Conformal invariance and self-avoiding walks in restricted geometries

1984 J. Phys. A: Math. Gen. 17 L933

(http://iopscience.iop.org/0305-4470/17/17/005)

J. Phys. A: Math. Gen. 17 (1984) L933-L938. Printed in Great Britain

LETTER TO THE EDITOR

Conformal invariance and self-avoiding walks in restricted geometries

J L Cardy† and S Redner‡

Center for Polymer Studies§ and Department of Physics, Boston University, Boston MA 02215, USA

Received 2 August 1984

Abstract. The predictions of conformal invariance for the statistics of self-avoiding random walks restricted to both semi-infinite and wedge-shaped geometries are tested by extrapolating exact enumerations. Close agreement is found, both for the angular distribution of the end-to-end vector, and for the dependence of the critical exponent γ_2 on the opening angle of the wedge.

Conformal invariance is believed to hold at the critical point of isotropic systems with short-range interactions (Polyakov 1970, Wegner 1976). It may be used to understand the effects of different geometries on the critical correlations (Cardy 1984a, b). In this letter we test some of these predictions for self-avoiding random walks (SAWs), which are related to the $n \to 0$ limit of the n-vector model (de Gennes 1979).

We first discuss a d-dimensional bulk geometry, bounded by a planar $(d-1)$-dimensional free surface, considering $d=2$ for simplicity (figure 1(c)). Choose Cartesian coordinates (x, y) so that the surface lies along $y=0$. According to the theory of surface critical phenomena (Binder 1983), the correlation function at the critical point between a spin on the boundary at $(0, 0)$ and one in the bulk at $(r \sin \theta, r \cos \theta)$ has the form

$$G(r, \theta, T_c) \sim r^{-\eta_\perp} f(\cos \theta), \tag{1}$$

as $r \to \infty$ at fixed θ. This is valid for $\cos \theta = x/r > 0$. However, for $\theta = \pi/2$, $G(r) \sim r^{-\eta_\parallel}$, and in order to achieve this r-dependence the angular function must vary as

$$f(\cos \theta) \sim \text{constant } (\cos \theta)^{\eta_\parallel - \eta_\perp}, \tag{2}$$

as $\cos \theta \to 0$. It is a consequence of conformal invariance that this θ-dependence is valid for *all* values of θ. To see this, let $z = x + iy$ and consider the analytic function

$$w(z) = rz/(r - z \sin \theta), \tag{3}$$

which maps the surface $\operatorname{Im} z = 0$ into itself. The point (r, θ) is mapped into $(r/\cos \theta, 0)$. Under such a conformal transformation, the correlation function (z) at T_c satisfies

$$G(z) = |w'(0)|^{\eta/2} |w'(z)|^{\eta/2} G[w(z)], \tag{4}$$

† Permanent address: Department of Physics, University of California, Santa Barbara, CA 93106, USA.
‡ Address from September 1984–January 1985: Schlumberger-Doll Research, PO Box 307, Ridgefield, CT 06877, USA.
§ Supported in part by grants from the ARO, NSF, and ONR.

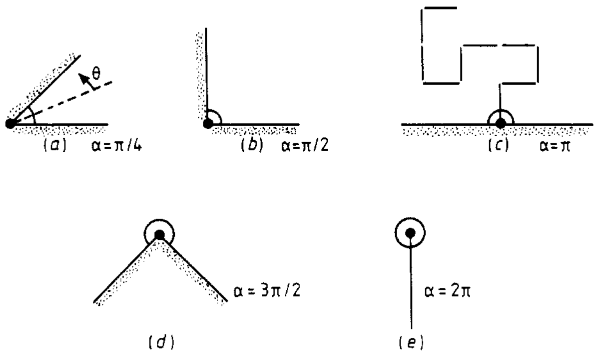

Figure 1. The various wedge geometries discussed in the text.

where η is the bulk exponent. Using the form (1) we find after a little algebra

$$f(\cos\theta)=f(1)(\cos\theta)^{\eta_\perp-\eta}, \tag{5}$$

which is equivalent to (2) extended to all values of θ, since $2\eta_\perp=\eta+\eta_\parallel$ (Binder 1983). Note that since we used only a special conformal transformation (fractional linear mapping) to derive (5) it is in fact valid for general dimension d (Cardy 1984b).

We now examine the consequences of these results for SAWs in the semi-infinite geometry of figure 1(c). The total number of SAWs of N steps beginning at $(0, 0)$ which terminate in a unit area at (r, θ) is given by

$$\int \mathrm{d}T\, \mathrm{e}^{NT} G(r, \theta, T). \tag{6}$$

For $T\neq T_c$, G has the scaling form $\xi^{-\eta_\perp}\phi(r/\xi, \theta)$ where $\xi=[(T_c-T)/T_c]^{-\nu}$. If we define $\rho_N(\theta)\,\mathrm{d}\theta$ to be the number of SAWs of N steps which end somewhere in the wedge $(\theta, \theta+\mathrm{d}\theta)$, then

$$\rho_N(\theta)=\int r\,\mathrm{d}r \int \mathrm{d}T\,\mathrm{e}^{NT}\xi^{-\eta_\perp}\phi(r/\xi, \theta). \tag{7}$$

For $N\to\infty$, the dominant contribution will come from $r\ll\xi$, where the θ-dependence of ϕ is given by (5). We therefore predict

$$\rho_N(\theta)\sim N^{\gamma_1-1}\mu_c^N(\cos\theta)^{\eta_\perp-\eta}, \tag{8a}$$

for $N\to\infty$ at fixed θ, where $\mu_c=\mathrm{e}^{T_c}$, and $\gamma_1=\nu(2-\eta_\perp)$. Exact enumerations of the total number of such walks ($\rho_N(\theta)$ integrated over θ) have been made for the square lattice (Barber *et al* 1978) and the triangular lattice (De Bell and Essam 1980), leading to the estimates $\gamma_1=0.945\pm0.005$ and $\gamma_1=0.956^{+0.014}_{-0.006}$ respectively. These estimates should be compared with the exact value $\gamma_1=61/64=0.9531\ldots$ obtained by Cardy (1984b).

In order to test the predictions of (8), we have enumerated all SAWs of up to 23 steps on the square lattice for which the starting point is on the planar interface (cf table 1), extending the data of Barber *et al* by two terms. As a preliminary, we have analysed the series for the total number of SAWs in order to obtain an independent

Table 1. Number of self-avoiding walks for N steps which start from the apex of a wedge of opening angle α.

N	α: $\pi/4$	$\pi/2$	π	$3\pi/4$	2π
1	1	2	3	4	3
2	2	4	7	10	9
3	3	10	19	28	25
4	8	24	49	74	69
5	14	60	131	202	189
6	36	146	339	534	515
7	70	366	899	1 442	1 395
8	177	912	2 345	3 822	3 767
9	372	2 302	6 199	10 258	10 147
10	942	5 800	16 225	27 202	27 273
11	2 056	14 722	42 811	72 718	73 191
12	5 222	37 368	112 285	192 840	196 093
13	11 736	95 304	296 051	514 228	524 877
14	29 878	243 168	777 411	1 363 342	1 403 127
15	68 576	622 518	2 049 025	3 629 316	3 748 503
16	175 038	1 594 622	5 384 855	9 619 264	10 004 097
17	408 328	4 094 768	14 190 509	25 575 326	26 686 881
18	1 044 533	10 521 384	37 313 977	67 765 590	71 131 217
19	2 468 261	27 085 436	98 324 565	180 001 304	189 527 987
20	6 326 688	69 768 478	258 654 441	476 807 826	504 650 261
21	15 107 015	179 982 688	681 552 747	1265 567 600	1343 361 337
22	38 791 865	464 564 220	1793 492 411	3351 529 410	3573 930 495
23	93 432 564	1200 563 864	4725 856 129	8890 447 682	9506 241 449
24	240 296 399	3104 192 722			
25	583 001 850	8034 256 412			
26	1501 520 574				
27	3665 682 736				

estimate of γ_1. By using square-root ratio analysis, together with the best available estimate for the bulk value of $\mu_c \cong 2.6385$ (Sykes *et al* 1972, Guttmann 1984), we conclude that $\gamma_1 = 0.955 \pm 0.003$. The quoted error bar on γ_1 is merely a subjective estimation of a possible error based on the scattering of the various residue values in a dlog Padé analysis.

In order to test the θ-dependence in (8a), we note that for $d=2$, the exact values for $\eta_\perp$ and η are known, leading to the prediction

$$\rho_N(\theta)\,\mathrm{d}\theta \sim \mu_c^N N^{-3/64}(\cos\theta)^{25/48}\,\mathrm{d}\theta \tag{8b}$$

for the number of N-step SAWS which terminate in the angular range $(\theta, \theta+\mathrm{d}\theta)$. In terms of this angular distribution, the moments

$$\langle\cos^{2j}\theta\rangle \sim \int_0^{\pi/2} \cos^{2j}\theta\rho_N(\theta)\,\mathrm{d}\theta\left(\int_0^{\pi/2}\rho_N(\theta)\,\mathrm{d}\theta\right)^{-1} \tag{9a}$$

can be expressed in terms of gamma functions and subsequently reduced to the closed form

$$\langle\cos^{2j}\theta\rangle = [(a+1)(a+3)\ldots(a+(2j-1))]/[(a+2)(a+4)\ldots(a+2j)], \tag{9b}$$

with $a = 25/48$ from (8*b*). The predicted values of these moments for $j = 1$–4 are shown in column II of table 2.

Table 2. The moments $\langle\cos^{2j}\theta\rangle$ of the angular distribution of end-points as $N \to \infty$: (I) Extrapolation results. These numbers carry an error of ± 0.01; (II) exact predictions of conformal invariance; (III) moments for an isotropic distribution and (IV) mean-field theory (free random walks).

j	I	II	III	IV
1	0.610	0.6033	0.5000	0.6667
2	0.479	0.4698	0.3750	0.5333
3	0.406	0.3978	0.3125	0.4571
4	0.359	0.3511	0.2734	0.4063

From our enumeration data for the total number of SAWS which start at the origin and terminate at a given point (x, y), we have calculated $\langle\cos^{2j}\theta\rangle$ at each value of N and extrapolated to $N \to \infty$ by a Neville-type analysis. These estimates are shown in column I. For each of these values, we tentatively assign an error of ± 0.01 based on the scattering of estimates by various methods of analysis. Even though there appears to be a small systematic difference between the series estimates for the moments and the predictions of conformal invariance, the overall agreement is quite reasonable, particularly in view of the values of a given by other approximate theories. If the surface had no effect, so that the distribution of end-points would be isotropic (corresponding to $a = 0$) the moments shown in column III would be obtained. On the other hand, neglecting the self-repulsion of the walks (mean-field theory) would give a dipolar distribution, resulting from an image effect. This corresponds to $a = 1$, and the resulting moments are shown in column IV.

In addition, we have examined the N-dependence of various measures of mean end-to-end distances to test whether the interface affects the correlation length exponent ν. Such a study was performed previously by Guttmann *et al* (1978) for the half- and quarter-space geometries. We considered the mean-square end-to-end distance $\langle R_N^2\rangle$, and the mean-square displacements parallel and perpendicular to the interface $\langle R_{\parallel N}^2\rangle$ and $\langle R_{\perp N}^2\rangle$, respectively. These quantities all appear to diverge with exponent values 2ν very close to the expected bulk value of 1.50. Moreover, the asymptotic value of the ratio $\langle R_{\parallel N}^2\rangle/\langle R_{\perp N}^2\rangle$ provides an independent test of the angular dependence of the two-point correlation function. Our extrapolations of this ratio are in good agreement with the value predicted by conformal invariance.

Further tests of conformal invariance can be obtained by considering SAWS in a wedge-shaped geometry with opening angle α. That the correlation functions involving spins near the corner should exhibit critical exponents dependent on α was pointed out by Cardy (1983) in the context of mean-field theory and the ε-expansion. For $d = 2$, this geometry is related to the surface case by the conformal mapping $w = z^{\pi/\alpha}$. It is then straightforward to apply (4) to obtain for the wedge geometry

$$\rho_N(\theta)\,\mathrm{d}\theta \sim N^{\gamma_2(\alpha)-1}\mu_c^N[\cos(\pi\theta/\alpha)]^{\eta_\perp-\eta}\,\mathrm{d}\theta, \tag{10}$$

where the boundaries of the wedge are at $\theta = \pm\alpha/2$, and

$$\gamma_2(\alpha) = (\pi/\alpha)\gamma_1 - (\pi/\alpha - 1)(\nu + \gamma/2). \tag{11}$$

To test these predictions, we have enumerated SAWs on the square lattice with the following wedge geometries: $\alpha = \pi/4$, $\pi/2$, $3\pi/2$, and 2π, the last case corresponding to SAWs which originate at one end of an excluded semi-infinite line (cf figure 1). We then employed a number of standard extrapolations to estimate the values of μ_c and $\gamma_2(\alpha)$. One expects that μ_c should be independent of α, that is, the connective constant should coincide with the bulk value. This has been shown rigourously for $\alpha > \pi$ by Whittington (1975) (see also Hammersley *et al* 1982, Whittington and Hammersley 1984). From our analysis we find $\mu_c(\pi/4) \cong 2.625$, $\mu_c(\pi/2) \cong 2.635$, and values of $\mu_c(\alpha) \gtrsim 2.6375$ for larger α, very close to the bulk value for μ_c. The weak α-dependence strongly suggests that asymptotically μ_c is independent of α and equal to the bulk value.

Our estimates for $\gamma_2(\alpha)$ are shown in table 3, and compared with the rigorous predictions of conformal invariance. The case $\alpha = \pi/4$ is somewhat pathological due to the lack of symmetry of the square lattice with respect to the $\theta = 0$ axis. However, for the other geometries, the series estimates strongly support the conformal invariance result.

Table 3. Comparison of the series estimates and the conformal invariance predictions for the exponent $\gamma_2(\alpha)$ governing the total number of N-step walks. $\mu^N N^{\gamma_2 - 1}$, in a wedge of opening angle α.

	$\gamma_2(\alpha)$ Estimated	$\gamma_2(\alpha)$ Predicted
$\pi/4$	-0.350 ± 0.150	$-29/64 \cong -0.453$
$\pi/2$	0.510 ± 0.005	$31/64 \cong 0.484$
π	0.955 ± 0.003	$61/64 \cong 0.953$
$3\pi/2$	1.100 ± 0.002	$71/64 \cong 1.094$
2π	1.189 ± 0.002	$76/64 \cong 1.188$

Finally we have looked at the angular moments $\langle \cos^{2j}(\pi\theta/\alpha) \rangle$ for the various geometries. These moments should coincide with those quoted in (9*b*) for the half-space geometry because the range of angular integration and the angular variable itself are rescaled in the same way compared to the half-space expression (9*a*). Our analysis of the first four moments does suggest that for a given j the estimates for differing geometries coincide. There are some weak dependences of a given moment on the geometry, which we attribute to non-asymptotic effects.

It is also worth mentioning that the divergence of the distance measures mentioned for the half-space problem all appear to be governed by the bulk value of the correlation length exponent with the possible exception of the (pathological) $\pi/4$ wedge geometry.

In conclusion, we have shown that the predictions of conformal invariance for SAWs near a boundary are verified by exact enumeration methods, to within numerical accuracy. It would be interesting to extend these results to other quantities such as monomer density correlations in a long macromolecule near a surface.

One of us (JLC) thanks the Center for Polymer Studies and the Department of Physics, Boston University, for its hospitality.

Note. After this paper was completed, we learned of work by Guttmann and Torrie (1984) in which results similar to some of those given in this paper are obtained. We thank Dr Guttmann for communicating his results prior to publication.

References

Barber M N, Guttmann A J, Middlemiss K M, Torrie G M and Whittington S G 1978 *J. Phys. A: Math. Gen.* **11** 1833

Binder K 1983 *Phase transitions and critical phenomena* vol 8, ed C Domb and J Lebowitz (London: Academic) p 1

Cardy J L 1983 *J. Phys. A: Math. Gen.* **16** 3617

—— 1984a *J. Phys. A: Math. Gen.* **17** L385

—— 1984b *Nucl. Phys. B* [FS] to be published

De Bell K and Essam J W 1980 *J. Phys. C: Solid State Phys.* **13** 4811

de Gennes P G 1979 *Scaling concepts in polymer physics* (Ithaca, NY: University Press)

Guttmann A J 1984 *J. Phys. A: Math. Gen.* **17** 455

Guttmann A J, Middlemiss K M, Torrie G M and Whittington S G 1978 *J. Chem. Phys.* **69** 5375

Guttmann A J and Torrie G M 1984 *J. Phys. A: Math. Gen.* **17** 3541

Hammersley J M, Torrie G M and Whittington S G 1982 *J. Phys. A: Math. Gen.* **15** 539

Polyakov A M 1970 *Pisma ZhETP* **12** 538 (*JETP Lett.* **12** 381)

Sykes M F, Guttmann A J, Watts M G and Roberts P D 1972 *J. Phys. A: Math. Gen.* **5** 653

Wegner F 1976 *Phase transitions and critical phenomena* vol 6 ed C Domb and M S Green (London: Academic)

Whittington S G 1975 *J. Chem. Phys.* **63** 779

Whittington S G and Hammersley J M 1984 *J. Phys. A: Math. Gen.* to be submitted