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LETTER TO THE EDITOR

Tests of hyperuniversality for self-avoiding walks

V Privman† and S Redner‡

† Department of Physics, 405-47, California Institute of Technology, Pasadena, CA 91125, USA

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

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Abstract. A universal combination of amplitudes for the end-to-end distance of N -step self-avoiding walks and for the number of N step self-avoiding polygons is estimated numerically for various lattices. In $d = 2$, universality of this amplitude combination is confirmed to good accuracy, while in $d = 3$, the data are consistent with universality but the error limits are rather large.

For finite-width, square-lattice strips we also calculate universal critical point correlation amplitudes by fixed-fugacity Monte Carlo simulations. In addition, these amplitudes are calculated analytically either exactly or approximately by Cardy's conformal mapping approach. Numerical values agree well with the theoretical predictions.

In addition to the famous hyperscaling exponent relations, e.g. $2 - \alpha = d\nu$ (see a review by Fisher 1974a, and references therein) there is a group of universal critical point amplitude combinations in the bulk (Stauffer *et al* 1972, Ferer *et al* 1973) and finite-size systems (Nightingale and Blöte 1983, Privman and Fisher 1984, Cardy 1984a, Privman 1985, and references therein) which all have a common property: they hold generally only below the upper critical dimension $d_c (= 4)$. Above d_c , these relations are usually violated, by the mechanism of a dangerous irrelevant variable, a feature which implies the non-existence of a scaling limit in the field-theoretical sense (Fisher 1974b, Privman and Fisher 1983, Binder *et al* 1985).

Specifically, one can define a number of divergent length scales near a critical point. These include (a) the correlation length $\xi(T, l)$; (b) an appropriate power of the singular part of the reduced free energy density $f^{(s)}(T, l)$, namely, $|f^{(s)}|^{-1/d}$; (c) the system size, l , for finite-size systems. Below d_c , all these lengths scale in the same way, i.e. their ratios approach *universal* constants as $T \rightarrow T_c$ and $l \rightarrow \infty$. Our present work addresses several aspects of the above amplitude universality property, usually termed hyperuniversality, for self-avoiding walks (SAWS).

We first describe the universal amplitude combination derivable from the root-mean-square end-to-end distance of N step walks, $\langle R_N^2 \rangle^{1/2}$, and the number of distinct unrooted N step polygons, p_N . Square (SQ), triangular (TR), two-choice square (L), simple cubic (SC), body- and face-centred cubic (BCC and FCC) lattice SAWS are then considered and the universal amplitude combination is estimated from existing enumeration data.

Next we consider universal finite-size amplitudes for correlation function moments on two-dimensional, $l \times \infty$, lattice strips, which are related to those calculated by Cardy (1984a) from conformal covariance of correlation functions. We calculate one of these

amplitudes exactly by Cardy's method. Numerical fixed-fugacity Monte Carlo (MC) simulations of SAWS on SQ lattice strips are also performed to calculate amplitudes. Finally the comparison of these results with theoretical values is reported.

We consider $\langle R_N^2 \rangle$ and p_N previously defined, and also the total number, c_N , of N step SAWS. As $N \rightarrow \infty$, we have

$$\langle R_N^2 \rangle \approx AN^{2\nu}, \quad (1)$$

$$c_N \approx C\mu^N N^{\gamma-1}, \quad (2)$$

$$p_N \approx B\mu^N N^{\alpha-3} = B\mu^N N^{-(d\nu+1)}, \quad (3)$$

where μ is the (non-universal) attrition parameter, while A , B and C are non-universal scaling amplitudes. Note that the assumption $d < d_c (= 4)$ was used in writing (3). Furthermore, relation (3) as written is valid for *close-packed lattices*: TR and FCC, only. Generalisation to other lattices will be discussed later.

We now define a universal amplitude relation, the validity of which *relies strongly* on the existence of the underlying field theory for SAWS in the fixed fugacity, z , formulation, namely the $n \rightarrow 0$ limit of the n -vector model (de Gennes 1972, des Cloizeaux 1975). The second-moment *correlation length*, ξ_2 , in the $n \rightarrow 0$ limit corresponds to

$$\xi_2^2(z) \equiv (2d)^{-1} \sum_N \langle R_N^2 \rangle c_N z^N / \sum_N c_N z^N, \quad (4)$$

while the quantity

$$f(z) \equiv k_B T v^{-1} \sum_N p_N z^N, \quad (5)$$

where v is the unit cell volume, has the critical behaviour of the free energy density. As $z \rightarrow z_c^-$, where $z_c \equiv 1/\mu$, one finds the critical-point singularities

$$\xi_2(z) \sim (z_c - z)^{-\nu} \quad \text{and} \quad f^{(s)} \sim (z_c - z)^{2-\alpha} = (z_c - z)^{d\nu}, \quad (6)$$

where (s) denotes the singular part. The two-scale factor universality relates the (undisplayed) amplitudes in (6) by asserting that

$$\Lambda \equiv \lim_{z \rightarrow z_c^-} [f^{(s)} \xi_2^d (k_B T)^{-1}] \quad (7)$$

is a *universal* constant (Stauffer *et al* 1972, Ferer *et al* 1973). In the fixed-fugacity formulation, we convert the sums in (4) and (5) to integrals and employ the asymptotic forms (1) and (3) to find

$$\Lambda = P\Gamma(\alpha - 2)[\Gamma(\gamma + 2\nu)/2d\Gamma(\gamma)]^{d/2}, \quad (8)$$

where $\Gamma(\cdot)$ is the usual gamma function. Thus we conclude that

$$P \equiv (\sigma^{-1} v^{-1} B) A^{d/2} \quad (9)$$

must be *universal* (with $\sigma \equiv 1$ for close-packed lattices).

Let us now discuss the loose-packed lattices SQ, BCC and SC. In this case (3) is valid for large *even* N , but $p_N \equiv 0$ for *odd* N . Thus (5) is a series in z^2 so that $f(z)$ has two equal strength singularities, at $z = \pm z_c$. If B from (3) is used in (9), we must put

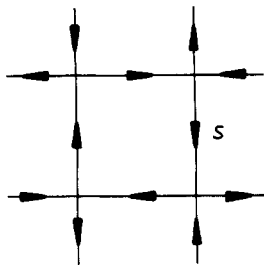
$$\sigma(\text{SQ, BCC and SC}) = 2 \quad (10)$$

in (9) to account for the difference between $f(z)$ and $f^{(s)}(z)$. For the remaining, L or

2-choice square lattice, described in detail, e.g. by Enting and Guttmann (1985) only p_4 and $p_{12}, p_{16}, p_{20}, \dots$ are non-zero. This indicates four singularities in $f(z)$, at $z = \pm z_c, \pm iz_c$ so that

$$\sigma(L) = 4. \tag{11}$$

The data for $\langle R_N^2 \rangle$ are usually given as $\langle R_N^2 \rangle = \rho_N s^2$, where s is the step length while ρ_N is dimensionless. In these units, $v(\text{SQ}) = 1s^2, v(\text{TR}) = (\sqrt{3}/2)s^2, v(\text{SC}) = 1s^3, v(\text{FCC}) = (1/\sqrt{2})s^3, v(\text{BCC}) = (4/3\sqrt{3})s^3$. The L lattice requires special consideration since it is not a regular lattice. The prescription of obtaining SAWS on it as the $n \rightarrow 0$ limit of some n -vector model is not known, so that the choice of v to use in (5) and (9) is ambiguous. When the L lattice is considered with directed bonds, one sees that the 'primitive' lattice vectors, connecting *equivalent sites*, lie along the diagonals. Thus the value of $v(L) = 2s^2$ seems plausible and will be used below.



To estimate $A^{d/2}$ and $(\sigma v)^{-1}B$ in (9) from enumeration data of $\langle R_N^2 \rangle$ and p_N , one needs the values of ν and μ as inputs. In quoting values of ν and μ , the symbol \approx will denote the choice of representative 'central' estimates, error bars being too small to influence appreciably our results. We take $\nu(d=2) = \frac{3}{4}$ (Nienhuis 1982) and $\nu(d=3) \approx 0.5875$ (Majid *et al* 1983). For μ , we use $\mu(\text{SQ}) \approx 2.638155$ and $\mu(\text{L}) \approx 1.5657$ (Enting and Guttmann 1985), $\mu(\text{TR}) \approx 4.15075$ (Guttmann 1984), and $\mu(\text{FCC}) \approx 10.0346, \mu(\text{BCC}) \approx 6.5295, \mu(\text{SC}) \approx 4.6834$ (Watts 1975, and references therein).

In order to estimate $A^{d/2}$ and $B/\sigma v$, we employ existing data and plot the approximating sequences $(\langle R_N^2 \rangle N^{-2\nu})^{d/2}$ and $\sigma^{-1} v^{-1} p_N \mu^{-N} N^{d\nu+1}$, respectively, against $1/N^\theta$ (Martin and Watts 1971, Sykes *et al* 1972, Grassberger 1982, Majid *et al* 1983, Enting and Guttmann 1985, Rapaport 1985a, b, Majid 1985). For several values of the effective convergence exponent θ , within ranges to be described below, we smoothly extrapolated the trend of the data points as $1/N^\theta \rightarrow 0$ to obtain estimates of $A^{d/2}$ and $B/\sigma v$.

In two dimensions, the value of the 'irrelevant' correction-to-scaling exponent Δ_1 is controversial (consult literature listed by Privman 1984a, and more recent work by Rapaport 1985a, and by Kremer and Lyklema 1985). Estimates for Δ_1 range from below $\frac{2}{3}$ to $\frac{3}{2}$, although the conclusion $\Delta_1 < 1$ seems plausible. In addition, the analytic-power, $1/N$ correction term will also be present. Thus we extrapolated against $N^{-\theta}$ with $0.5 \leq \theta \leq 1.0$, and assigned equal weight to estimates obtained with θ varying within this range. This gives

$$A_{\text{SQ}} = 0.765 \pm 0.015, \quad (B/\sigma v)_{\text{SQ}} = 0.283 \pm 0.004, \tag{12a, b}$$

$$A_{\text{TR}} = 0.708 \pm 0.021, \quad (B/\sigma v)_{\text{TR}} = 0.306 \pm 0.007, \tag{13a, b}$$

$$A_{\text{L}} = 0.670 \pm 0.015, \quad (B/\sigma v)_{\text{L}} = 0.36 \pm 0.03. \tag{14a, b}$$

A more refined estimate of A_{TR} can be obtained by elaborate techniques since the TR lattice $\langle R_N^2 \rangle$ series is both relatively long and non-oscillating. The estimates

$$A_{\text{TR}} = 0.707 \pm 0.006 \quad \text{and} \quad A_{\text{TR}} \approx 1/\sqrt{2} (\approx 0.707) \quad (15a, b)$$

have been reported by Privman (1984b) and Djordjevic *et al* (1983), respectively. We will use this estimate, (15a), in place of (13a).

In three dimensions the (smooth, non-oscillating) FCC $\langle R_N^2 \rangle$ series has been subject to a detailed analysis by Majid *et al* (1983). They find

$$A_{\text{FCC}} = 1.05 \pm 0.03, \quad (16)$$

and $\Delta_1 \approx 0.47$. The value of Δ_1 near $\frac{1}{2}$ is consistent with other studies (cited by Majid *et al* 1983). By scanning the range of θ near $\frac{1}{2}$, we estimate

$$A_{\text{FCC}}^{3/2} = 1.03 \pm 0.06, \quad (B/\sigma v)_{\text{FCC}} = 0.054 \pm 0.017, \quad (17a, b)$$

$$A_{\text{BCC}}^{3/2} = 1.07 \pm 0.05, \quad (B/\sigma v)_{\text{BCC}} = 0.074 \pm 0.015, \quad (18a, b)$$

$$A_{\text{SC}}^{3/2} = 1.18 \pm 0.10, \quad (B/\sigma v)_{\text{SC}} = 0.067 \pm 0.007. \quad (19a, b)$$

The error limits here are rather subjective and were obtained by varying θ in the range $0.2 \leq \theta \leq 0.7$. Note that (16) corresponds to $A_{\text{FCC}}^{3/2} = 1.076 \pm 0.046$; we will use this in place of (17a). Rapaport (1985a, b) also reported MC estimates of A for several lattices: his values are consistent with (12a), (13a), (15), (18a) and (19a).

Turning now to the amplitude combination P in (9), we obtain, in two dimensions,

$$P(\text{SQ}) = 0.217 \pm 0.007, \quad (20)$$

$$P(\text{TR}) = 0.216 \pm 0.007, \quad (21)$$

$$P(\text{L}) = 0.24 \pm 0.025. \quad (22)$$

Thus P is indeed universal in $d = 2$. For three-dimensional lattices, we find

$$P(\text{FCC}) = 0.06 \pm 0.02, \quad (23)$$

$$P(\text{BCC}) = 0.08 \pm 0.02, \quad (24)$$

$$P(\text{SC}) = 0.08 \pm 0.015. \quad (25)$$

Although the error bars do overlap for $d = 3$, the deviation of the central FCC value is alarming: further numerical work is called for. Note that the existing ϵ -expansion results (Aharony 1974) are not sufficient for calculating P or Λ of (8) and (9) due to a different normalisation of the critical-point amplitudes involved.

We now turn to the calculation of the amplitudes for SAW correlation function moments in finite strips for the purposes of testing universality. Consider a lattice strip of width l , located at $|y| \leq \frac{1}{2}l$ and $-\infty < x < \infty$ in the xy plane. Cardy (1984a) used conformal covariance of correlation functions in $d = 2$ to establish the asymptotic (large l) relations

$$\xi_0^{(p)}(z_c) \approx (\pi\eta)^{-1}l, \quad (26)$$

$$\xi_0^{(f)}(z_c) \approx 2(\pi\eta_{\parallel})^{-1}l, \quad (27)$$

where ξ_0 is the correlation length defined by the decay of the correlation function

$$G_l(x, y; z) \sim \exp(-|x|/\xi_0(z)), \quad (28)$$

for $|x| \gg l$. The superscripts (p) and (f) denote periodic and free boundary conditions, respectively. For SAWS, $\eta = \frac{5}{24}$ (Nienhuis 1982) and $\eta_{\parallel} = \frac{5}{4}$ (Cardy 1984b). The bulk ($l = \infty$) critical-point $z_c \equiv 1/\mu$ value must be used in (26)-(27).

In our numerical studies, somewhat different quantities are calculated: we consider the average squared end-to-end distance, which corresponds to the $n \rightarrow 0$ limit of the n -vector model quantity

$$\langle r^2 \rangle_c \equiv \left(\sum_{x,y} (x^2 + y^2) G_l(x, y; z_c) \right) / \left(\sum_{x,y} G_l(x, y; z_c) \right), \tag{29}$$

and also the average projection of the end-to-end vector along the strip,

$$\langle x^2 \rangle_c \equiv \left(\sum_{x,y} x^2 G_l(x, y; z_c) \right) / \left(\sum_{x,y} G_l(x, y; z_c) \right), \tag{30}$$

where $\langle \cdot \rangle_c$ denotes a quantity evaluated at z_c . Note that $\langle x^2 \rangle_c$ is equivalent to $2\xi_2^2(z_c)$ defined in (4) since the strip is one dimensional. The correlation lengths $\xi_0(z_c)$ and $\xi_2(z_c)$, although distinct, should not be very different. Therefore we can employ (26) and (27) to obtain *approximate* estimates

$$\langle (x^2)_c^{1/2} / l \rangle^{(p)} \approx \sqrt{2} / \pi \eta \approx 2.16, \tag{31}$$

$$\langle (x^2)_c^{1/2} / l \rangle^{(f)} \approx 2\sqrt{2} / \pi \eta_{\parallel} \approx 0.72, \tag{32}$$

with $\langle r^2 \rangle_c^{1/2} / l$ having close values (obviously $\langle r^2 \rangle_c^{1/2} > \langle x^2 \rangle_c^{1/2}$). Cardy (1985) devised an expansion for small η which can be used to establish the approximate equality (31) (here $\eta = \frac{5}{24} \approx 0.208$).

The asymptotic behaviour of $\langle x^2 \rangle_c^{(p)}$ can, in fact, be calculated in the closed form. Let (ρ, θ) denote polar coordinates in the $d = 2$ plane. Then the conformal mapping of the plane onto a strip reads (Cardy 1984a)

$$x = (l/2\pi) \ln(\rho/a), \tag{33}$$

$$y = l\theta/2\pi. \tag{34}$$

Here a is an arbitrary *fixed* reference point at $(\rho, \theta) = (a, 0)$, while $0 < \rho < \infty$ and $-\pi \leq \theta \leq \pi$. Cardy argued that the asymptotic behaviour of $G_l(x, y; z_c)$ is given by

$$G_l(x, y; z_c) \approx (l/2\pi\rho)^{-\eta/2} (l/2\pi a)^{-\eta/2} \bar{G}_{\infty}(\bar{\rho}; z_c), \tag{35}$$

where the prefactors involve the dilation of the conformal mapping, $l/2\pi\rho$, while \bar{G}_{∞} denotes the bulk correlation function with respect to $(\rho, \theta) \equiv (a, 0)$, instead of the origin. Thus \bar{G}_{∞} depends asymptotically on

$$\bar{\rho} \equiv (\rho^2 + a^2 - 2a\rho \cos \theta)^{1/2} \tag{36}$$

and, at z_c , is given by

$$\bar{G}_{\infty}(\bar{\rho}; z_c) \approx \text{constant} \times (\bar{\rho})^{-\eta}. \tag{37}$$

Now (35) with (33), (34), (36) and (37) reduces evaluation of the numerator and the denominator in relation (29) for $\langle x^2 \rangle_c^{(p)}$ to complicated double integrals. It turns out that the integrals can be calculated in closed form. We will not give details of this tedious calculation except to mention that a great simplification is achieved by changing

the integration variables to polar coordinates (ρ, θ) , via (33)-(34). One obtains

$$(2\pi)^2 l^{-2} \langle x^2 \rangle_c^{(p)} \approx \psi' \left(\frac{\eta}{4} \right) - \frac{\pi^2}{2 \sin^2(\pi\eta/4)}, \tag{38}$$

where the function $\psi'(x) \equiv \sum_{k=0}^{\infty} (x+k)^{-2}$ has been described, e.g. by Gradshteyn and Ryzhik (1980: see p 944). For saws $(\eta = \frac{5}{24})$ we find

$$\langle (x^2)_c^{1/2} / l \rangle^{(p)} \approx 2.160\ 02 \dots, \tag{39}$$

which is very close to the approximate estimate (31). Indeed, we can now explicitly verify that (31) is the asymptotically leading contribution to (38) as $\eta \rightarrow 0$.

Finally, let us point out that predictions of the conformal mapping theory for the critical behaviour of saws at an *edge* have recently been tested by numerical studies (Cardy and Redner 1984, Guttmann and Torrie 1984).

To test the theoretical predictions, we report here numerical estimation of $\langle x^2 \rangle_c^{(p)}$ for sq-lattice strips of width $l = 3, 5, 7, 9, 11, 13, 15$ and of $\langle x^2 \rangle_c^{(f)}$ and $\langle r^2 \rangle_c^{(f)}$ for $l = 3, 5, 7, 9, 11, 15, 19, 25$ (lattice rows). We employ the fixed fugacity, z , MC method which has been introduced by Redner and Reynolds (1981) and described in detail by Berretti and Sokal (1985). The value of $z_c \equiv 1/\mu$ is required as an input: we used the central estimate of Enting and Guttmann (1985) listed above. A total of about 100 hours of CPU time on the IBM 3081 machine were used (80 and 20 hours for periodic and free boundary conditions, respectively).

Our results are summarised in figure 1 where numerical estimates are plotted against l^{-1} . The free boundary condition data seem linear for the l values studied. Extrapolation suggests

$$\langle (x^2)_c^{1/2} / l \rangle^{(f)} \approx 0.71 \pm 0.01, \tag{40}$$

$$\langle (r^2)_c^{1/2} / l \rangle^{(f)} \approx 0.75 \pm 0.01, \tag{41}$$

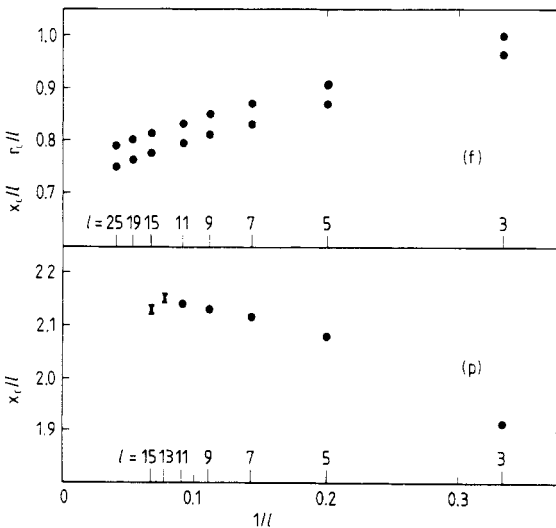


Figure 1. Values of $\langle x^2 \rangle_c^{1/2} / l \equiv x_c / l$ and $\langle r^2 \rangle_c^{1/2} / l \equiv r_c / l$ as functions of l^{-1} . Results for periodic and free boundary conditions are given separately and marked (p) and (f), respectively. One-standard-deviation error ranges do not exceed the size of the symbols, except for the two data points indicated.

as $l \rightarrow \infty$. These values are in agreement with the approximate theoretical prediction (32).

Non-monotonicity of the periodic boundary condition data for $l = 13$ and 15 may indicate that either one-standard-deviation error bars are overly optimistic or that there is some oscillatory behaviour for $l \geq 15$ before the asymptotic value of (39) is approached. Nevertheless, the numerical values for $l \geq 7$ deviate by no more than 3% from the theoretical prediction.

In summary, we presented a discussion and a numerical study of several critical-point amplitude combinations which must be universal for saws in $d = 2$ and 3 . In two dimensions, hyperuniversality is confirmed numerically with reasonable accuracy. In three dimensions, the results are not really definitive and further numerical tests will be useful. We also exploited conformal invariance to show that amplitude of end-to-end distance for saws on finite strips are universal and depend only on the corresponding bulk exponent η . These predictions are in excellent agreement with our numerical simulations.

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