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LETTER TO THE EDITOR

Universal distance ratios for two-dimensional self-avoiding walks: corrected conformal-invariance predictions

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Abstract. We correct a combinatorial error in the Cardy–Saleur conformal-invariance prediction of a universal amplitude ratio for two-dimensional self-avoiding walks. We present high-precision Monte Carlo data that confirm the corrected prediction.

One of the most important results of two-dimensional conformal field theory is the c-theorem of Zamolodchikov [1-3]. Using this theorem, Cardy [4] and Cardy and Saleur [5] have predicted certain universal amplitude combinations for two-dimensional self-avoiding walks. Recently, however, Guttmann and Yang [6] and Lam [7] have presented numerical evidence suggesting that the Cardy–Saleur prediction is strongly violated. In this letter we resolve the contradiction. We show that the Cardy–Saleur logic is correct, but is marred by a combinatorial error involving factors of 2. We then present Monte Carlo data—which are consistent with the estimates of Guttmann–Yang and Lam, but much more precise—that confirm to high accuracy the corrected conformal-invariance prediction.

The c-theorem [1-3] states that on the space of continuum (renormalized) two-dimensional field theories parametrized by coupling constants $g=(g^1,\ldots,g^n)$, there exists a scalar function $C(g)$ and a non-degenerate symmetric matrix function $G_{ij}(g)$ (both of which can be defined explicitly in terms of two-point correlation functions) such that:

(a) at each conformal-invariant renormalization-group fixed point g_* (i.e. $\beta(g_*)=0$), $C(g_*)$ equals the central charge c of the Virasoro algebra in the corresponding conformal field theory;

(b) in a neighbourhood of g_*, the function $C(g)$ is related to the renormalization-group β-function $\beta(g)$ by

$$C(g)=C(g_*)-6(g-g_*)^iG_{ij}(g)\beta^j(g)+\mathrm{O}((g-g_*)^3) \qquad (1)$$

$$\frac{\partial C(g)}{\partial g^i}=-12G_{ij}(g)\beta^j(g)+\mathrm{O}((g-g_*)^2) \qquad (2)$$

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(so that in particular $C(g)$ is stationary at RG fixed points);

(c) for arbitrary g,

$$C(g) \equiv \beta^i(g)\frac{\partial C(g)}{\partial g^i} = -12\beta^i(g)G_{ij}(g)\beta^j(g) \tag{3}$$

(d) the change in $C(g)$ between fixed points g_{*1} and g_{*2} connected by the RG flow is

$$\begin{aligned} C(g_{*2}) - C(g_{*1}) &= -\frac{3}{2}\int_0^\infty R^3\langle\Theta(0)\Theta(R)\rangle^{\mathrm{conn}}\,\mathrm{d}R \\ &= -\frac{3}{4\pi}\int r^2\langle\Theta(0)\Theta(r)\rangle^{\mathrm{conn}}\,\mathrm{d}^2r \end{aligned} \tag{4}$$

where Θ is the trace of the stress tensor, and the connected correlation functions are evaluated at any theory along the RG trajectory running from g_{*1} to g_{*2};

(e) if the theory at g satisfies reflection positivity (sometimes called 'unitarity') [8-10], then $G_{ij}(g)$ is positive-definite (so that in particular $C(g)$ strictly decreases along the RG flow, and is stationary only at RG fixed points).

We emphasize that statements (a)-(d) should hold *whether or not* the theories in question are reflection-positive. This is an important point, because the self-avoiding walk is *not* reflection-positive: this can be seen either by direct calculation of the two-point function on the lattice [11], or by noting that the relevant representations of the Virasoro algebra ($c=0$, $h\neq 0$ [12-14]) lie outside the Friedan-Qiu-Shenker [15] classification.

Cardy [4] and Cardy-Saleur [5] apply the c-theorem to an n-vector model near its critical point: the continuum-limit Hamiltonian is

$$\mathscr{H} = \mathscr{H}^* + t\int \varepsilon(r)\,\mathrm{d}^2r + h\int s^1(r)\,\mathrm{d}^2r \tag{5}$$

where $\mathscr{H}^*$ is the fixed-point Hamiltonian, and ε and s are the energy and spin operators. The trace of the stress tensor is

$$\Theta(r) = 2\pi[y_t t\varepsilon(r) + y_h h s^1(r)] \tag{6}$$

where y_t, y_h are the RG eigenvalues ($y = 2 - x$ where x is the scaling dimension). They then apply the sum rule (4): here g_{*1} is the O(n) fixed point $\mathscr{H}^*$ and g_{*2} is the trivial high-temperature fixed point, so the central charges are $C(g_{*1}) = c(n) = 1 - 6/m(m+1)$ where $n = 2\cos(\pi/m)$ [16-18] and $C(g_{*2}) = 0$. It follows that

$$\int r^2[y_t^2t^2\langle\varepsilon(0)\varepsilon(r)\rangle_{t,h}^{\mathrm{conn}} + y_h^2h^2\langle s^1(0)s^1(r)\rangle_{t,h}^{\mathrm{conn}} + 2y_ty_hth\langle s^1(0)\varepsilon(r)\rangle_{t,h}^{\mathrm{conn}}]\,\mathrm{d}^2r = \frac{1}{3\pi}c(n) \tag{7}$$

independent of t, h in the scaling region. Evaluating (7) at $h=0$, we obtain

$$y_t^2t^2\int r^2\langle\varepsilon(0)\varepsilon(r)\rangle_{t,0}^{\mathrm{conn}}\,\mathrm{d}^2r = \frac{1}{3\pi}c(n). \tag{8}$$

Differentiating (7) twice with respect to h and then setting $h=0$, we obtain

$$\begin{aligned} y_t^2t^2\int (r_1-r_2)^2\langle s^1(0)s^1(r)\varepsilon(r_1)\varepsilon(r_2)\rangle_{t,0}^{\mathrm{conn}}\,\mathrm{d}^2r\,\mathrm{d}^2r_1\,\mathrm{d}^2r_2 + 2y_h^2\int r^2\langle s^1(0)s^1(r)\rangle_{t,0}^{\mathrm{conn}}\,\mathrm{d}^2r \\ -4y_ty_ht\int r_1^2\langle s^1(0)s^1(r)\varepsilon(r_1)\rangle_{t,0}^{\mathrm{conn}}\,\mathrm{d}^2r\,\mathrm{d}^2r_1 = 0. \end{aligned} \tag{9}$$

The next step is to translate these continuum expressions onto the lattice. The lattice O(n) Hamiltonian is $\mathcal{H}=-\beta\sum_{\langle ij\rangle}s_i\cdot s_j-h\sum_i s_i^1$, where s is an n-component isotropic spin normalized to $|s|^2=n$; the energy operator is $\varepsilon(r)=s_i\cdot s_j$ where $r=\langle ij\rangle$. The sum rules (7)–(9) can then be carried over immediately to the lattice, where they hold in the limit $t\equiv\beta_c-\beta\to 0$, $h\to 0$.

To obtain predictions for self-avoiding walks (SAWs), we use the well known representation of the SAW as the $n\to 0$ limit of the O(n) model [19–22]. Cardy's first prediction [4] is obtained by letting $n\to 0$ in (8): both sides of (8) vanish at $n=0$, but extracting the term of order n it is found that

$$\lim_{N\to\infty} Np_N\langle R_b^2\rangle_N\beta_c^N=\frac{5}{16\pi^2} \tag{10}$$

where p_N is the number of N-step self-avoiding polygons and $\langle R_b^2\rangle_N$ is their mean bond-weighted squared radius of gyration. This prediction is confirmed numerically to a few parts in 10^4 [4, 23].

The Cardy–Saleur prediction [5] is obtained by letting $n\to 0$ in (9). The correlation functions become sums over self-avoiding walks: all loops disappear, as do the subtracted terms in the connected correlations. For example, the quantity $\langle s^1(0)s^1(r)\varepsilon(r_1)\rangle_{t,0}^{\text{conn}}$ becomes a sum over self-avoiding walks with endpoints at 0 and r and a bond at r_1. At this point Cardy and Saleur argue that 'each insertion of $\varepsilon(r)$ can be connected to the polymer in two ways, giving rise to factors of 2'. This statement is *incorrect*: while it is true that a bond $r_1=\langle ij\rangle$ can be connected to the walk in two ways, this gives rise to *two different* SAWs: one goes from $0\to i\to j\to r$ and the other from $0\to j\to i\to r$. Therefore, in computing the coefficient for *any given* SAW appearing in the sum over all SAWs, *no factor of 2 appears.* The correct conformal-invariance prediction is therefore not

$$F_\infty\equiv\lim_{N\to\infty}\frac{(2+y_t/y_h)\langle R_g^2\rangle_N-\langle R_m^2\rangle_N+\frac{1}{8}\langle R_e^2\rangle_N}{\langle R_e^2\rangle_N}=0 \tag{11}$$

but rather

$$F'_\infty\equiv\lim_{N\to\infty}\frac{(2+y_t/y_h)\langle R_g^2\rangle_N-2\langle R_m^2\rangle_N+\frac{1}{2}\langle R_e^2\rangle_N}{\langle R_e^2\rangle_N}=0. \tag{12}$$

Here $\langle R_g^2\rangle_N$, $\langle R_e^2\rangle_N$ and $\langle R_m^2\rangle_N$ are, respectively, the mean-square radius of gyration, the mean-square end-to-end distance, and the mean-square distance of a monomer from the origin, taken in the ensemble of all N-step SAWs starting at the origin and ending anywhere. The eigenvalues $y_t=\frac{4}{3}$ and $y_h=\frac{91}{48}$ are known from either Coulomb gas [24] or conformal-invariance [13, 16] methods.

Let us define the amplitude ratios

$$A_N=\frac{\langle R_g^2\rangle_N}{\langle R_e^2\rangle_N} \tag{13}$$

$$B_N=\frac{\langle R_m^2\rangle_N}{\langle R_e^2\rangle_N} \tag{14}$$

$$F_N=\left(2+\frac{y_t}{y_h}\right)A_N-B_N+\tfrac{1}{8} \tag{15}$$

$$F'_N=\left(2+\frac{y_t}{y_h}\right)A_N-2B_N+\tfrac{1}{2}. \tag{16}$$

These ratios become universal (i.e. dependent only on the spatial dimension d) in the limit $N\to\infty$. The ratios A_N and B_N have long been of interest in polymer physics [25].

By enumeration of walks on the square lattice ($N\leqslant 21$) and the triangular lattice ($N\leqslant 15$) together with the usual extrapolation methods, Guttmann and Yang [6] obtain the estimates

$$A_\infty = 0.1396 \pm 0.0010$$

$$B_\infty = 0.4375 \pm 0.0020$$

and thus

$$F_\infty = 0.0649 \pm 0.0047$$
$$F'_\infty = 0.0024 \pm 0.0067.$$

These estimates disagree with the original Cardy-Saleur prediction by more than thirteen error bars, but agree excellently with the corrected prediction. Lam [7] used the incomplete-enumeration Monte Carlo algorithm [26, 27] to generate walks of length up to $N = 100$ on the square lattice. After extrapolation he finds

$$A_\infty = 0.1398 \pm 0.0005$$

$$B_\infty = 0.4399 \pm 0.0010$$

and thus

$$F_\infty = 0.0633 \pm 0.0024$$

$$F'_\infty = -0.0016 \pm 0.0034$$

where the error bars are apparently one standard deviation. (By extrapolating F_N directly he gets $F_\infty = 0.0633 \pm 0.0010$.)

In both cases, however, one might worry about the possible systematic errors due to corrections to scaling, which could be significant for these moderately short walks. To test this, we performed a high-precision Monte Carlo study of SAWs on the square lattice using much longer walks ($250\leqslant N\leqslant 4000$). By far the most efficient algorithm for this purpose is the *pivot algorithm*, which is able to produce one 'effectively independent' configuration in a computer time of order N [28]. Using this algorithm Madras and Sokal [28] have computed A_N for $200\leqslant N\leqslant 10\,000$ and obtained the very precise estimate

$$A_\infty = 0.140\,29 \pm 0.000\,12$$

(95% confidence interval); corrections to scaling were unobservably small (i.e. much smaller than the statistical errors) for $N\geqslant 200$. Here we provide additional data for A_N, and measure also B_N, F_N and F'_N.

In table 1 we report the raw data from our runs. The integrated autocorrelation time for each observable is always of order 20–40. The error bars are determined by

Table 1. The results of our runs. Errors are ± one standard deviation.

N	Iterations	$\langle R_g^2\rangle_N$	$\langle R_e^2\rangle_N$	$\langle R_m^2\rangle_N$	$F_N\langle R_e^2\rangle_N$	$F'_N\langle R_e^2\rangle_N$
250	5.25×10^7	429.83 ± 0.16	3064.7 ± 1.4	1346.8 ± 0.6	198.20 ± 0.38	0.61 ± 0.75
500	5.25×10^7	1212.49 ± 0.47	8646.2 ± 4.1	3801.5 ± 1.8	557.01 ± 1.1	-2.1 ± 2.1
1000	5.25×10^7	3425.1 ± 1.3	$24\,429\pm11$	$10\,739\pm5.0$	1574.1 ± 3.0	-3.7 ± 6.0
2000	5.25×10^7	9696.4 ± 5.9	$69\,023\pm50$	$30\,350\pm21$	4487 ± 14	-10 ± 27
4000	1.02×10^7	$27\,380\pm39$	$194\,830\pm341$	$85\,718\pm144$	$12\,702\pm90$	46 ± 175

Table 2. Our estimates as a function of the length of the walks. Errors (one standard deviation) are shown in parentheses.

N	A_N	B_N	F_N	F'_N
250	0.140 25 (10)	0.439 47 (32)	0.064 67 (12)	0.000 20 (24)
500	0.140 23 (11)	0.439 67 (33)	0.064 42 (13)	−0.000 25 (25)
1000	0.140 21 (11)	0.439 58 (33)	0.064 43 (13)	−0.000 15 (25)
2000	0.140 30 (12)	0.439 71 (35)	0.064 57 (15)	−0.000 14 (28)
4000	0.140 63 (28)	0.440 00 (84)	0.065 20 (34)	0.000 23 (64)

standard methods of time-series analysis [28, appendix C], using a self-consistent rectangular window of width $15\tau_{\mathrm{int}}$. The estimates of $\langle R_g^2\rangle_N$ and $\langle R_e^2\rangle_N$ are in good agreement with those of Madras and Sokal [28], but are more precise.

In table 2 we report the corresponding estimates for the amplitude ratios. Error bars on a ratio $\langle A\rangle/\langle B\rangle$ are determined by applying the usual autocorrelation analysis to the time series $A/\langle A\rangle - B/\langle B\rangle$. We see no statistically significant corrections to scaling in these ratios. Averaging all the data, we find

$$A_\infty = 0.140\,26 \bullet 0.000\,11$$

$$B_\infty = 0.439\,62 \pm 0.000\,33$$

$$F_\infty = 0.064\,54 \pm 0.000\,13$$

$$F'_\infty = -0.000\,06 \pm 0.000\,25$$

where the error bars are 95% confidence intervals (2σ).

Our results are in perfect agreement with the estimates of Guttmann–Yang and Lam, but are more precise. The original Cardy–Saleur prediction is incorrect, but the corrected prediction is verified to a few parts in 10^4. Conformal invariance is vindicated†.

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† For another check of the sum rule (4), see [29].

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