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

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Abstract. We simulated self-avoiding walks on the square lattice with fixed endpoints by means of a dynamic Monte Carlo algorithm. From these data we obtain an evaluation of the effective coordination number μ and the critical exponents α and ν. We can therefore test the hyperscaling relation $2-\alpha = d\nu$ with a careful estimate of systematic and statistical errors.

Among the scaling relations for critical exponents, the most subtle ones are the so-called hyperscaling relations, in which the dimensionality d of the system appears explicitly. While the ordinary scaling laws are expected to hold in all models, the validity of hyperscaling in a given model is a profound dynamical question: in the renormalisation group framework it depends on the existence or not of dangerous irrelevant variables (Fisher 1973, 1983, Knops *et al* 1977). Various forms of hyperscaling have been proven rigorously to hold for two-dimensional Ising models (Aizenman 1982) and to fail for Ising models in dimension $d>4$ (Aizenman 1982, Fröhlich 1982, Aragão de Carvalho *et al* 1983, Aizenman and Graham 1983, Hattori 1983, Aizenman and Fernández 1986, Fröhlich and Sokal 1986, Fernández *et al* 1986); the validity of hyperscaling for the three-dimensional Ising model is a long-standing controversy (Baker 1977, Lévy *et al* 1982, Fisher and Chen 1985, Guttmann 1986a).

In this paper we concentrate on the hyperscaling relation for the specific heat, which is written variously as

$$d\nu = 2-\alpha \tag{1a}$$

or as

$$d\nu = 2-\alpha_{\text{sing}}. \tag{1b}$$

Here ν, α and α_{sing} are the critical exponents for the correlation length, the specific heat and the singular part of the specific heat, respectively. We emphasise, along with Fisher (1967), the distinction between α and α_{sing}: for example, for Ising models and self-avoiding walks in dimension $d>4$ it is expected that $\nu=\frac{1}{2}$, $\alpha=0$, $\alpha_{\text{sing}}=2-\frac{1}{2}d<0$, so that ($1a$) fails but ($1b$) holds. It is not entirely clear whether the heuristic arguments

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for hyperscaling (Kadanoff 1966, Fisher 1967, Hall 1975) are intended to yield (1*a*) or (1*b*). The only available rigorous results are the lower bound

$$\alpha \geqslant \max(2 - d\nu, 0) \tag{2}$$

(Josephson 1967a, b, Stell 1972, Sokal 1981, Hara *et al* 1985 footnote 25) and the upper bound

$$\begin{aligned} &\alpha \leqslant (2-d/2)\gamma \qquad && d \leqslant 4 \\ &\alpha \leqslant 0 && d \geqslant 4 \end{aligned} \tag{3}$$

(Sokal 1979, 1982) for Ising and related models. Since it is known rigorously that $\nu \geqslant \frac{1}{2}$, at least for models satisfying reflection positivity (Glimm and Jaffe 1974, 1977, Fisher 1969, Fröhlich *et al* 1976, Sokal 1982), it follows that (1*a*) must fail for dimension $d > 4$. The validity of (1*a*) and (1*b*) for the three-dimensional Ising model is still somewhat controversial (Zinn-Justin 1979, Lévy *et al* 1982, Fisher and Chen 1985).

The main numerical techniques used so far to study the critical exponent α have been the series extrapolation (Sykes *et al* 1972a, b, Zinn-Justin 1979, Lévy *et al* 1982, Guttmann 1984, 1986b, Enting and Guttmann 1985, Fisher and Chen 1985) and the field theoretic renormalisation group (Le Guillou and Zinn-Justin 1980). Relatively little Monte Carlo work on α has been done; it is the purpose of this paper to begin to fill this gap.

The model we shall consider is the self-avoiding walk (SAW) on the square lattice ($d = 2$). In polymer physics SAW have been introduced as a model for polymer molecules with excluded volume (de Gennes 1979). In field theory they appear as the $n \searrow 0$ limit of an O(n)-invariant σ model (de Gennes 1972, des Cloizeaux 1975, Aragão de Carvalho *et al* 1983). We consider the present study a warm-up for the physically more interesting (and potentially controversial) case of SAW in dimension $d = 3$.

Criticality for this model means the limit of an infinite number of steps. If $C_N(x)$ is the number of N-step SAW starting from the origin and ending at the site x, one expects an asymptotic behaviour of the type

$$C_N(x) \sim \mu^N N^{\alpha_{\rm sing}-2} \tag{4}$$

where μ is called the effective coordination number, which depends on the given lattice. Note that it is $\alpha_{\rm sing}$ which appears in (4); for the SAW we always have $\alpha = \max(\alpha_{\rm sing}, 0)$.

The radius of gyration of a walk is the square root of the mean-square distance from its barycentre of the sites along the walk. The mean radius of gyration $S_N(x)$ for walks of N steps starting from the origin and ending at the site x is believed to scale as

$$S_N(x) \sim N^\nu. \tag{5}$$

The exponents α and ν are believed to depend only on the dimension d of the lattice. In formulae (4) and (5) N must have the same parity as x, otherwise $C_N(x) = 0$. Notice that μ and ν can alternatively be obtained by considering N-step walks starting from the origin but ending anywhere, because their number and their mean radius of gyration are believed to scale as

$$\begin{aligned} &C_N \sim \mu^N N^{\gamma-1} \\ &S_N \sim N^\nu \end{aligned} \tag{6}$$

with γ a new universal exponent.

Nienhuis (1982, 1984) has determined the exact critical exponents for the universality class of the two-dimensional SAW, making use of renormalisation group ideas. He finds $\nu = \frac{3}{4}$ and, assuming hyperscaling, $\alpha_{\text{sing}} = \frac{1}{2}$. Direct numerical estimates of ν and α_{sing} are in agreement with these values. Derrida (1981) obtains

$$\begin{aligned} \mu &= 2.638\,17 \pm 0.000\,21 \\ \nu &= 0.7503 \pm 0.0002 \end{aligned} \tag{7}$$

based on a finite-size scaling (also called phenomenological renormalisation) computation (but see Berretti and Sokal (1985) for a critique). Enting and Guttmann (1985) obtain

$$\begin{aligned} \mu &= 2.638\,16 \pm 0.000\,10 \\ \alpha_{\text{sing}} &= 0.500 \pm 0.005 \end{aligned} \tag{8}$$

based on an exact enumeration of self-avoiding rings on the square lattice up to 46 steps (i.e. $C_N(x)$ for x a nearest neighbour of the origin up to $N = 45$). Assuming $\alpha_{\text{sing}} = \frac{1}{2}$ they obtain the more precise estimate

$$\mu = 2.638\,155 \pm 0.000\,025. \tag{9}$$

Unfortunately their method does not give any information on the mean radius of gyration. This quantity has been studied for rings only up to 28 steps (Privman and Rudnick 1985); the resulting estimate is

$$\nu = 0.750 \pm 0.0015. \tag{10}$$

Monte Carlo studies of SAW with free endpoint (Havlin and Ben-Avraham 1983, Rapaport 1985, Berretti and Sokal 1985, Madras and Sokal 1986) give values for μ and ν in agreement with the above estimates.

In this paper we report the results of a simulation on SAW with fixed endpoints which have been chosen to be nearest neighbours ($|x| = 1$). We use a Monte Carlo algorithm due to Berg and Foerster (1981), Aragão de Carvalho *et al* (1983) and Aragão de Carvalho and Caracciolo (1983) (hereafter referred to as BFACF). This algorithm is of the chain-deformation type, and generates SAW in a modified grand canonical ensemble (N is variable) with grand partition function

$$\Xi(\beta) = \sum_{\omega:0\to x} N(\omega)\beta^{N(\omega)} \tag{11}$$

where ω is a SAW starting at the origin and ending at x, and $N(\omega)$ is the number of steps in ω. The BFACF algorithm has recently been proven to be ergodic in the two-dimensional case (Madras 1986). In dimension $d = 3$ the BFACF algorithm is not ergodic when $|x|_\infty \equiv \max(|x_1|, |x_2|, |x_3|) = 1$, due to the possibility of knots (Sokal 1986). The ergodicity in $d = 3$ for $|x|_\infty \geq 2$, or in $d \geq 4$, is an open question.

The dynamical properties of the BFACF algorithm are rather subtle. Let A be an observable and t the Monte Carlo time, and let

$$\rho_{AA}(t) = \frac{\langle A(0)A(t)\rangle - \langle A(0)\rangle^2}{\langle A(0)^2\rangle - \langle A(0)\rangle^2} \tag{12}$$

be its normalised time-autocorrelation function measured at equilibrium. For most Monte Carlo algorithms $\rho_{AA}(t)$ decays exponentially ($\sim \exp(-t/\tau)$), but for the BFACF algorithm τ is infinite, i.e. the lowest excitation is *massless* (Sokal and Thomas 1986). Nevertheless, the integrated autocorrelation time

$$\tau_{\text{int}} = \tfrac{1}{2} \sum_{t=-\infty}^{+\infty} \rho_{AA}(t) \tag{13}$$

appears to be finite, for *reasonable* observables A. It is this quantity which determines the statistical error bars in the Monte Carlo determination of $\langle A \rangle$ (Binder 1979, Berretti and Sokal 1985). We expect that $\tau_{\text{int},A}$ scales as

$$\tau_{\text{int},A} \sim c_A \langle N \rangle^{p_A}. \tag{14}$$

It is found empirically (Caracciolo and Sokal 1986) that $p_A \approx 3$, at least for the observables $A = N$, N^2, N^3; the constant c_A does of course depend on A. Further information on the dynamical behaviour can be found in Caracciolo and Sokal (1986) and Sokal and Thomas (1986).

We chose $\beta = 0.376$ and performed 1.4×10^8 Monte Carlo iterations for thermalisation; we then performed 3.5×10^{10} iterations, taking data once every 1.4×10^5 iterations. This took ≈ 300 h of CPU time on an IBM 3033 computer. At this value of β,

$$\langle N \rangle = 65.74 \pm 1.64. \tag{15}$$

The autocorrelation time is found to be

$$\tau_{\text{int},N} = (1.87 \pm 0.14) \times 10^6 \tag{16}$$

(Caracciolo and Sokal 1986), indicating that the thermalisation interval was adequate. Following Berretti and Sokal (1985) (see also Caracciolo and Glaus 1985, Glaus 1985, Guttmann *et al* 1986) we computed maximum-likelihood estimates of μ and α_{sing} by assuming that for $N \geqslant N_{\min}$ one has exactly

$$C_N(x) = a_0(x) \mu^N N^{\alpha_{\text{sing}}-2} (1 + a_1(x)/N) \chi(N = x \bmod 2). \tag{17}$$

In tables 1 and 2 we show the estimators for μ and α_{sing} as functions of $N_{\min}$ and a_1. Using the *flatness criterion* (Berretti and Sokal 1985, Guttmann *et al* 1986), we find

$$\begin{aligned} \mu &= 2.6375 \pm 0.0005 \pm 0.0024 \\ \alpha_{\text{sing}} &= 0.520 \pm 0.046 \pm 0.150. \end{aligned} \tag{18}$$

Here the first error is the systematic error due to excluded corrections to scaling (95% subjective confidence limits) and the second error is the statistical error (95% confidence limits, evaluated at $N_{\min} = 49$). If we impose the best series-extrapolation estimate $\mu = 2.638\,156$ (Guttmann 1986b) and perform a one-parameter maximum-likelihood analysis, we find (table 3)

$$\alpha_{\text{sing}} = 0.465 \pm 0.030 \pm 0.057. \tag{19}$$

The estimates (18) and (19) are consistent with the series-extrapolation predictions (though with much larger error bars) and with the presumed exact value $\alpha_{\text{sing}} = \frac{1}{2}$.

To estimate the critical exponent ν, we assumed that for $N \geqslant N_{\min}$ we have exactly

$$\log S_N(x) = \nu \log(N + b_1(x)) + b_0(x) \tag{20}$$

and performed a least-squares fit. In figure 1 we plot the estimates for ν as a function of $N_{\min}$ for a range of values of b_1. We find

$$\nu = 0.750 \pm 0.002 \pm 0.009 \tag{21}$$

Table 1. Maximum-likelihood estimates for μ as a function of N_{min} and a_l (see (17)). The last entry in each column is the statistical error bar (95% confidence limit).

	N_{min}							
a_l	9	19	29	39	49	59	69	79
−2.00	2.6384	2.6380	2.6378	2.6378	2.6376	2.6375	2.6374	2.6373
−1.75	2.6383	2.6379	2.6378	2.6378	2.6376	2.6375	2.6374	2.6373
−1.50	2.6381	2.6378	2.6377	2.6377	2.6376	2.6375	2.6374	2.6372
−1.25	2.6380	**2.6377**	**2.6377**	**2.6377**	**2.6376**	2.6374	2.6373	2.6372
−1.00	2.6378	**2.6377**	**2.6376**	**2.6377**	**2.6375**	2.6374	2.6373	2.6372
−0.75	2.6377	**2.6376**	**2.6376**	**2.6376**	**2.6375**	2.6374	2.6373	2.6372
−0.50	2.6375	**2.6375**	**2.6375**	**2.6376**	**2.6375**	2.6374	2.6373	2.6372
−0.25	2.6374	**2.6375**	**2.6375**	**2.6376**	**2.6375**	2.6374	2.6373	2.6372
0.00	2.6372	**2.6374**	**2.6374**	**2.6375**	**2.6374**	2.6373	2.6373	2.6371
0.25	2.6371	**2.6373**	**2.6374**	**2.6375**	**2.6374**	2.6373	2.6372	2.6371
0.50	2.6370	**2.6373**	**2.6374**	**2.6375**	**2.6374**	2.6373	2.6372	2.6371
0.75	2.6368	2.6372	2.6373	2.6374	2.6374	2.6373	2.6372	2.6371
1.00	2.6367	2.6372	2.6373	2.6374	2.6374	2.6373	2.6372	2.6371
	0.0014	0.0017	0.0019	0.0022	0.0024	0.0030	0.0034	0.0038

Table 2. Maximum-likelihood estimates for α_{sing} as a function of N_{min} and a_l (see (17)). The last entry in each column is the statistical error bar (95% confidence limit).

	N_{min}							
a_l	9	19	29	39	49	59	69	79
−2.00	0.448	0.475	0.487	0.487	0.498	0.512	0.521	0.535
−1.75	0.461	0.483	0.492	0.491	0.502	0.515	0.524	0.537
−1.50	0.473	0.490	0.497	0.495	0.506	0.518	0.527	0.540
−1.25	0.485	**0.497**	**0.502**	**0.500**	**0.509**	0.521	0.530	0.543
−1.00	0.497	**0.503**	**0.507**	**0.504**	**0.513**	0.524	0.533	0.545
−0.75	0.508	**0.510**	**0.513**	**0.508**	**0.517**	0.528	0.536	0.548
−0.50	0.519	**0.517**	**0.518**	**0.512**	**0.520**	0.531	0.539	0.550
−0.25	0.530	**0.524**	**0.523**	**0.516**	**0.524**	0.534	0.542	0.553
0.00	0.540	**0.530**	**0.528**	**0.521**	**0.527**	0.537	0.545	0.556
0.25	0.551	**0.536**	**0.533**	**0.525**	**0.531**	0.540	0.547	0.558
0.50	0.561	**0.543**	**0.537**	**0.529**	**0.534**	0.543	0.550	0.561
0.75	0.571	0.549	0.542	0.533	0.538	0.546	0.553	0.563
1.00	0.580	0.555	0.547	0.537	0.541	0.550	0.556	0.566
	0.047	0.072	0.098	0.123	0.150	0.207	0.255	0.316

Table 3. Maximum-likelihood estimates for $\alpha_{\rm sing}$ as a function of $N_{\rm min}$ and a_1 (see (17)), with $\mu = 2.638\,156$ imposed. The last entry in each column is the statistical error bar (95% confidence limit).

	$N_{\rm min}$									
a_1	9	19	29	39	49	59	69	79	89	99
−3.50	0.407	0.441	0.450	0.452	0.455	0.457	0.457	0.457	0.458	0.459
−3.25	0.416	0.446	0.454	0.454	0.457	0.459	0.459	0.459	0.460	0.460
−3.00	0.424	**0.450**	**0.457**	**0.457**	**0.459**	**0.461**	**0.460**	**0.460**	0.461	0.461
−2.75	0.433	**0.455**	**0.460**	**0.460**	**0.461**	**0.463**	**0.462**	**0.462**	0.462	0.463
−2.50	0.441	**0.459**	**0.463**	**0.462**	**0.464**	**0.465**	**0.464**	**0.463**	0.464	0.464
−2.25	0.449	**0.463**	**0.467**	**0.465**	**0.466**	**0.467**	**0.466**	**0.465**	0.465	0.465
−2.00	0.457	**0.468**	**0.470**	**0.467**	**0.468**	**0.468**	**0.467**	**0.466**	0.467	0.467
−1.75	0.464	**0.472**	**0.473**	**0.470**	**0.470**	**0.470**	**0.469**	**0.468**	0.468	0.468
−1.50	0.472	**0.476**	**0.476**	**0.472**	**0.472**	**0.472**	**0.471**	**0.469**	0.470	0.469
−1.25	0.479	**0.480**	**0.479**	**0.475**	**0.474**	**0.474**	**0.472**	**0.471**	0.471	0.470
−1.00	0.486	0.484	0.482	0.477	0.477	0.476	0.474	0.473	0.472	0.472
−0.75	0.493	0.488	0.485	0.480	0.479	0.478	0.476	0.474	0.474	0.473
−0.50	0.500	0.492	0.488	0.482	0.481	0.480	0.477	0.476	0.475	0.474
	0.025	0.033	0.042	0.050	0.057	0.067	0.076	0.086	0.097	0.109

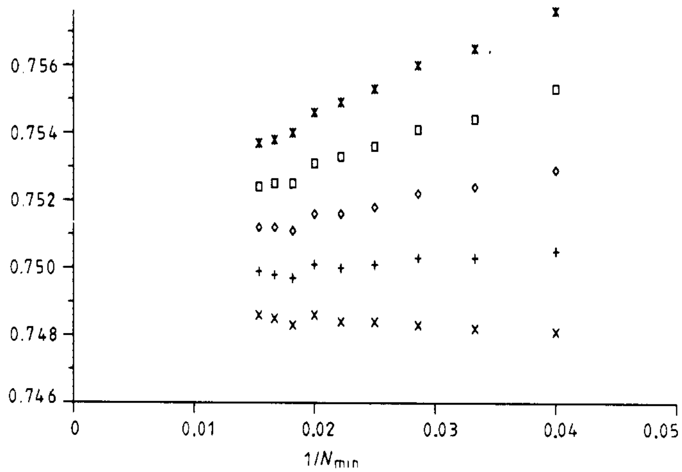

Figure 1. Least-squares estimates for ν as a function of $N_{\rm min}$ and b_1 (see (20)). Error bars are statistical errors only (95% confidence limits). ×, $b = 0$; +, $b = 0.25$; ◇, $b = 0.5$; □, $b = 0.75$; *, $b = 1.0$.

(statistical error bar evaluated at $N_{\rm min} = 49$), in good agreement with the presumed exact value $\nu = \frac{3}{4}$.

Our data are entirely consistent with the hyperscaling relation (1*a*) and (1*b*). It is to be emphasised, however, that our error bars on μ and $\alpha_{\rm sing}$ are very large, and our walks are rather short, compared to a similar study of SAW with *free* endpoints (Berretti and Sokal 1985). This difference can be attributed to the larger dynamic critical exponent of the BFACF algorithm ($\tau_{{\rm int},N} \sim \langle N \rangle^{\approx 3}$) as compared to the Berretti–Sokal algorithm ($\tau \sim \langle N \rangle^2$). Perhaps the simulation of walks with fixed endpoints is intrinsically more difficult than for free endpoints, or perhaps new algorithms better than the BFACF algorithm can be devised. The question is an important one, and upon it may depend the feasibility of a high-precision Monte Carlo test of the hyperscaling relation (1) for the three-dimensional SAW.

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