005$ and $\gamma_{11} = -0.19^{+0.03}_{-0.02}$ for the square lattice SAW series. Those estimates were made under the assumption that $\mu = 2.6385$. Using our refined estimate of the connective constant μ, these become $\gamma_1 = 0.953 \pm 0.006$ and $\gamma_{11} = -0.19 \pm 0.02$.

It is enlightening to consider the values of the scaling indices in the light of these results and Neinhuis (1982) exact values for the bulk exponents, $\gamma = 43/32$, $\nu = 3/4$. From the bulk exponents and (1.6a) we obtain $y_0 = 91/48$. Given that all known bulk exponents for the square lattice SAW and Ising models are rational fractions with denominators given by powers of two, it is to be expected that γ_1 and γ_{11} also display this feature. Assuming then that $\gamma_1 = a/64$, where a is an unknown integer to be determined, our estimate 0.953 ± 0.006 gives $a = 60.9 \pm 0.6$, which suggests $a = 61$ exactly and hence that the scaling index $y_1 = 3/8$. This implies that $\gamma_{11} = -3/16 = -0.1875$, in precise agreement with our series estimate. If a were taken to be 60 or 62 instead of 61, this would give $\gamma_{11} = -0.21875$ or -0.15625 respectively, both of which are outside the error bounds for γ_{11}, and $\gamma_1 = 0.9375$ or 0.96875 either of which would require a doubling of our already conservative error estimates. Accordingly, we believe that these values are exact, that is,

$$\gamma_{11} = -3/16, \qquad \gamma_1 = 61/64, \qquad y_0 = 91/48 \qquad y_1 = 3/8. \tag{3.4}$$

The assumptions underlying these results are supported by the recent work of Friedan *et al* (1984) who have shown that the critical exponents of many two-dimensional models follow from the conformal invariance of the system. The simple, rational, form of the exponents then follows from this observation.

Turning now to the wedge series, $C_2(\alpha)$, $C_{21}(\alpha)$ and $C_{22}(\alpha)$, these have been analysed in precisely the same manner as described above. There is a steady deterioration in the quality of the data as α decreases, and, for fixed α, as one proceeds through the hierarchy $C_2(\alpha) \to C_{21}(\alpha) \to C_{22}(\alpha)$. As an indication, we show the detailed results of our analysis of $C_2(\pi/4)$ and $C_{21}(\pi/2)$ for the square lattice in table 3. From these results, we estimate $\gamma_2(\pi/4) = -0.46 \pm 0.02$ and $\gamma_{21}(\pi/2) = -0.67 \pm 0.04$. In table 4 we summarise our results for all series, both for the square and simple cubic lattices. In order to determine the nature of the angular dependence of the scaling index y_2, and hence the exponents γ_2, γ_{21} and γ_{22}, we first note that, if the wedge angle $\alpha = \pi$, the wedge problem degenerates into the surface problem. That is, $\gamma_2(\pi) = \gamma_1$ and $\gamma_{21}(\pi) = \gamma_{11}$. From (1.6*b*) and (1.6*d*) we therefore obtain $y_2(\pi) = y_1 - 1$. Now for the two-dimensional Ising model Barber *et al* (1984) have obtained $y_2 = -\pi/2\alpha$. It seems likely that a similar, simple angular dependence could prevail for the SAW problem too. To pursue this possibility further, we note (3.4) that $y_2(\pi) = y_1 - 1 = -5/8$ for the two-dimensional SAW model, which would imply that $y_2(\alpha) = -5\pi/8\alpha$ for this model. We thereby obtain for the exponents

$$\gamma_2(\alpha) = 91/64 - 15\pi/32\alpha, \qquad \gamma_{21}(\alpha) = 9/32 - 15\pi/32\alpha,$$
$$\gamma_{22}(\alpha) = -15\pi/16\alpha. \tag{3.5}$$

Table 3. Results of analysis for exponent $\gamma_2(\pi/4)$ and $\gamma_{21}(\pi/2)$ for the square lattice SAW series.

		$C_2(\pi/4)$			$C_{21}(\pi/2)$	
n	λ_n	Linear extrapolants	Quadratic extrapolants	λ_n	Linear extrapolants	Quadratic extrapolants
15	−0.0886	−0.4161	−0.3874	−0.1944	−0.5836	−0.5850
16	−0.1087	−0.4103	−0.3702	−0.2185	−0.5808	−0.5609
17	−0.1262	−0.4057	−0.3709	−0.2397	−0.5784	−0.5600
18	−0.1416	−0.4032	−0.3831	−0.2585	−0.5777	−0.5727
19	−0.1553	−0.4029	−0.4001	−0.2754	−0.5791	−0.5908
20	−0.1676	−0.4043	−0.4171	−0.2907	−0.5821	−0.6091
21	−0.1791	−0.4068	−0.4310	−0.3048	−0.5861	−0.6245
22	−0.1896	−0.4099	−0.4409	−0.3178	−0.5907	−0.6362
23	−0.1994	−0.4132	−0.4471	−0.3298	−0.5954	−0.6444
24	−0.2084	−0.4162	−0.4502	−0.3411	−0.5999	−0.6497
25	−0.2168	−0.4191	−0.4514	−0.3516	−0.6041	−0.6530
26				−0.3615	−0.6080	−0.6548

Table 4. Summary of exponent estimates. 'Exact' results come from $\gamma_0 = 91/48$, $y_1 = 3/8$, $y_2(\alpha) = -5\pi/8\alpha$. Conjectured results derive from the assumed form $y_2(\alpha) = \frac{1}{2} - 0.847 \pm 0.017$.

Exponent	Square lattice: Series estimates	Square lattice: 'Exact' results	Simple cubic lattice: Series estimates	Simple cubic lattice: 'Conjectured' estimates
$\gamma_2(\pi)$	0.952 ± 0.006	0.953 125	0.676 ± 0.009	0.67 ± 0.02
$\gamma_2(\pi/2)$	0.484 ± 0.012	0.484 375	0.16 ± 0.03	0.17 ± 0.03
$\gamma_2(\pi/2)$†	0.483 ± 0.012	0.484 375		
$\gamma_2(\pi/4)$	-0.46 ± 0.01	−0.453 125	-0.9 ± 0.2	-0.82 ± 0.07
$\gamma_{21}(\pi)$	-0.19 ± 0.02	−0.1875	-0.4 ± 0.3	-0.40 ± 0.04
$\gamma_{21}(\pi/2)$	-0.67 ± 0.04	−0.656 25	-1.0 ± 0.3	-0.90 ± 0.06
$\gamma_{21}(\pi/4)$	-1.59 ± 0.05	−1.593 75	< -1.3	-1.90 ± 0.09
$\gamma_{22}(\pi)$			-1.0 ± 0.1	-1.00 ± 0.03
$\gamma_{22}(\pi/2)$			-2.1 ± 0.2	-1.99 ± 0.07
$\gamma_{22}(\pi/4)$			-3.0 ± 0.3	-3.98 ± 0.14

† Lattice rotated by $\pi/4$ with respect to coordinate system.

Evaluating these for $\alpha = \frac{1}{2}\pi, \frac{1}{4}\pi$ we obtain the values shown in table 4. It can be seen that the agreement with all square lattice series results is excellent, and we confidently conjecture that these results are exact.

To further test this conjecture, we have again followed a method introduced in B1, and formed products which are independent of the connective constant and should have vanishing critical exponent. That is, denoting

$$
\begin{aligned}
C_2(x, \alpha) &= \sum_{n \geq 0} c_n^2(\alpha) x^n, \\
C_{21}(x, \alpha) &= \sum_{n \geq 0} c_n^{21}(\alpha) x^n, \\
C_{22}(x, \alpha) &= \sum_{n \geq 0} c_n^{22}(\alpha) x^n
\end{aligned}
\tag{3.6}
$$

then from (1.6*d*, *e*, *f*) we find

$$[c_n^2(\pi)]^2 c_n^2(\pi/4)/[c_n^2(\pi/2)]^3 \sim \text{constant } n^{\phi} \tag{3.7}$$

$$[c_n^{21}(\pi)]^2 c_n^{21}(\pi/4)/[c_n^{21}(\pi/2)]^3 \sim \text{constant } n^{\phi} \tag{3.8}$$

$$[c_n^{22}(\pi)]^2 c_n^{22}(\pi/4)/[c_n^{22}(\pi/2)]^3 \sim \text{constant } n^{2\phi} \tag{3.9}$$

where

$$\phi = \nu[2y_2(\pi) + y_2(\pi/4) - 3y_2(\pi/2)]. \tag{3.10}$$

If $y_2(\alpha)$ is a linear function of $1/\alpha$, $y_2(\alpha) = a + b\pi/\alpha$, then $\phi = 0$. We have formed these products, and estimated ϕ from the ratios of alternate terms and their linear and quadratic extrapolants. In order to save space we do not show the resultant sequences. For the square lattice we find from $C_2(x, \alpha)$ that $|\phi| < 0.008$, and from $C_{21}(x, \alpha)$ that $|\phi| < 0.02$. For the simple cubic lattice we find from $C_2(x, \alpha)$ that $|\phi| < 0.015$, from $C_{21}(x, \alpha)$ that $|\phi| < 0.03$ and from $C_{22}(x, \alpha)$ that $|\phi| < 0.06$.

The estimates are steadily decreasing in magnitude, and are already sufficiently close to zero that they provide additional strong support for our conjecture that $\phi = 0$

for both the square and simple cubic lattices. To investigate the assumption that $y_2(\alpha) = a + b\pi/\alpha$ further, we point out that there exist numerous products of the form

$$c_n^{2m}(\alpha)/c_n^{2m}(\alpha/2) \sim \text{constant } n^\theta \qquad m = 0, 1, 2 \tag{3.11}$$

where $c_n^{20}(\alpha)$ denotes $c_n^2(\alpha)$ etc and

$$\begin{aligned} \theta &= \nu[y_2(\alpha) - y_2(\alpha/2)] = -\nu b\pi/\alpha \qquad (m = 0, 1) \\ &= 2\nu[y_2(\alpha) - y_2(\alpha/2)] = -2\nu b\pi/\alpha \qquad (m = 2). \end{aligned} \tag{3.12}$$

We have formed several instances of such products, and analysed the resulting sequences for θ in the same manner as our analysis for ϕ. For the square lattice data, we obtain for $m = 0$, $\alpha = \pi$, the result $-\nu b\pi/\alpha = -0.467 \pm 0.003$, or $b = -0.623 \pm 0.004$. From $y_2(\pi) = y_1 - 1 = -5/8$, it follows that $a = -0.002 \pm 0.004$. This then provides strong support for our result $y_2(\alpha) = -5\pi/8\alpha$.

For the SC lattice series, we obtain the following results:

$$\begin{array}{ll} \theta(m=0, \alpha=\pi) = 0.498 \pm 0.009, & \theta(m=0, \alpha=\frac{1}{2}\pi) = 0.99 \pm 0.02 \\ \theta(m=1, \alpha=\pi) = 0.50 \pm 0.02, & \theta(m=1, \alpha=\frac{1}{2}\pi) = 1.0 \pm 0.1 \\ \theta(m=2, \alpha=\pi) = 1.01 \pm 0.04, & \theta(m=2, \alpha=\frac{1}{2}\pi) = 2.0 \pm 0.4. \end{array} \tag{3.13}$$

These are all consistent with the assumed linear form for $y_2(\alpha)$, and yield $b = (-0.498 \pm 0.009)/\nu$. Using the current RG estimate of $\nu = 0.588 \pm 0.0015$, we find $b = -0.847 \pm 0.017$. In order to determine a we need an exponent estimate. Our direct analysis of the three-dimensional series utilised the same methods as did the two-dimensional analysis (and B1) and the results are also shown in table 4. From $\gamma_2(\pi) = \gamma_1 = 0.676 \pm 0.009$ and the RG estimates (Le Guillou and Zinn-Justin 1980) $\gamma = 1.1615 \pm 0.0020$ and $\nu = 0.588 \pm 0.0015$, we obtain $y_0 = 2.488 \pm 0.004$, $y_1 = 0.662 \pm 0.022$ and $y_2(\pi) = -0.338 \pm 0.022$. Then from $y_2(\alpha) = a + b\pi/\alpha$, and $b = -0.847 \pm 0.017$, we get $a = 0.509 \pm 0.039$. These results then give

$$\begin{array}{lll} & \gamma_2(\pi/2) = 0.178 & \gamma_2(\pi/4) = -0.818 \\ \gamma_{21}(\alpha) = -0.40 & \gamma_{21}(\pi/2) = -0.89 & \gamma_{21}(\pi/4) = -1.88 \\ \gamma_{22}(\alpha) = -0.99 & \gamma_{22}(\pi/2) = -1.98 & \gamma_{22}(\pi/4) = -3.97. \end{array} \tag{3.14}$$

These are all in good agreement with our series results, apart from $\gamma_{22}(\pi/4)$ where the series seems strangely well-converged at an exponent value of -3.0. As we have remarked previously, this is the lowest quality data of all, and accordingly this discrepancy can be dismissed, and we conclude that the simple form assumed for y_2 is probably correct.

4. Discussion and conclusion

For the two-dimensional self avoiding walk data in a simple wedge geometry of wedge angle α, we find the critical behaviour to be described by the scaling form (1.4), (1.5) with $\nu = 3/4$, $y_0 = 91/48$, $y_1 = 3/8$ and $y_2 = -5\pi/8\alpha$, from which all exponents follow by the usual scaling laws, as derived in § 1.

In this study, the lattice axes have been chosen to coincide with the axes of the cartesian coordinate system used in defining the wedge. In order to test whether this choice has any effect on the exponent values, we generated data for the case $\alpha = \frac{1}{2}\pi$ but with the lattice rotated by $\frac{1}{4}\pi$ with respect to the coordinate system. Thus the wedge boundaries were the square lattice diagonals. Repeating the analyses of the previous section for $C_2(\pi/2)$ defined in this way, we find $\gamma_2(\pi/2) = 0.483 \pm 0.012$, (see table 4) in excellent agreement with the conjectured exact result $\gamma_2(\pi/2) = 0.484\,375$. We also generated the series $C_{12}(\pi/2)$ for this geometry, but as all odd terms vanish, the series was too short for all but the crudest analysis, which was consistent with our exact value.

In three dimensions, the assumption of a simple linear form for $y_2(\alpha)$ is well supported by the data. We find that the three-dimensional data are also well represented by the scaling form (1.4), (1.5), where both RG and series estimates have been used to estimate the scaling indices. These are shown in table 5.

Table 5. Scaling indices for two- and three-dimensional N-vector models in a wedge. The two-dimensional results are believed to be exact. In three dimensions, y_0 derives from RG estimates, y_1 and y_2 from series analysis estimates.

	Mean field	$N=0$ (SAW)	$N=1$ (Ising)	$N=2$ (PCH)	$N=3$ (CH)	$N=\infty$ (Spherical)
$d=2$						
y_0	2	$1.895\,83\dot{3}$	1.875	—	—	—
y_1	0	0.375	0.5	—	—	—
y_2	$-\pi/\alpha$	$-5\pi/8\alpha$	$-\pi/2\alpha$	—	—	—
$d=3$						
y_0	2.5	2.488 ± 0.004	2.485 ± 0.004	2.484 ± 0.004	2.483 ± 0.004	2.5
y_1	0.5	0.66 ± 0.02	0.71 ± 0.02	?	?	?
y_2	$0.5 - \pi/\alpha$	$0.5 + b\pi/\alpha$	$0.5 + b\pi/\alpha$	?	?	?
		$b = -0.847 \pm 0.017$	$b = -0.79 \pm 0.02$			

For the two-dimensional Ising model confined to a wedge, Barber *et al* (1984) have found analogous behaviour, described by the scaling form (1.4) and (1.5), where the appropriate scaling indices are also shown in table 5.

It is instructive to compare the results of the scaling index $y_2(\alpha)$ with the mean-field value, $y_2(\alpha) = 1 - \frac{1}{2}d - \pi/\alpha$. For $d = 2$, this gives $y_2(\alpha) = -b\pi/\alpha$, with $b = 1$, which is precisely of the form found for both the Ising and SAW models—with, of course, a different constant b. For $d = 3$, the mean-field result is $y_2(\alpha) = \frac{1}{2} - b\pi/\alpha$, with $b = 1$, which again is precisely of the form found for the SAW model. Our series results are not sufficiently accurate that we can confidently assert that the leading constant is exactly $\frac{1}{2}$ for the SAW model, but since mean-field theory accurately predicts the leading constant for both $d = 2$ models, it seems at least plausible that this should also be true for $d = 3$ models. This would allow the ready evaluation of more accurate exponent estimates than given in (3.14), and these are shown in the last column of table 4. More significantly, it would then follow that $y_2(\alpha) = \frac{1}{2} + b\pi/\alpha$ for all three-dimensional N-vector models, where $b = b(N)$. For the Ising model, we can estimate $b(1)$ using the series for γ_1 given by Whittington *et al* (1979). Their analysis gave $\gamma_1 = 0.78 \pm 0.02$ and we have re-analysed the series using the highly accurate value for the critical temperature obtained by several recent Monte Carlo studies (e.g. Pawley *et al* 1983),

$v_c = \tanh(J/kT_c) = 0.218\,90$, and by comparing the behaviour of the exponent estimates with those of the (longer) SAW series. In that way we estimate $\gamma_1 = 0.755 \pm 0.010$. Then using the RG results $\gamma = 1.241 \pm 0.002$, $\nu = 0.630 \pm 0.0015$, we get $y_0 = 2.485 \pm 0.004$, and our estimate of γ_1 gives $y_1 = 0.713 \pm 0.023$, so that $y_2(\pi) = 1 - y_1 = -0.287 \pm 0.023$. The assumption that $y_2(\alpha) = \frac{1}{2} + b\pi/\alpha$ then yields $b = -0.787 \pm 0.023$. In the last column of table 4 we list the exponents that follow from this assumption.

The assumption that $y_2(\alpha) = \frac{1}{2} + b\pi/\alpha$ could perhaps be tested by determining $y_2(\alpha)$ for the spherical model, but the well known difficulties of interpreting the spherical model in a non-translationally invariant geometry militate against this procedure.

A more convincing argument follows from Cardy's one-loop expansion for y_2,

$$y_2 = d/2 - 1 - \delta + [(5\delta^2 + 1)(N+2)]\varepsilon/12\delta(N+8) + O(\varepsilon^2) \tag{4.1}$$

for the N-vector model, where $\delta = \pi/\alpha$. We note that the order ε term contains no constant part, implying that the constant part is given *solely* by the leading (mean-field) term. This observation is, we believe, a convincing argument for $y_2(\infty) = \frac{1}{2}$.

We have no explanation for the surprisingly complex form of the $O(\varepsilon)$ term in (4.1). Our analysis suggests that $y_2(\alpha) = a + b\delta$, with $a = d/2 - 1$ and $b = b(N, d)$. However Cardy has pointed out other difficulties with his expansion that occur when the angle $\alpha \leq 12°$. Possibly these difficulties can be traced to the problem of defining such manifestly geometric concepts as edges and wedges within the framework of a continuum theory. Penultimately, we make the amusing observation that

$$y_2 = d/2 - 1 - \delta + [3(N+2)]\delta\varepsilon/4(N+8) \tag{4.2}$$

fits all available data exactly for $d = \varepsilon = 2$, and only differs from the best numerical results by a few percent for $d = 3$.

It is worth noting that, while $\gamma_2(\pi) = \gamma_1$, $\gamma_2(2\pi) \neq \gamma$. The reason for this is that $\gamma_2(2\pi)$ is the exponent characterising the number of SAW's that are rooted at the origin and never cross the semi-infinite hyperplane $x_2 = 0$, $x_1 > 0$.

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Addendum. After the completion of this work we were told of an as yet unpublished result of J Cardy, who has obtained $\eta_{11} = (2\nu + 1)/(4\nu - 1)$ from which the results we claim to be exact for the two-dimensional SAW model follow directly. Cardy has also obtained the angular dependence of $y_2(\alpha)$ for the two-dimensional SAW model reported here.

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