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Monte Carlo test of a hyperscaling relation for the two-dimensional self-avoiding walk: II

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Abstract. By using a novel Monte Carlo algorithm which uses non-local moves to decrease the critical slowing-down, we simulate two-dimensional self-avoiding walks (SAWs) in a variable-length fixed-endpoint ensemble. This allows us to determine with reasonable accuracy the critical exponent α_{sing}. As a byproduct, we obtain also accurate measurements of the exponent ν and the connective constant μ. We thus get a direct check of the hyperscaling relation $d\nu = 2 - \alpha_{sing}$. Estimates of α_{sing} and μ are obtained by a maximum-likelihood fit which combines data generated at different fugacities.

Over the past decade, great progress has been made in improving the available precision in Monte Carlo estimates of the critical behaviour of statistical mechanical models. In part this progress has been due to the vast increases in available computer power; but probably more important (at least in the long run) has been the development of new and vastly more efficient algorithms [1].

In [2, 3] we have introduced a new Monte Carlo procedure to sample the ensemble of self-avoiding walks (SAWs) with variable length and fixed endpoints. Our algorithm is a hybrid of an earlier algorithm [4–6], whose elementary moves are local deformations of the SAW, with non-local moves that cut the walk into pieces and reassemble them (see also [7–9]).

The purely local algorithm, hereafter called BFACF, shows a severe critical slowing-down, more precisely [3, section 3.1]

$$\tau \gtrsim \langle N \rangle^{4\nu} \sim \begin{cases} \langle N \rangle^3 & \text{for } d = 2 \\ \langle N \rangle^{\approx 2.4} & \text{for } d = 3 \\ \langle N \rangle^2 & \text{for } d \geq 4 \end{cases} \tag{1}$$

where τ is the integrated autocorrelation time (for suitable observables) and $\langle N \rangle$ is the average length of the walk. The introduction of non-local moves, inspired by the

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pivot algorithm [10] for generating walks with fixed length and *free* endpoints, has the effect of speeding up the slowest modes of the BFACF algorithm and thereby changing the dynamic universality class of the algorithm. Indeed, for an optimal choice of the percentage of non-local moves we could obtain

$$\tau \sim \langle N \rangle^{\approx 2.3} \tag{2}$$

in dimension $d = 2$. In practice at $\langle N \rangle \approx 150$ there is already a factor-of-6 reduction in the CPU time to obtain a fixed statistical error, with respect to the BFACF algorithm.

In this paper we show concretely how this algorithmic improvement translates into a reduced statistical error in our estimates of static critical quantities, compared to a previous study [11] using the BFACF algorithm. Our principal concern is, as before, the critical exponent α_{sing}, which governs the critical behaviour of the SAW analogue of the singular part of the specific heat. This exponent can be efficiently estimated *only* in a variable-length fixed-endpoint ensemble. As a byproduct we also obtain estimates of the connective constant μ and the critical exponent ν. (These quantities can, however, be estimated more efficiently by other algorithms: see [12] for μ and [10] for ν.) In particular, we can test the hyperscaling relation

$$d\nu = 2 - \alpha_{\text{sing}} \tag{3}$$

as discussed in more detail in [11]. In this paper we study dimension $d = 2$ (square lattice); this is a warm-up for a study (now in progress) of $d = 3, 4$.

Our ensemble consists of all SAWs (of arbitrary length) starting at the origin and ending at a chosen point x, with probability

$$\pi_\beta(\omega) = \Xi(\beta, x)^{-1} (|\omega| + 1)\beta^{|\omega|} . \tag{4}$$

Here $|\omega|$ denotes the number of bonds in the walk ω, β is a user-chosen fugacity, and

$$\Xi(\beta, x) = \sum_{N=0}^{\infty} (N + 1)\beta^N c_N(x) \tag{5}$$

is the partition function for this ensemble, where $c_N(x)$ is the number of N-step SAWs starting from the origin and ending at x. It is expected that $c_N(x)$ has the asymptotic behaviour

$$c_N(x) \sim \mu^N N^{\alpha_{\text{sing}}-2} \qquad x \text{ fixed} \neq 0 \tag{6}$$

as $N \to \infty$†. Here we take x to be a nearest neighbour of the origin.

To estimate μ and α_{sing} we adopt the maximum-likelihood method, as suggested in [12, section 4.2]. We assume that for $N > N_{\min}$ the relation

$$c_N(x) = \begin{cases} a_0(x)\mu^N N^{\alpha_{\text{sing}}-2}[1 + a_1(x)/N] & \text{for } N \text{ odd} \\ 0 & \text{for } N \text{ even} \end{cases} \tag{7}$$

holds, where thanks to a_1 we mimic a correction to scaling that is difficult to make more precise within our errors. By varying $N_{\min}$ and a_1 we can probe the sensitivity of our estimates to corrections to scaling.

† Here N and x are assumed to have the same parity modulo 2, since otherwise $c_N(x) = 0$.

In our case we have at our disposal measurements obtained from runs at various values of the fugacity β. Maximum-likelihood estimators $\hat{\mu}$ and $\hat{\alpha}$ are obtained by solving for each $N_{\min}$ and a_1 the two coupled equations

$$\sum_i l_i \langle N \rangle_{\mathrm{obs},\beta_i} = \sum_i l_i \langle N \rangle_{\hat{\mu},\hat{\alpha},\beta_i}$$
$$\sum_i l_i \langle \log N \rangle_{\mathrm{obs},\beta_i} = \sum_i l_i \langle \log N \rangle_{\hat{\mu},\hat{\alpha},\beta_i} \tag{8}$$

where l_i is the number of 'effectively independent' measurements available for $N > N_{\min}$ at fugacity β_i, which are used to compute the observed averages $\langle \cdot \rangle_{\mathrm{obs},\beta_i}$; and $\langle \cdot \rangle_{\mu,\alpha,\beta}$ are the theoretical averages computed from the probability distribution (4) restricted to $N > N_{\min}$, with the $c_N(x)$ as in (7). The statistical error bars on $\hat{\mu}$ and $\hat{\alpha}$ are obtained from maximum-likelihood theory [12, section 4.2].

In tables 1 and 2 we report, respectively, $\langle N \rangle_{\mathrm{obs}}$ and $\langle \log N \rangle_{\mathrm{obs}}$ for various β and $N_{\min}$, along with their *true* statistical errors (i.e. taking proper account of autocorrelations). These raw data may be useful to readers who wish to reanalyse our data (e.g. using different methods to account for corrections to scaling), or to readers planning their own simulations. In table 3 we give the number of 'effectively independent' measurements in our data, that is, the total number of iterations divided by twice the integrated autocorrelation time $\tau_{\mathrm{int},N}$. In tables 4 and 5 we give, respectively, the estimators $\hat{\mu}$ and $\hat{\alpha}$, as functions of $N_{\min}$ and a_1.

Table 1. $\langle N \rangle_{\mathrm{obs}}$ as a function of β and the cut $N_{\min}$. Errors are ± one standard deviation.

	β			
$N_{\min}$	0.3744	0.3760	0.3771	0.3778
20	79.57±0.91	105.02±1.09	147.62±1.60	210.93±3.74
30	92.07±1.03	118.28±1.20	162.23±1.71	227.29±3.96
40	103.94±1.15	130.90±1.30	175.80±1.82	242.27±4.15
50	115.57±1.28	142.87±1.40	188.77±1.93	256.55±4.34
60	126.84±1.41	154.58±1.51	201.22±2.03	270.20±4.53
70	137.98±1.55	166.04±1.61	213.52±2.14	283.66±4.71
80	148.96±1.69	177.27±1.72	225.45±2.24	296.62±4.89
90	159.75±1.84	188.43±1.83	237.07±2.35	309.19±5.07
100	170.47±2.00	199.31±1.94	248.65±2.45	321.64±5.24
110	181.15±2.18	210.15±2.06	260.05±2.56	333.98±5.42

Using the *flatness criterion* advocated in [12, sections 4.2 and 5.3] and [13], we find that corrections to scaling are reasonably well taken into account with $-1.5 \lesssim a_1 \lesssim -0.5$, yielding the estimates

$$\mu = 2.638\,15 \pm 0.000\,08 \pm 0.000\,36 \tag{9}$$
$$\alpha_{\mathrm{sing}} = 0.497 \pm 0.017 \pm 0.034 \tag{10}$$

where the first error is the systematic error due to omitted corrections to scaling (95% subjective confidence limit as defined in [12, footnote 17]) and the second error is the statistical error (95% confidence limit) evaluated at $N_{\min} = 60$.

Table 2. $\langle \log N \rangle_{obs}$ as a function of β and the cut N_{min}. Errors are ± one standard deviation.

	β			
N_{min}	0.3744	0.3760	0.3771	0.3778
20	4.122±0.009	4.337±0.009	4.599±0.010	4.872±0.016
30	4.326±0.009	4.520±0.009	4.761±0.009	5.016±0.015
40	4.485±0.009	4.664±0.008	4.888±0.009	5.128±0.015
50	4.617±0.009	4.782±0.008	4.995±0.009	5.223±0.014
60	4.730±0.009	4.885±0.008	5.086±0.008	5.305±0.014
70	4.829±0.009	4.975±0.008	5.167±0.008	5.378±0.014
80	4.918±0.009	5.055±0.008	5.240±0.008	5.444±0.013
90	4.997±0.010	5.129±0.008	5.306±0.008	5.503±0.013
100	5.070±0.010	5.196±0.008	5.367±0.008	5.558±0.013
110	5.138±0.010	5.257±0.008	5.423±0.008	5.609±0.013

Table 3. Number of 'effectively independent' measurements obtained for each β, as a function of the cut N_{min}. Also indicated are the total number of iterations in the combined runs at each β.

	β			
N_{min}	0.3744	0.3760	0.3771	0.3778
20	21051	30546	33947	15358
30	17082	26166	30310	14111
40	14106	22694	27371	13087
50	11753	19894	24888	12200
60	9887	17534	22755	11422
70	8361	15530	20859	10716
80	7106	13809	19194	10087
90	6068	12306	17719	9519
100	5196	11011	16376	8994
110	4458	9866	15164	8507
Total Iterations (10^9)	8.2	17.2	47.5	32.7

By fixing μ at the best available estimate [14] $\mu = 2.638\,1585$, we get a better estimate for α_{sing}:

$$\alpha_{sing} = 0.496 \pm 0.009 \pm 0.015\,. \tag{11}$$

Conversely, by fixing $\alpha_{sing} = \frac{1}{2}$ as expected [15], we get a better estimate for μ:

$$\mu = 2.638\,12 \pm 0.000\,07 \pm 0.000\,16\,. \tag{12}$$

As a byproduct of our simulations, we can obtain estimates of the critical exponent ν governing the size of typical SAWs. The mean-square radius of gyration

$$\langle S_N^2 \rangle \equiv \frac{1}{c_N(x)} \sum_{\omega} S_N^2(\omega) \tag{13}$$

Table 4. Maximum-likelihood estimator $\hat{\mu}$ as a function of the parameter a_1 and the cut $N_{\min}$. Values in boldface indicate the 'flatness region'. Statistical error $\Delta\hat{\mu}$ is a 95% confidence interval (2σ).

	a_1								
$N_{\min}$	−1.50	−1.25	−1.00	−0.75	−0.50	−0.25	0.00	0.25	$\Delta\hat{\mu}$
20	2.63826	2.63822	2.63819	2.63816	2.63812	2.63809	2.63805	2.63802	0.00025
30	2.63821	2.63818	2.63816	2.63814	2.63811	2.63809	2.63807	2.63805	0.00028
40	**2.63818**	**2.63816**	**2.63814**	**2.63812**	**2.63811**	2.63809	2.63807	2.63806	0.00031
50	**2.63816**	**2.63814**	**2.63813**	**2.63812**	**2.63810**	2.63809	2.63808	2.63806	0.00034
60	**2.63816**	**2.63815**	**2.63814**	**2.63813**	**2.63812**	2.63811	2.63810	2.63809	0.00036
70	**2.63814**	**2.63813**	**2.63812**	**2.63811**	**2.63810**	2.63809	2.63808	2.63807	0.00039
80	**2.63813**	**2.63813**	**2.63812**	**2.63811**	**2.63810**	2.63809	2.63809	2.63808	0.00042
90	**2.63815**	**2.63815**	**2.63814**	**2.63813**	**2.63812**	2.63812	2.63811	2.63810	0.00044
100	**2.63817**	**2.63817**	**2.63816**	**2.63815**	**2.63815**	2.63814	2.63814	2.63813	0.00047
110	**2.63819**	**2.63818**	**2.63818**	**2.63817**	**2.63816**	2.63816	2.63815	2.63815	0.00050

Table 5. Maximum-likelihood estimator $\hat{\alpha}$ as a function of the parameter a_1 and the cut $N_{\min}$. Values in boldface indicate the 'flatness region'. Statistical error $\Delta\hat{\alpha}$ is a 95% confidence interval (2σ).

	a_1								
$N_{\min}$	−1.50	−1.25	−1.00	−0.75	−0.50	−0.25	0.00	0.25	$\Delta\hat{\alpha}$
20	0.4826	0.4879	0.4931	0.4982	0.5033	0.5083	0.5133	0.5182	0.0159
30	0.4878	0.4919	0.4959	0.4999	0.5038	0.5077	0.5116	0.5155	0.0203
40	**0.4912**	**0.4945**	**0.4979**	**0.5012**	**0.5045**	0.5077	0.5110	0.5142	0.0248
50	**0.4931**	**0.4960**	**0.4989**	**0.5017**	**0.5046**	0.5074	0.5103	0.5131	0.0295
60	**0.4922**	**0.4948**	**0.4974**	**0.4999**	**0.5024**	0.5049	0.5074	0.5100	0.0344
70	**0.4964**	**0.4987**	**0.5010**	**0.5033**	**0.5056**	0.5079	0.5102	0.5124	0.0396
80	**0.4967**	**0.4988**	**0.5009**	**0.5031**	**0.5051**	0.5072	0.5093	0.5114	0.0451
90	**0.4936**	**0.4956**	**0.4976**	**0.4995**	**0.5014**	0.5033	0.5053	0.5072	0.0509
100	**0.4906**	**0.4924**	**0.4942**	**0.4960**	**0.4978**	0.4996	0.5014	0.5032	0.0570
110	**0.4884**	**0.4901**	**0.4918**	**0.4935**	**0.4952**	0.4969	0.4986	0.5002	0.0635

where

$$S_N^2(\omega) \equiv \frac{1}{N+1}\sum_{i=0}^{N}\left(\omega_i - \frac{1}{N+1}\sum_{j=0}^{N}\omega_j\right)^2 \tag{14}$$

is believed to have the asymptotic behaviour

$$\langle S_N^2\rangle \sim N^{2\nu} \tag{15}$$

as $N \to \infty$. In addition, for our two-dimensional walks we can define the *signed* area $\mathcal{A}(\omega)$ enclosed by the closed loop $(\omega_0, \omega_1, \ldots, \omega_N, \omega_0)$, namely

$$\mathcal{A}(\omega) \equiv \text{`}\int y\,\mathrm{d}x\text{'} \equiv \sum_{i=1}^{N+1}\omega_i^{(2)}\left(\omega_i^{(1)} - \omega_{i-1}^{(1)}\right) \tag{16}$$

where $\omega_{N+1} \equiv \omega_0$ and the superscripts refer to the one- and two-components of vectors in $\mathbf{Z}^2$. Clearly $\langle\mathcal{A}\rangle = 0$ by reflection symmetry. It is believed that $\langle|\mathcal{A}|\rangle$ has the

asymptotic behaviour

$$\langle |\mathcal{A}| \rangle \sim N^{2\nu} \tag{17}$$

as $N \to \infty$. See also [16].

To estimate the exponent ν we made a least-squares fit of the data with $N > N_{\min}$ to the relations

$$\langle \log S_N^2 \rangle_N = 2\nu \log(N + b_1) + \log b_0 \tag{18}$$

$$\langle \log |\mathcal{A}| \rangle_N = 2\nu \log(N + c_1) + \log c_0 \tag{19}$$

with b_1, c_1 fixed. Note that once more we are simulating corrections to scaling by means of a simple $1/N$ correction.

In table 6 we show the estimates $\hat{\nu}$ obtained from measurements of the radius of gyration S_N. These estimates agree with those of reference [11], but now it has been possible to penetrate deeper into the critical regime. It appears that the value $b_1 \approx 0.30$ accounts well for the corrections to scaling, at least in the regime of N probed by our simulations ($50 \lesssim N \lesssim 500$). The curves for b_1 above or below 0.30 show, as expected, a slight slope in opposite directions. The whole picture is remarkably smooth, and gives us confidence in the quality of the results. We conclude that

$$\nu = 0.7505 \pm 0.0007 \pm 0.0006 \tag{20}$$

$$b_0 = 0.0548 \pm 0.0004 \pm 0.0003\,. \tag{21}$$

Table 6. Least-squares estimator $\hat{\nu}$ as a function of the parameter b_1 and the cut $N_{\min}$, derived from the data of the squared radius of gyration S_N^2. Statistical error $\Delta\hat{\nu}$ is a 95% confidence interval (2σ).

	b_1								
$N_{\min}$	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	$\Delta\hat{\nu}$
20	0.74854	0.74903	0.74951	0.75000	0.75049	0.75097	0.75146	0.75194	0.00033
30	0.74903	0.74941	0.74978	0.75016	0.75054	0.75091	0.75129	0.75166	0.00040
40	0.74925	0.74956	0.74987	**0.75018**	**0.75049**	**0.75081**	0.75112	0.75143	0.00048
50	0.74943	0.74970	0.74997	**0.75024**	**0.75051**	**0.75077**	0.75104	0.75131	0.00055
60	0.74966	0.74990	0.75014	**0.75037**	**0.75061**	**0.75085**	0.75108	0.75132	0.00062
70	0.74972	0.74993	0.75014	**0.75035**	**0.75057**	**0.75078**	0.75099	0.75120	0.00070
80	0.74967	0.74986	0.75006	**0.75025**	**0.75044**	**0.75064**	0.75083	0.75102	0.00077
90	0.74979	0.74997	0.75014	**0.75032**	**0.75050**	**0.75068**	0.75085	0.75103	0.00085
100	0.74986	0.75002	0.75019	**0.75035**	**0.75051**	**0.75068**	0.75084	0.75101	0.00093
110	0.74987	0.75002	0.75017	**0.75033**	**0.75048**	**0.75063**	0.75079	0.75094	0.00101

The results of a similar analysis for the area $|\mathcal{A}|$ are exhibited in table 7. In this case there is a substantial curvature as a function of $N_{\min}$, so that the potential systematic error is much larger. We estimate

$$\nu = 0.7511 \pm 0.0012 \pm 0.0008 \tag{22}$$

$$c_0 = 0.1351 \pm 0.0020 \pm 0.0011\,. \tag{23}$$

Table 7. Least-squares estimator $\hat{\nu}$ as a function of the parameter b_1 and the cut $N_{\min}$, derived from the data of the area $|\mathcal{A}|$. Statistical error $\Delta\hat{\nu}$ is a 95% confidence interval (2σ).

	b_1								
$N_{\min}$	0.25	0.30	0.35	0.40	0.45	0.50	0.55	0.60	$\Delta\hat{\nu}$
20	0.75008	0.75056	0.75105	0.75153	0.75201	0.75250	0.75321	0.75357	0.00042
30	0.74989	0.75027	0.75064	0.75101	0.75138	0.75176	0.75220	0.75241	0.00052
40	0.74985	0.75015	0.75046	0.75077	0.75108	0.75139	0.75170	0.75186	0.00061
50	0.74993	0.75020	0.75046	0.75072	0.75099	0.75126	0.75150	0.75161	0.00070
60	0.75007	0.75031	0.75055	0.75078	0.75102	0.75125	0.75143	0.75151	0.00079
70	0.75020	0.75041	0.75062	0.75082	0.75104	0.75125	0.75137	0.75142	0.00088
80	0.75015	0.75034	0.75054	0.75073	0.75093	0.75112	0.75125	0.75133	0.00098
90	0.75024	0.75042	0.75059	0.75077	0.75094	0.75112	0.75125	0.75132	0.00108
100	0.75052	0.75068	0.75085	0.75101	0.75117	0.75134	0.75147	0.75153	0.00118
110	0.75065	0.75081	0.75095	0.75111	0.75126	0.75142	0.75155	0.75162	0.00129

Our estimates of μ, α_{sing} and ν are more precise than those in [11] by a factor 6.6, 3.7 and 8.5, respectively. The CPU time was roughly the same in both cases (of the order of 1000 hours on a VAX 8650 running VMS Fortran).

While this is about the best one can do nowadays for the determination of α_{sing}, better determinations of μ and ν can be obtained by using other Monte Carlo algorithms (with less severe critical slowing-down) working in different ensembles. In particular, the Berretti–Sokal algorithm for the variable-length free-endpoint ensemble [12] is most suited for the computation of μ, while the pivot algorithm for the fixed-length free-endpoint ensemble [10] is by far the most efficient algorithm for the study of ν.

For the two-dimensional SAW, the exponents $\alpha_{\text{sing}} = \frac{1}{2}$ and $\nu = \frac{3}{4}$ are believed to be exact [15]. But it is worthwhile to examine the numerical determinations of α_{sing}, ν and μ, as an indicator of the precision and reliability of the various numerical methods. An unbelievably precise estimate of μ and α_{sing} comes from the exact enumeration of self-avoiding polygons (SAPs) on the square lattice up to $N = 56$, a heroic computation by Guttmann and Enting [14]. They estimate

$$\mu = 2.638\,159 \pm 0.000\,005 \tag{24}$$

$$\alpha_{\text{sing}} = 0.500\,06 \pm 0.000\,06 \tag{25}$$

$$\nu = 0.753 \pm 0.007\,. \tag{26}$$

By assuming $\alpha_{\text{sing}} = \frac{1}{2}$, they get a more precise estimate of μ:

$$\mu = 2.638\,1585 \pm 0.000\,0010\,. \tag{27}$$

These estimates are in perfect agreement with ours; for μ and α_{sing} they are vastly more precise, while for ν they are significantly less precise†. In the past year, Enting and Guttmann [17] obtained an even more precise estimate of α_{sing}, by enumerating

† These comparisons of error bars should, however, be interpreted cautiously. Guttmann and Enting [14] do not attach any specific confidence level (even an admittedly subjective one) to their error bar, so its meaning is ambiguous. Our error bars are, by contrast, always 95% confidence limits.

SAPs on the honeycomb lattice up to $N = 82$: using the exactly known connective constant $\mu = (2+\sqrt{2})^{1/2}$ [15, 18], they found

$$\alpha_{\text{sing}} = 0.499\,98 \pm 0.000\,02\,. \tag{28}$$

Other methods yield an accuracy comparable to ours. By a finite-size-scaling method (also called phenomenological renormalisation), Derrida [19] obtained

$$\mu = 2.638\,17 \pm 0.000\,21 \tag{29}$$

$$\nu = 0.7503 \pm 0.0002 \tag{30}$$

(but see the criticisms in [12, section 6.1]). By a Monte Carlo study of SAWs with variable length and free endpoints, Berretti and Sokal [12] obtained

$$\mu = 2.638\,20 \pm 0.000\,04 \pm 0.000\,30 \tag{31}$$

$$\nu = 0.7590 \pm 0.0062 \pm 0.0042 \tag{32}$$

(95% confidence limits). By a Monte Carlo study using the pivot algorithm to generate SAWs with fixed length and free endpoints, Madras and Sokal [10] obtained

$$\nu = 0.7496 \pm 0.0007 \tag{33}$$

(95% confidence limits), where the error is purely statistical (corrections to scaling were unobservably small because they used extremely long walks).

The exponent α_{sing} has, therefore, a curious status: for two-dimensional SAWs (and *only* these!), it has been determined by series-extrapolation methods far more precisely than any other exponent; but Monte Carlo measurements of this exponent are few—only [11] and the present paper, as far as we know—and are considerably *less* precise than for the other exponents. The principal cause of this lack of precision is the severe critical slowing-down exhibited by all known algorithms for simulating the variable-length fixed-endpoint ensemble. Even so, the non-local algorithm used here did provide a factor-of-6 gain in efficiency compared with the previous work.

Our simultaneous and independent determination of ν and α_{sing} allows us to confirm, by Monte Carlo methods, the series-extrapolation studies that establish numerically the hyperscaling relation (3) in dimension two. Analogous checks in dimensions three and four are now in progress.

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