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## Criticality of self-avoiding walks with an excluded infinite needle

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**Abstract.** We study the effect of repulsion for self-avoiding walks and random walks from excluded sets. We show, in particular, that the mean displacement away from an excluded infinite needle of self-avoiding random walks in three dimensions has to diverge along the privileged axis as  $N^\sigma$ , where  $N$  is the number of steps and  $\sigma$  is a sub-leading critical exponent for the two-point function. This exponent has been determined by using a high-precision Monte Carlo simulation ( $\sigma = 0.370 \pm 0.011$ ). Its knowledge is used to improve the measure of universal quantities, like the exponent  $\nu$  ( $\nu = 0.5867 \pm 0.0025$ , in agreement with the  $\epsilon$ -expansion estimate and with experimental data) and amplitude ratios. We verify also that for simple random walks the excluded needle introduces instead logarithmic violations to scaling.

### 1. Introduction

In this paper we will investigate the repulsion of self-avoiding walks (SAWs) from an excluded half-line. This work is motivated by the intriguing result by Considine and Redner [1] who found that, in three dimensions, the mean displacement of a SAW along the axis away from the excluded set diverges with the number of steps  $N$  as  $N^\sigma$ , with the new critical exponent  $\sigma \approx 0.35$ . However, this result was obtained by using enumeration data with  $N \leq 17$  and the observed behaviour may only be a short-series effect. Indeed, in the corresponding random-walk model they found that the asymptotic behaviour is reached only for very large  $N$  because of strong corrections to scaling.

In two dimensions, the same model has been fully clarified [2] by means of conformal techniques (see [3] for an introduction). No new exponent appears as  $\sigma = \nu = \frac{3}{4}$ .

Less understood is the model in which the excluded set reduces to a point. The effect of repulsion, when this point is chosen to be a nearest-neighbour of the origin of the SAW, has also been studied as *persistence* of the walk in the direction of the first step. From the available data, the mean displacement in the direction of the first step

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is interpreted to scale either as a power of  $N$  with a small exponent [4], or as a  $\log N$  [5], in analogy to what is known exactly for the simple random walk [6]†.

In section 2 we shall clarify how these different behaviours can be understood by looking at the relevance of the perturbation which the excluded set introduces, at the fixed point which governs the scaling behaviour of the model without this constraint. In particular, we shall see that the exponent  $\sigma$  is simply related to the sub-leading correction to the two-point correlation function of the corresponding continuum limit which emerges from the scaling. It will also follow that in two-dimensions with an excluded point a power-law behaviour (and not a logarithmic growth) must be expected for SAWs.

A high-precision Monte Carlo test has confirmed our expectations. In section 3 we present the results which lead to the determination of  $\sigma$ , while in section 4 we will use the relation between  $\sigma$  and the sub-leading corrections to the two-point function to better extrapolate the behaviour of universal quantities. For example, the exponent  $\nu$  turns out to be lower than previously observed, but in agreement with the  $\varepsilon$ -expansion result and with experimental data from polymers.

As an extra test of our ideas, we also simulated the simple random walk in the presence of an excluded needle in three dimensions, because in this case we believe that the perturbation due to the excluded needle is not irrelevant but marginal. Indeed, the presence of logarithmic corrections to scaling at the fixed point is confirmed in section 5.

## 2. Excluded set and corrections to scaling

In the terminology of the field-theoretic approach to critical phenomena, the criticality of the SAW is governed by the fixed point of the  $O(n)$   $\sigma$ -model analytically continued to  $n=0$  [11–14]. The presence of an excluded region corresponds to a perturbation due to the introduction of an operator which creates vacancies in the  $O(n)$  model. Let us suppose for concreteness that the excluded region  $\mathcal{R}$  is cylindrically symmetric about some axis (as is the case for an excluded point or half-line, and is true more generally for an excluded wedge or cone); then it is convenient to use polar coordinates  $(r, \theta)$  oriented along this axis. Now consider the correlation function between a spin at the origin and one in the bulk at location  $(r, \theta)$ ; this function will have the scaling form

$$G_{\mathcal{R}}(\rho, \theta; \beta) \sim \rho^{-(d-2+\eta_{\mathcal{R}})} F_{\mathcal{R}}(\rho/\xi(\beta), \theta) + \rho^{-(d-2+\eta'_{\mathcal{R}})} F'_{\mathcal{R}}(\rho/\xi(\beta), \theta) + \dots \quad (1)$$

Here  $\beta$  is the inverse temperature, and  $\xi \sim (\beta_c - \beta)^{-\nu}$  is the correlation length in the unperturbed theory; the critical inverse temperature  $\beta_c$  and the exponent  $\nu$  are not modified by the presence of the vacancies‡. However, the behaviour of the other quantities depends on whether the perturbation is relevant or irrelevant [16]:

(i) If the perturbation is relevant, then the leading spin-spin decay exponent  $\eta_{\mathcal{R}}$  differs from its bulk value  $\eta$  (and as a consequence the leading susceptibility exponent  $\gamma_{\mathcal{R}} = (2 - \eta_{\mathcal{R}})\nu$  differs from its bulk value  $\gamma = (2 - \eta)\nu$ ). Likewise, the leading scaling

† More recent work concerning persistency properties of trails and silhouettes, which belong to the same universality class of SAW, can be found in [7] and [8], respectively in two and three dimensions. See also [9] and [10], where persistency is used to locate the transition temperatures.

‡ Unless the excluded region  $\mathcal{R}$  is so big that the remaining set  $\mathbb{Z}^d \setminus \mathcal{R}$  is effectively a space of lower dimensionality. See [15] for how thin a set has to be before  $\mu = 1/\beta_c$  changes.

function  $F_{\mathcal{R}}$  differs from its bulk value  $F$ ; in particular, it has a non-trivial angular dependence [17].

(ii) If the perturbation is *irrelevant*, then  $\eta_{\mathcal{R}}$  and  $F_{\mathcal{R}}$  are *unchanged* from their bulk values  $\eta$  and  $F$ . In particular, the leading scaling function  $F$  has *no angular dependence*. The effects of the perturbation show up only in the *non-leading* exponents and scaling functions  $\eta'_{\mathcal{R}}, \dots$  and  $F'_{\mathcal{R}}, \dots$ , which *can* differ from their bulk values.

In either case,  $\eta_{\mathcal{R}}$  and  $F_{\mathcal{R}}$  (and indeed all of the exponents  $\eta'_{\mathcal{R}}, \dots$  and scaling functions  $F'_{\mathcal{R}}, \dots$  except for an unknown amplitude) are universal in the sense that they depend only on the *global* properties of the excluded region  $\mathcal{R}$ , such as its dimensionality and its opening angle.

More subtle is the case in which the perturbation is *marginal*:  $\eta_{\mathcal{R}}$  is equal to the bulk value but the universal scaling behaviour may be broken by logarithmic violations and observables associated with the perturbation can show a complete breaking of universality, in the sense that they can have critical exponent with an explicit dependence from the coupling of the perturbation [18, 19].

Let us now discuss the relevance of the perturbation introduced by an excluded region  $\mathcal{R}$  for SAWs and random walks. Let us remember that on pure dimensional grounds it is easy to establish that the probability of intersection of two random objects, extending at infinity respectively in  $d'$  and  $d''$  dimensions, in a lattice of dimension  $d$ , is not null only if

$$d' + d'' \geq d. \quad (2)$$

Let  $d''$  be the dimension of the chosen region  $\mathcal{R}$  on the lattice.

First let us consider the case of a random walk. It is well known that its Hausdorff dimension is two. This means that a random walk may intersect the region  $\mathcal{R}$  outside any bounded volume if

$$d \leq d'' + 2. \quad (3)$$

For strict inequality we expect that the operator which creates the vacancies in the region  $\mathcal{R}$  to be relevant at the fixed point which governs the criticality of the walks. Marginality should correspond to the case of equality. Let  $\mathcal{R}$  be a single point, i.e.  $d'' = 0$ . Then we expect marginality in  $d = 2$  (which shows up in logarithmic corrections [6]) and irrelevant corrections in  $d = 3$  (which implies the appearance of a *persistence length* as in [1]). If  $\mathcal{R}$  is a *half-line*,  $d'' = 1$ , thus in two dimensions there is a change in the universality class (which shows up in a variation of the value of  $\eta$ , while  $\nu$  stays unaltered), marginality would occur in  $d = 3$  and irrelevant corrections in  $d \geq 4$ , in close agreement with Considine and Redner's calculations for  $d = 2, 3$  [1].

Now, the Hausdorff dimension of a SAW is  $d' = 1/\nu$ , where

$$\begin{aligned} \nu = 1 & \quad \text{for } d = 1 \\ \nu = \frac{3}{4} & \quad \text{for } d = 2 \\ \nu \approx 0.6 & \quad \text{for } d = 3 \\ \nu = \frac{1}{2}(\log) & \quad \text{for } d = 4 \\ \nu = \frac{1}{2} & \quad \text{for } d > 4. \end{aligned} \quad (4)$$

(The Flory formula  $\nu \approx 3/(d+2)$  for  $d \leq 4$  is an excellent approximation, though not exact in general.) Therefore, we expect an excluded point to be a relevant perturbation

if  $d \leq 1/\nu$ ; this occurs only in dimension  $d = 1$ . Likewise, we expect an excluded half-line or line to be a relevant perturbation if  $d \leq 1/\nu + 1$ ; this occurs only in dimension  $d = 1, 2$ , indeed in the interesting case  $d = 2$  there appears an explicit  $\theta$ -dependence of  $F_{\mathcal{R}}$  [17], from which it follows that all quantities, even and odd, have the same behaviour given by (11) [2]. (If the Flory formula were exact, these perturbations would be relevant for  $d \leq 1$  and  $d \leq \frac{5}{2}$ , respectively.) Above these dimensions the perturbation is irrelevant and thus we expect the leading exponents to remain equal to their bulk value.

Now let  $z = \rho \cos \theta$  be the end-point coordinate of the SAW which feels the asymmetry due to the presence of the excluded region, and  $r = \rho \sin \theta$ , i.e. the end-point coordinate of the SAW, respectively longitudinal and transversal with respect to the exclusion axis. The average value

$$\langle r^k z^h \rangle(\beta) = \sum_N \langle r^k z^h \rangle_N C_N \beta^N \tag{5}$$

where  $C_N$  is the total number of SAWs of  $N$  steps beginning at the origin and ending anywhere, is given by

$$\frac{\int dV \rho^{k+h} \cos^h \theta \sin^k \theta G(\rho, \theta; \beta)}{\int dV G(\rho, \theta; \beta)} \tag{6}$$

By using the form (1) for the two-point function, we obtain

$$\langle r^k z^h \rangle(\beta) = A_1(h, k) \xi^{k+h}(\beta) + A_2(h, k) \xi^{k+h+\eta-\eta'}(\beta) + \dots \tag{7}$$

where  $A_1(h, k)$  and  $A_2(h, k)$  are moments of the scaling functions  $F_{\mathcal{R}}$  and  $F'_{\mathcal{R}}$ , respectively:

$$A_1(h, k) = \frac{\int dV \rho^{k+h-(d-2+\eta_{\mathcal{R}})} \cos^h \theta \sin^k \theta F_{\mathcal{R}}(\rho, \theta)}{\int dV \rho^{-(d-2+\eta_{\mathcal{R}})} F_{\mathcal{R}}(\rho, \theta)} \tag{8}$$

$$A_2(h, k) = \frac{\int dV \rho^{k+h-(d+2+\eta'_{\mathcal{R}})} \cos^h \theta \sin^k \theta F'_{\mathcal{R}}(\rho, \theta)}{\int dV \rho^{-(d-2+\eta_{\mathcal{R}})} F_{\mathcal{R}}(\rho, \theta)} \tag{9}$$

Since  $\xi \sim N^\nu$ , we find

$$\langle r^k z^h \rangle_N \sim A_1(h, k) N^{(h+k)\nu} + A_2(h, k) N^{(h+k+\eta-\eta')\nu} + \dots \tag{10}$$

Now, if the perturbation is *relevant*, then  $F_{\mathcal{R}}$  has non-trivial angular dependence, and presumably all of the moments  $A_1(h, k)$  are non-zero (barring miraculous cancellations). In this case

$$\langle r^k z^h \rangle_N \sim N^{(h+k)\nu} \tag{11}$$

for all  $h, k$ . On the other hand, if the perturbation is *irrelevant*, then  $F$  has no angular dependence, so  $A_1(h, k) = 0$  for  $h$  odd; but presumably all of the moments  $A_2(h, k)$  are non-zero (again barring miraculous cancellations). Hence we have

$$\langle r^k z^h \rangle_N \sim \begin{cases} N^{(h+k)\nu} & \text{for } h \text{ even} \\ N^{\sigma+(h+k-1)\nu} & \text{for } h \text{ odd} \end{cases} \tag{12}$$

where  $\sigma = (\eta - \eta' + 1)\nu$ . This second case, as we have shown, corresponds to SAWs in two dimensions with an excluded point and in three dimensions with an excluded needle. Thus in both cases we expect  $\langle z \rangle$  to scale as  $N^\nu$  with  $\sigma \neq \nu$  and no logarithms, in contrast to what happens for simple random walks.

Another effect of the sub-leading correction induced by the excluded point in two dimensions and by the half-line in three dimensions is the appearance of a non-rotational invariant sub-leading correction to even quantities with exponent  $\Delta = (\eta' + \eta)\nu = \nu - \sigma$ . For instance, by considering in the three-dimensional case the end-to-end distance, we will have

$$\langle z^2 \rangle_N = AN^{2\nu} \left( 1 + \frac{B}{N^{\Delta_n}} + \dots \right) \quad (13)$$

$$\langle r^2 \rangle_N = 2AN^{2\nu} \left( 1 + \frac{B'}{N^{\Delta_n}} + \dots \right) \quad (14)$$

with  $B \neq B'$ , where the dots include rotational-symmetric corrections (possibly with a lower exponent) and non-rotational invariant terms with a larger exponent. The subscript  $n$  shows that we refer to the problem with an excluded needle. It follows that  $\sigma = \nu - \Delta_n$  can be also computed measuring  $\langle r^2 \rangle_N / \langle z^2 \rangle_N - 2$  which scales like  $N^{-\Delta_n} = N^{-(\nu+\sigma)}$ . This will provide an important consistency check for our reasoning.

For the three-dimensional case the relation between this exponent  $\Delta_n$  and the sub-leading corrections in the bulk is not clear and is presently under investigation [20]. The situation is simpler in two dimensions with an excluded point. Here  $\langle R_e^2 \rangle$  in the bulk is equal to  $\langle z^2 \rangle + \langle r^2 \rangle$  computed with an excluded point. Indeed, the exclusion of a point that is a nearest-neighbour to the origin of the SAW is equivalent to fix the first link of the walk, but quantities like  $\langle R_e^2 \rangle$  are insensitive to the direction of the first step. It follows that the exponent  $\Delta_p$  which occurs in presence of an excluded point will appear as a sub-leading exponent also for quantities in the bulk, as long as  $B + B' \neq 0$ .

If this is the case the value obtained by Grassberger [4] for  $\sigma$  in  $\langle z \rangle = aN^\sigma$ , i.e.  $\sigma = 0.063 \pm 0.010$ , could be interpreted in terms of the irrelevant operators which have been recently found by Saleur [21] through an investigation of the transfer matrix. He found that the thermal operators of the theory have dimensions  $X_i = 2h_{3,i+2}$  where  $h_{r,s}$  is given by the Kac formula [22, 23] with central charge  $c = 0$ :

$$h_{r,s} = \frac{(2r-3s)^2 - 1}{24}. \quad (15)$$

The lowest operator has dimension  $X_1 = \frac{2}{3}$  and corresponds to the energy operator, while the second has dimension  $X_2 = \frac{35}{12}$ , thus giving rise to a sub-leading exponent  $\Delta_p = (X_2 - 2)\nu = \frac{11}{16}$ . This would imply  $\sigma = \nu - \Delta_p = \frac{1}{16} = 0.0625$ , in good agreement with Grassberger's value. Thus, Grassberger's result seems to confirm the presence of a term with  $\Delta = \frac{11}{16}$  for bulk quantities and indeed there is some numerical evidence that this is the case [24-27]. This possibility is actually under investigation [28].

### 3. Detection of the sub-leading corrections

In order to test the ideas presented in the previous section we have studied the three-dimensional case with an excluded needle by means of a high-precision Monte Carlo simulation on a cubic lattice using very long SAWs ( $100 \leq N \leq 16\,000$ ). We have performed our simulations on an IBM 4381 using a total of roughly 1500 hours of CPU time for SAWs and 100 for the simulation of simple random walks.

By far the most efficient algorithm for simulating SAWs with free endpoints and fixed length  $N$  is the *pivot algorithm*, which is able to produce an effectively independent

**Table 1.** Autocorrelation times for different observables and the percentage of accepted pivot moves for SAWs in  $d = 3$ . The error ranges correspond to the 95% confidence interval (two standard deviations).

$N$	$\tau_{\text{int},z}$	$\tau_{\text{int},z^2}$	$\tau_{\text{int},z^3}$	$\tau_{\text{int},R_g^2}$	$f$
100	$6.10 \pm 0.10$	$4.41 \pm 0.06$	$5.10 \pm 0.08$	$15.5 \pm 0.4$	0.582
150	$6.60 \pm 0.12$	$4.64 \pm 0.07$	$5.38 \pm 0.08$	$17.5 \pm 0.5$	0.557
250	$7.17 \pm 0.09$	$4.95 \pm 0.05$	$5.85 \pm 0.07$	$20.1 \pm 0.4$	0.527
500	$7.93 \pm 0.11$	$5.33 \pm 0.06$	$6.38 \pm 0.08$	$23.0 \pm 0.5$	0.488
1 000	$8.42 \pm 0.17$	$5.93 \pm 0.10$	$6.65 \pm 0.12$	$26.7 \pm 1.0$	0.453
2 000	$9.59 \pm 0.21$	$6.60 \pm 0.12$	$7.79 \pm 0.15$	$29.9 \pm 1.1$	0.419
4 000	$9.98 \pm 0.30$	$7.07 \pm 0.18$	$8.09 \pm 0.22$	$32.2 \pm 1.7$	0.386
16 000	$11.36 \pm 1.11$	$7.98 \pm 0.80$	$9.39 \pm 0.88$	$35.6 \pm 5.3$	0.319

**Table 2.** The results of our runs in  $d = 3$  for SAWs. The error ranges are 95% confidence intervals (two standard deviations).

$\langle \mathcal{O} \rangle_N$	$N$			
	100	150	250	500
Iterations	$5.2 \times 10^6$	$5.2 \times 10^6$	$1 \times 10^7$	$1 \times 10^7$
$\langle z \rangle_N$	$1.000 \pm 0.028$	$1.165 \pm 0.038$	$1.401 \pm 0.038$	$1.756 \pm 0.061$
$\langle z^2 \rangle_N$	$87.47 \pm 0.30$	$141.74 \pm 0.49$	$260.36 \pm 0.68$	$593.1 \pm 1.6$
$\langle z^3 \rangle_N$	$233.7 \pm 7.6$	$443 \pm 16$	$986 \pm 31$	$(278 \pm 11) \times 10^1$
$\langle z^4 \rangle_N$	$(2051 \pm 14) \times 10^1$	$(5400 \pm 38) \times 10^1$	$(1830 \pm 10) \times 10^2$	$(9517 \pm 53) \times 10^2$
$\langle z^5 \rangle_N$	$(842 \pm 35) \times 10^2$	$(259 \pm 12) \times 10^3$	$(1077 \pm 43) \times 10^3$	$(685 \pm 34) \times 10^4$
$\langle r^2 \rangle_N$	$183.45 \pm 0.47$	$295.71 \pm 0.80$	$541.1 \pm 1.1$	$1224.3 \pm 2.7$
$\langle zr^2 \rangle_N$	$133.4 \pm 5.5$	$258 \pm 12$	$559 \pm 22$	$1567 \pm 78$
$\langle R_g^2 \rangle_N$	$42.296 \pm 0.084$	$68.38 \pm 0.15$	$125.68 \pm 0.21$	$285.90 \pm 0.52$
$\langle R_e^2 \rangle_N$	$270.91 \pm 0.65$	$437.5 \pm 1.1$	$801.5 \pm 1.5$	$1817.5 \pm 3.6$
$\langle R_m^2 \rangle_N$	Data not available		$385.18 \pm 0.73$	$874.6 \pm 1.8$

  

$\langle \mathcal{O} \rangle_N$	$N$			
	1000	2000	4000	16 000
Iterations	$5 \times 10^6$	$1 \times 10^7$	$1 \times 10^7$	$7.5 \times 10^6$
$\langle z \rangle_N$	$2.34 \pm 0.13$	$2.98 \pm 0.12$	$3.93 \pm 0.22$	$6.54 \pm 0.64$
$\langle z^2 \rangle_N$	$1344.7 \pm 5.4$	$3031.9 \pm 7.6$	$6884 \pm 20$	$(3526 \pm 13) \times 10^1$
$\langle z^3 \rangle_N$	$(870 \pm 55) \times 10^1$	$(248 \pm 12) \times 10^2$	$(734 \pm 46) \times 10^2$	$(618 \pm 69) \times 10^3$
$\langle z^4 \rangle_N$	$(4908 \pm 41) \times 10^3$	$(2499 \pm 13) \times 10^4$	$(12906 \pm 78) \times 10^4$	$(3385 \pm 26) \times 10^6$
$\langle z^5 \rangle_N$	$(521 \pm 39) \times 10^5$	$(315 \pm 10) \times 10^6$	$(214 \pm 17) \times 10^7$	$(93 \pm 13) \times 10^9$
$\langle r^2 \rangle_N$	$2759.4 \pm 8.8$	$6220 \pm 12$	$14067 \pm 23$	$(7143 \pm 21) \times 10^1$
$\langle zr^2 \rangle_N$	$(480 \pm 39) \times 10^1$	$(1361 \pm 84) \times 10^1$	$(392 \pm 32) \times 10^2$	$(350 \pm 48) \times 10^3$
$\langle R_g^2 \rangle_N$	$647.9 \pm 1.8$	$1466.3 \pm 2.6$	$3323.2 \pm 6.7$	$16\,980 \pm 44$
$\langle R_e^2 \rangle_N$	$4103 \pm 12$	$9252 \pm 17$	$20\,951 \pm 46$	$(10\,669 \pm 30) \times 10^1$
$\langle R_m^2 \rangle_N$	$1974.4 \pm 6.1$	$4463.8 \pm 8.7$	$10\,102 \pm 22$	$(5143 \pm 15) \times 10^1$

configuration in a computer time of order  $N$  [29]. This algorithm can also be used in our case, in the presence of an excluded line: it is indeed very simple to see that the ergodicity proof given in [29] can be easily extended to this case. In tables 1–3 we report the raw data from our runs. The integrated autocorrelation times have been computed using a self-consistent rectangular window of width  $15\tau_{\text{int}}$  (see appendix C of [29] for details), and  $f$  represents the percentage of accepted pivot moves. Here  $R_g^2$  stands for the radius of gyration.

From the data of table 1 we can determine the dynamic behaviour of the algorithm. The dynamic exponents are obtained by fitting the data against  $KN^p(1+H/N^\Delta)$  for various, *fixed*, values of  $H$  and  $\Delta$  and then applying the *flatness criterion* advocated in sections 4.2 and 5.3 of [30]. We find

$$p_z = 0.123 \pm 0.021 \pm 0.006 \quad (16)$$

$$p_{z^2} = 0.142 \pm 0.020 \pm 0.005 \quad (17)$$

$$p_{z^3} = 0.128 \pm 0.024 \pm 0.006 \quad (18)$$

$$p_{R_g^2} = 0.144 \pm 0.035 \pm 0.011 \quad (19)$$

$$p_f = -0.1126 \pm 0.0017 \pm 0.0003 \quad (20)$$

where the first error is the systematic error due to unincluded corrections to scaling (95% subjective confidence limit as defined in footnote 17 of [30]) and the second error is the statistical error (95% confidence interval). The critical exponents agree with those found by Madras and Sokal for SAWs in the bulk, thus showing that the introduction of the excluded half-line does not change the dynamic universality class of the algorithm.

From the data of tables 2 and 3 we obtain the exponents and the amplitudes reported in table 4 ( $\langle \mathcal{O} \rangle = K_\sigma N^{\sigma_\sigma}$ ) by performing a least-squares fit. From these data it is immediately seen that quantities like  $\langle z^k r^h \rangle_N$  with  $k$  odd and  $h$  even scale like  $N^{\sigma+(k+h-1)\nu}$  where  $\sigma \approx 0.37$ . Specifically we have (we divide by appropriate powers of  $z$  in order to eliminate the  $\nu$ -dependence of the exponents)

$$\sigma(\langle z \rangle) = 0.367 \pm 0.011 \quad (21)$$

$$\sigma(\langle z^3 \rangle / \langle z^2 \rangle) = 0.372 \pm 0.013 \quad (22)$$

$$\sigma(\langle z^5 \rangle / \langle z^4 \rangle) = 0.377 \pm 0.017 \quad (23)$$

$$\sigma(\langle zr^2 \rangle / \langle r^2 \rangle) = 0.362 \pm 0.024 \quad (24)$$

**Table 3.** Values of  $\sigma(F_{A,B})$  where  $F_{A,B} = A/\langle A \rangle - B/\langle B \rangle$ . They are needed for the calculation of the error of the ratio  $\langle A \rangle / \langle B \rangle$ , as shown later in the text.

$\sigma(F)_N$	$N$							
	100	150	250	500	1000	2000	4000	16 000
$F_{R_g^2, R_g^2}$	0.000 63	0.000 65	0.000 49	0.000 53	0.000 78	0.000 50	0.000 58	0.000 74
$F_{R_m^2, R_g^2}$	Not available		0.000 52	0.000 55	0.000 85	0.000 53	0.000 62	0.000 79
$F_{z^3, z^2}$	0.001 74	0.001 79	0.001 36	0.001 40	0.002 04	0.001 33	0.001 51	0.001 91
$F_{z^3, z^2}$	0.016	0.018	0.015	0.020	0.031	0.021	0.031	0.055



**Table 4.** Critical exponents and amplitudes with error ranges (two standard deviations) for SAWs as recovered from a least-squares fit. The sum of weighted square deviations is also reported (the number of degrees of freedom is six, except for  $R_m^2$  where it is four).

$\langle O \rangle$	$\sigma_O$	$\Delta\sigma_O$	$K_O$	$\Delta K_O$	$\chi^2$
$\langle z \rangle$	0.367	0.011	0.184	0.012	3.0
$\langle z^3 \rangle$	1.555	0.012	0.182	0.013	4.3
$\langle z^3 \rangle / \langle z^2 \rangle$	0.372	0.013	0.481	0.036	4.3
$\langle z^5 \rangle$	2.747	0.015	0.273	0.026	9.2
$\langle z^5 \rangle / \langle z^4 \rangle$	0.377	0.017	0.725	0.077	6.8
$\langle zr^2 \rangle$	1.541	0.015	0.112	0.010	3.0
$\langle zr^2 \rangle / \langle r^2 \rangle$	0.362	0.024	0.139	0.018	3.4
$\langle r^2 \rangle$	1.175 2	0.000 6	0.821 3	0.003 2	28.1
$\langle z^2 \rangle$	1.181 7	0.000 7	0.381 4	0.001 8	48.7
$\langle z^4 \rangle$	2.366 7	0.001 4	0.385 2	0.003 9	69.6
$\langle R_g^2 \rangle$	1.177 4	0.000 5	1.120 2	0.004 3	47.2
$\langle R_g^2 \rangle$	1.181 7	0.000 6	0.184 1	0.000 6	94.4
$\langle R_m^2 \rangle$	1.177 0	0.000 7	0.581 0	0.001 5	14.2
$\langle r^2 \rangle / \langle z^2 \rangle - 2$	-0.226	0.029	0.271	0.048	4.5

giving the final estimate

$$\sigma = 0.370 \pm 0.011 \quad (25)$$

where the error range corresponds to the 95% confidence interval.

These results are in complete agreement with those obtained by Considine and Redner and thus we can confirm the presence of this sub-leading exponent.

As expected the even quantities  $\langle z^2 \rangle$ ,  $\langle r^2 \rangle$  and  $\langle R_g^2 \rangle$  scale as usual as  $N^{2\nu}$ , with  $\nu \approx \frac{3}{5}$ . The error ranges in table 4 are, however, too optimistic. The high value of  $\chi^2$  and the inconsistency between the values of  $\nu$  obtained from different observables (see for instance the estimates from  $\langle z^2 \rangle$  and  $\langle r^2 \rangle$  in table 4) show the necessity of the inclusion of correction terms to simple scaling. Moreover, fitting the data discarding the low- $N$  values shows a systematic decrease of the estimate, and this is a clear sign of the presence of sizeable sub-leading corrections. We will discuss this problem in the following section.

We have also measured the sub-leading exponent associated with the breaking of the rotational invariance, analysing the behaviour of the quantity  $\langle r^2 \rangle / \langle z^2 \rangle - 2$  which scales as  $N^{-\Delta}$ . A least-squares fit gives

$$\Delta_n = 0.226 \pm 0.029 \quad (26)$$

in good agreement with our more refined prediction  $\Delta_n = \nu - \sigma = 0.217 \pm 0.013$ , all error bars being 95% confidence intervals.

#### 4. Universal behaviour

As we have seen in the previous section a reliable determination of  $\nu$  requires the introduction of sub-leading corrections. Usually, keeping account of these terms is difficult because the sub-leading exponent is not known and it should be included as an extra parameter in the fits. Here, however, the situation is different; indeed, we know that a term  $1/N^\Delta$  with  $\Delta = \Delta_n = 0.22$  is certainly present. We do not know if this

is really the lowest sub-leading correction; indeed, rotational-invariant terms with lower  $\Delta$  cannot *a priori* be excluded. However, the low value of  $\Delta_n$  makes us confident that this is indeed the lowest correction.

We will thus suppose that the first sub-leading correction to the two-point function is non-rotational invariant, fitting our data as

$$\langle \mathcal{O} \rangle = KN^{2\nu} \left( 1 + \frac{H}{N^\Delta} \right) \tag{27}$$

with  $\Delta = 0.22$ , using the method described in [30]. In tables 5 and 6 we present the results for the end-to-end distance  $R_c^2$  and the radius of gyration  $R_g^2$ , by including each time only the data with  $N \geq N_{\min}$ . Using the flatness criterion we get

$$\nu(\langle r^2 \rangle) = 0.5873 \pm 0.0037 \pm 0.0004 \tag{28}$$

$$\nu(\langle z^2 \rangle) = 0.5890 \pm 0.0042 \pm 0.0004 \tag{29}$$

$$\nu(\langle z^4 \rangle) = 0.5875 \pm 0.0030 \pm 0.0005 \tag{30}$$

$$\nu(\langle R_c^2 \rangle) = 0.5870 \pm 0.0020 \pm 0.0003 \tag{31}$$

$$\nu(\langle R_g^2 \rangle) = 0.5856 \pm 0.0021 \pm 0.0003 \tag{32}$$

$$\nu(\langle R_m^2 \rangle) = 0.5865 \pm 0.0030 \pm 0.0004 \tag{33}$$

where the error ranges are respectively the systematic and the statistical ones and correspond to 95% confidence intervals. Here  $R_m^2$  is the average distance of a monomer from an end point of the walk.

In applying the flatness criterion we have discarded the data at  $N = 100$  and 150. Inclusion of these data produces estimates of  $\nu$  strongly varying from one observable to the other and not compatible among them. Indeed, the flatness regions include

**Table 5.** Least-square estimator  $\nu$  as a function of the parameter  $H$  and of the cut  $N_{\min}$ , derived from the data of the square end-to-end distance. The statistical error  $\Delta\nu$  is a 95% confidence interval and refers to all the data belonging to the same column. Below each value we report the  $\chi^2$  of the corresponding fit ( $\chi_n^2$  where  $n$  is the number of degrees of freedom). Values in bold face indicate the flatness region.

$H$	$N_{\min}$					
	100	150	250	500	1000	2000
0.04	0.589 68	0.589 31	0.588 92	0.588 44	0.588 52	0.588 61
	$\chi_6^2 = 61.3$	$\chi_5^2 = 35.6$	$\chi_4^2 = 13.3$	$\chi_3^2 = 3.4$	$\chi_2^2 = 3.3$	$\chi_1^2 = 3.2$
0.00	0.588 68	0.588 36	<b>0.588 02</b>	<b>0.587 61</b>	<b>0.587 79</b>	<b>0.587 93</b>
	$\chi_6^2 = 47.2$	$\chi_5^2 = 28.0$	$\chi_4^2 = 10.4$	$\chi_3^2 = 3.6$	$\chi_2^2 = 3.1$	$\chi_1^2 = 2.8$
-0.04	0.587 66	0.587 40	<b>0.587 09</b>	<b>0.586 78</b>	<b>0.587 05</b>	<b>0.587 23</b>
	$\chi_6^2 = 35.1$	$\chi_5^2 = 21.7$	$\chi_4^2 = 8.5$	$\chi_3^2 = 4.3$	$\chi_2^2 = 3.1$	$\chi_1^2 = 2.5$
-0.08	0.586 62	0.586 41	<b>0.586 16</b>	<b>0.585 93</b>	<b>0.586 30</b>	<b>0.586 52</b>
	$\chi_6^2 = 25.3$	$\chi_5^2 = 16.8$	$\chi_4^2 = 7.5$	$\chi_3^2 = 5.3$	$\chi_2^2 = 3.0$	$\chi_1^2 = 2.1$
-0.12	0.585 56	0.585 40	0.585 20	0.585 06	0.585 54	0.585 81
	$\chi_6^2 = 18.2$	$\chi_5^2 = 13.7$	$\chi_4^2 = 7.6$	$\chi_3^2 = 6.8$	$\chi_2^2 = 3.1$	$\chi_1^2 = 1.8$
-0.16	0.584 47	0.584 38	0.584 23	0.584 18	0.584 77	0.585 09
	$\chi_6^2 = 14.0$	$\chi_5^2 = 12.3$	$\chi_4^2 = 9.0$	$\chi_3^2 = 8.9$	$\chi_2^2 = 3.4$	$\chi_1^2 = 1.5$
$\Delta\nu$	0.000 27	0.000 30	0.000 35	0.000 46	0.000 68	0.000 82

**Table 6.** Results for the radius of gyration. See the caption of table 5 for the explanation of the symbols.

$H$	$N_{\min}$					
	100	150	250	500	1000	2000
0.00	0.590 84	0.590 45	0.589 97	0.589 35	0.589 05	0.588 95
	$\chi_6^2 = 94.4$	$\chi_5^2 = 61.4$	$\chi_4^2 = 22.6$	$\chi_3^2 = 3.9$	$\chi_2^2 = 2.2$	$\chi_1^2 = 2.0$
-0.10	0.588 23	0.587 98	0.587 62	0.587 23	0.587 19	0.587 19
	$\chi_6^2 = 43.3$	$\chi_5^2 = 30.3$	$\chi_4^2 = 9.0$	$\chi_3^2 = 1.3$	$\chi_2^2 = 1.3$	$\chi_1^2 = 1.3$
-0.14	0.587 14	0.586 96	<b>0.586 65</b>	<b>0.586 35</b>	<b>0.586 42</b>	<b>0.586 47</b>
	$\chi_6^2 = 28.2$	$\chi_5^2 = 21.0$	$\chi_4^2 = 5.6$	$\chi_3^2 = 1.1$	$\chi_2^2 = 1.0$	$\chi_1^2 = 1.0$
-0.18	0.586 03	0.585 92	<b>0.585 67</b>	<b>0.585 46</b>	<b>0.585 64</b>	<b>0.585 74</b>
	$\chi_6^2 = 16.8$	$\chi_5^2 = 13.8$	$\chi_4^2 = 3.5$	$\chi_3^2 = 1.5$	$\chi_2^2 = 1.0$	$\chi_1^2 = 0.8$
-0.22	0.584 90	0.584 85	<b>0.584 66</b>	<b>0.584 56</b>	<b>0.584 85</b>	<b>0.585 00</b>
	$\chi_6^2 = 9.6$	$\chi_5^2 = 9.1$	$\chi_4^2 = 3.1$	$\chi_3^2 = 2.6$	$\chi_2^2 = 1.0$	$\chi_1^2 = 0.5$
-0.26	0.583 74	0.583 76	0.583 63	0.583 64	0.584 05	0.584 25
	$\chi_6^2 = 7.2$	$\chi_5^2 = 7.1$	$\chi_4^2 = 4.3$	$\chi_3^2 = 4.3$	$\chi_2^2 = 1.2$	$\chi_1^2 = 0.4$
$\Delta\nu$	0.000 24	0.000 27	0.000 32	0.000 43	0.000 63	0.000 76

points got from fits with relative low goodness (high  $\chi^2$ ). Thus, probably at  $N = 100$  and 150 additional corrections to scaling are still sizeable†: we expect corrections with exponents  $N = 2\Delta \approx 0.4$ ,  $N = 3\Delta$  and so on, which can still be relevant at these low values of  $N$ .

From the data we obtain the final estimate

$$\nu = 0.5867 \pm 0.0025. \quad (34)$$

This value for  $\nu$  is less than the value obtained in the absence of an excluded half-line with Monte Carlo methods [29, 31], exact enumeration [32] and with that obtained by considering self-avoiding polygons [33]. However, notice that the determinations based on Monte Carlo data did not take into account sub-leading non-analytic corrections which, if included, as noticed in [33], lower the estimate of  $\nu$ . We do not feel qualified to pass a judgement on the series extrapolation method, but we suspect that at the currently available series length ( $N \leq 21$ ) a strong sub-leading correction could explain the discrepancy (see [34]). Notice that our value is in agreement with the estimate obtained from the  $\varepsilon$ -expansion [35] and with the experimental value  $\nu = 0.586 \pm 0.004$  [36].

We have also computed the ratios

$$A_N = \langle R_g^2 \rangle / \langle R_e^2 \rangle \quad (35)$$

$$B_N = \langle R_m^2 \rangle / \langle R_e^2 \rangle \quad (36)$$

which are believed to converge as  $N \rightarrow \infty$  to constants depending only on the universality class. Here again a simple weighted mean gives a very high  $\chi^2$ , showing the necessity of the inclusion of a correction term. We have thus fitted our data against  $K + H/N^\Delta$  with  $\Delta$  ranging within a large interval. The results for  $A$  are reported in table 7. We get

$$A = 0.1605 \pm 0.0011 \pm 0.0003 \quad (37)$$

$$B = 0.4826 \pm 0.0022 \pm 0.0005. \quad (38)$$

† We thank Alan Sokal for suggesting this possibility to us.

**Table 7.** Values of  $A$  for various values of  $\Delta$  and  $N_{\min}$ . Errors (two standard deviations, 95% confidence level) are shown in parentheses.  $\Delta = \infty$  corresponds to the weighted average.

$\Delta$	$N_{\min}$					
	100	150	250	500	1000	2000
$\infty$	0.157 54 (7) $\chi^2_7 = 923.8$	0.157 71 (7) $\chi^2_6 = 691.5$	0.157 90 (7) $\chi^2_5 = 479.6$	0.158 23 (8) $\chi^2_4 = 218.7$	0.158 55 (10) $\chi^2_3 = 55.2$	0.158 67 (11) $\chi^2_2 = 22.9$
1.00	0.158 39 (9) $\chi^2_6 = 174.0$	0.158 58 (10) $\chi^2_5 = 87.9$	0.158 72 (11) $\chi^2_4 = 46.4$	0.158 93 (13) $\chi^2_3 = 9.6$	0.159 06 (17) $\chi^2_2 = 4.5$	0.159 10 (23) $\chi^2_1 = 4.2$
0.75	0.158 64 (10) $\chi^2_6 = 104.0$	0.158 80 (11) $\chi^2_5 = 48.0$	0.158 92 (12) $\chi^2_4 = 25.5$	0.159 12 (15) $\chi^2_3 = 4.6$	0.159 21 (21) $\chi^2_2 = 3.0$	0.159 21 (27) $\chi^2_1 = 3.0$
0.50	0.159 10 (12) $\chi^2_6 = 43.3$	0.159 25 (14) $\chi^2_5 = 17.0$	0.159 34 (15) $\chi^2_4 = 9.6$	0.159 50 (19) $\chi^2_3 = 2.4$	0.159 49 (28) $\chi^2_2 = 2.4$	0.159 43 (35) $\chi^2_1 = 2.0$
0.30	0.160 00 (18) $\chi^2_6 = 13.9$	0.160 12 (20) $\chi^2_5 = 5.8$	0.160 16 (22) $\chi^2_4 = 5.2$	0.160 24 (29) $\chi^2_3 = 4.5$	0.160 04 (42) $\chi^2_2 = 2.7$	0.159 85 (52) $\chi^2_1 = 1.3$
0.25	0.160 44 (20) $\chi^2_6 = 10.8$	0.160 56 (23) $\chi^2_5 = 5.9$	0.160 57 (26) $\chi^2_4 = 5.8$	0.160 61 (34) $\chi^2_3 = 5.7$	0.160 30 (50) $\chi^2_2 = 2.9$	0.160 07 (61) $\chi^2_1 = 1.1$
0.24	0.160 55 (21) $\chi^2_6 = 10.4$	0.160 66 (24) $\chi^2_5 = 6.1$	0.160 68 (27) $\chi^2_4 = 6.1$	0.160 70 (35) $\chi^2_3 = 6.0$	0.160 37 (51) $\chi^2_2 = 2.9$	0.160 12 (63) $\chi^2_1 = 1.1$
0.23	0.160 67 (22) $\chi^2_6 = 10.1$	0.160 78 (24) $\chi^2_5 = 6.3$	0.160 79 (28) $\chi^2_4 = 6.3$	0.160 80 (36) $\chi^2_3 = 6.3$	0.160 44 (53) $\chi^2_2 = 3.0$	0.160 18 (66) $\chi^2_1 = 1.1$
0.22	0.160 80 (23) $\chi^2_6 = 9.9$	0.160 91 (25) $\chi^2_5 = 6.6$	0.160 91 (29) $\chi^2_4 = 6.6$	0.160 91 (83) $\chi^2_3 = 6.6$	0.160 52 (56) $\chi^2_2 = 3.0$	0.160 24 (68) $\chi^2_1 = 1.1$
0.21	0.160 95 (23) $\chi^2_6 = 9.8$	0.161 05 (26) $\chi^2_5 = 7.0$	0.161 04 (30) $\chi^2_4 = 7.0$	0.161 03 (39) $\chi^2_3 = 7.0$	0.160 61 (58) $\chi^2_2 = 3.1$	0.160 31 (71) $\chi^2_1 = 1.0$
0.20	0.161 10 (25) $\chi^2_6 = 9.8$	0.161 20 (28) $\chi^2_5 = 7.4$	0.161 19 (31) $\chi^2_4 = 7.4$	0.161 16 (41) $\chi^2_3 = 7.3$	0.160 70 (61) $\chi^2_2 = 3.1$	0.160 39 (74) $\chi^2_1 = 1.0$
0.19	0.161 28 (26) $\chi^2_6 = 9.9$	0.161 37 (29) $\chi^2_5 = 7.9$	0.161 35 (33) $\chi^2_4 = 7.8$	0.161 30 (43) $\chi^2_3 = 7.7$	0.160 81 (64) $\chi^2_2 = 3.2$	0.160 48 (78) $\chi^2_1 = 1.0$
0.18	0.161 47 (27) $\chi^2_6 = 10.1$	0.161 56 (30) $\chi^2_5 = 8.4$	0.161 53 (34) $\chi^2_4 = 8.2$	0.161 46 (45) $\chi^2_3 = 8.0$	0.160 93 (67) $\chi^2_2 = 3.2$	0.160 57 (82) $\chi^2_1 = 0.9$
0.17	0.161 69 (28) $\chi^2_6 = 10.3$	0.161 77 (32) $\chi^2_5 = 9.0$	0.161 73 (36) $\chi^2_4 = 8.7$	0.161 64 (48) $\chi^2_3 = 8.4$	0.161 06 (70) $\chi^2_2 = 3.3$	0.160 67 (86) $\chi^2_1 = 0.9$
0.10	0.164 40 (46) $\chi^2_6 = 15.0$	0.164 43 (52) $\chi^2_5 = 15.0$	0.164 25 (59) $\chi^2_4 = 13.3$	0.163 90 (79) $\chi^2_3 = 11.5$	0.162 71 (116) $\chi^2_2 = 3.7$	0.162 00 (142) $\chi^2_1 = 0.7$

Our value for  $A$  is in good agreement with the estimates in the bulk (see [29]). For  $B$  the only previous available estimate comes from an old work by Domb and Hiøe [37]. Their value ( $B = 0.472 \pm 0.002$ ) is slightly lower than our prediction; however, the discrepancy can be easily explained by the limited number of terms ( $N \leq 10$ ) of their series.

Let us mention that a direct fit to the data for  $\Delta$  gives the result

$$\Delta = 0.20 \pm 0.09 \quad (39)$$

where the error is two standard deviations. We thus have a check on the assumption that the first sub-leading correction to mean square-displacement is non-rotational invariant.

Let us discuss the error of the ratios  $\langle A \rangle / \langle B \rangle$ . It is straightforward to show that, if  $A$  and  $B$  are generic observables, the following relation holds:

$$\sigma^2\left(\frac{\bar{A}}{\bar{B}}\right) = \frac{\langle A \rangle^2}{\langle B \rangle^2} \left[ \frac{\sigma^2(\bar{A})}{\langle A \rangle^2} + \frac{\sigma^2(\bar{B})}{\langle B \rangle^2} - 2 \frac{\text{cov}(\bar{A}, \bar{B})}{\langle A \rangle \langle B \rangle} \right] \quad (40)$$

where  $\bar{A}$  and  $\bar{B}$  are the estimators of  $\langle A \rangle$  and  $\langle B \rangle$  defined as the mean values of the time series of  $A$  and  $B$  (see [29]).

The term in square brackets is simply given by the variance  $\sigma^2(F_{A,B})$  of the estimator of  $F_{A,B}$  where

$$F_{A,B} = \frac{A}{\langle A \rangle} - \frac{B}{\langle B \rangle} \quad (41)$$

can be treated as a generic observable of our model. Applying the Schwartz inequality  $|\text{cov}(\bar{A}, \bar{B})| \leq \sigma(\bar{A})\sigma(\bar{B})$  we get the upper bound

$$\sigma^2\left(\frac{\bar{A}}{\bar{B}}\right) \leq \frac{\langle A \rangle^2}{\langle B \rangle^2} \left[ \frac{\sigma(\bar{A})}{\langle A \rangle} + \frac{\sigma(\bar{B})}{\langle B \rangle} \right]^2. \quad (42)$$

When  $A$  is an 'odd' observable (like  $z^3$ ) and  $B$  is an 'even' one (like  $z^2$ ), they scale respectively as  $N^{2h\nu+\sigma}$  and  $N^{(2h+1)\nu}$  and we have

$$\sigma^2(\bar{A}) \approx N^{2(2h+1)\nu+p_A} \quad \langle A \rangle^2 \approx N^{2(2h\nu+\sigma)} \quad (43)$$

$$\sigma^2(\bar{B}) \approx \langle B \rangle^2 N^{p_B} \approx N^{2(2h\nu)+p_B} \quad (44)$$

where  $p$  is the dynamic critical exponent associated with the variable, so that  $\sigma^2(\bar{A})/\langle A \rangle^2 \gg \sigma^2(\bar{B})/\langle B \rangle^2$ ,  $|\text{cov}(\bar{A}, \bar{B})|/\langle A \rangle \langle B \rangle$  and

$$\sigma^2\left(\frac{\bar{A}}{\bar{B}}\right) \approx \frac{\langle A \rangle^2}{\langle B \rangle^2} \frac{\sigma^2(\bar{A})}{\langle A \rangle^2} \quad (45)$$

When instead  $A$  and  $B$  are both even,  $\sigma^2(F_{A,B})$  is not so simple to handle and there is no other choice than to measure it. Our data are reported in table 3. In this case the exact factor  $\sigma^2(F_{A,B})$  given in table 3 is about 8-9 times smaller than the estimate obtained by the Schwartz inequality, as suggested in [29]. The relation (45) for  $\sigma^2(z^3/z^2)$  is also well verified.

## 5. Random walk with an excluded needle

We found it also interesting to simulate the same model with an excluded needle for simple random walks. In this case the introduction of vacancies should appear as a marginal perturbation to the model without constraints and thus the behaviour of observables associated with the perturbation is noteworthy, as they can show a non-universal behaviour.

By a direct computation in the continuum limit, the authors of [1] find

$$\langle z \rangle_N \approx \frac{N^\nu}{\ln N} \times \left[ 1 + O\left(\frac{1}{\ln N}\right) \right] \quad (46)$$

$$\langle R_g^2 \rangle_N \approx N^{2\nu} \times \left[ 1 + O\left(\frac{1}{\ln N}\right) \right] \quad (47)$$

where, of course,  $\nu = \frac{1}{2}$ .

In table 8 we report the raw data from our runs.

Our data for  $z$  cannot, of course, exclude a power-law scaling (a least-squares fit produces an exponent close to that of  $\sigma$  obtained from SAW), but we can see an increase of the effective exponent with  $N_{\min}$  towards  $\frac{1}{2}$ . However, a fit of the form  $\langle z \rangle_N = KN^\nu/\ln N$  gives an estimate for the exponent  $\nu$  which changes monotonically with

**Table 8.** The results of our runs in  $d = 3$  for random walks with an infinite needle excluded. The error ranges are 95% confidence intervals (two standard deviations).

$N$	$\langle \mathcal{O} \rangle_N$	
	$\langle z \rangle_N$	$\langle R_g^2 \rangle_N$
50	$0.7097 \pm 0.0089$	$8.6693 \pm 0.0090$
100	$0.916 \pm 0.013$	$17.151 \pm 0.020$
250	$1.274 \pm 0.021$	$42.608 \pm 0.050$
500	$1.631 \pm 0.030$	$84.97 \pm 0.10$
1 000	$2.107 \pm 0.044$	$169.59 \pm 0.21$
2 000	$2.720 \pm 0.064$	$338.81 \pm 0.43$
4 000	$3.584 \pm 0.091$	$677.09 \pm 0.86$
8 000	$4.70 \pm 0.18$	$1353.2 \pm 2.4$
12 000	$5.41 \pm 0.22$	$2026.5 \pm 3.7$
16 000	$6.04 \pm 0.26$	$2702.2 \pm 4.9$

**Table 9.** Least-square estimator  $\nu$  as a function of the cut  $N_{\min}$ , derived from the data for  $z$  by a fit of the form  $z = KN^\nu / \ln N$ . The statistical error  $\Delta\nu$  is a 95% confidence interval.

$N_{\min}$	100	250	500	1000	2000	4000
$\nu$	0.523	0.513	0.510	0.506	0.502	0.489
	$\chi^2_7 = 22.4$	$\chi^2_6 = 4.3$	$\chi^2_5 = 2.5$	$\chi^2_4 = 1.7$	$\chi^2_3 = 1.5$	$\chi^2_2 = 0.3$
$\Delta\nu$	0.007	0.009	0.012	0.016	0.022	0.031

**Table 10.** Least-square estimator  $\nu$  as a function of the parameter  $H$  and of the cut  $N_{\min}$ , derived from the data for the radius of gyration by a fit of the form  $KN^{2\nu} (1 + H/\ln N)$ . The statistical error  $\Delta\nu$  is a 95% confidence interval. Values in bold face indicate the flatness region.

$H$	$N_{\min}$						
	100	250	500	1000	2000	4000	8000
0.00	0.498 56	0.498 95	0.499 14	0.499 25	0.499 23	0.499 11	0.498 83
	$\chi^2_7 = 55.9$	$\chi^2_6 = 8.6$	$\chi^2_5 = 1.9$	$\chi^2_4 = 0.8$	$\chi^2_3 = 0.7$	$\chi^2_2 = 0.6$	$\chi^2_1 = 0.4$
0.08	0.499 45	0.499 70	0.499 80	0.499 85	0.499 77	0.499 61	0.499 29
	$\chi^2_7 = 23.2$	$\chi^2_6 = 3.4$	$\chi^2_5 = 1.3$	$\chi^2_4 = 1.1$	$\chi^2_3 = 0.9$	$\chi^2_2 = 0.6$	$\chi^2_1 = 0.4$
0.11	<b>0.499 77</b>	<b>0.499 97</b>	<b>0.500 05</b>	<b>0.500 07</b>	<b>0.499 97</b>	<b>0.499 79</b>	<b>0.499 44</b>
	$\chi^2_7 = 15.1$	$\chi^2_6 = 2.5$	$\chi^2_5 = 1.4$	$\chi^2_4 = 1.4$	$\chi^2_3 = 1.0$	$\chi^2_2 = 0.6$	$\chi^2_1 = 0.4$
0.14	<b>0.500 09</b>	<b>0.500 24</b>	<b>0.500 29</b>	<b>0.500 29</b>	<b>0.500 17</b>	<b>0.499 97</b>	<b>0.499 60</b>
	$\chi^2_7 = 9.2$	$\chi^2_6 = 2.0$	$\chi^2_5 = 1.6$	$\chi^2_4 = 1.6$	$\chi^2_3 = 1.1$	$\chi^2_2 = 0.6$	$\chi^2_1 = 0.4$
0.17	<b>0.500 41</b>	<b>0.500 51</b>	<b>0.500 53</b>	<b>0.500 50</b>	<b>0.500 37</b>	<b>0.500 16</b>	<b>0.499 78</b>
	$\chi^2_7 = 5.3$	$\chi^2_6 = 2.0$	$\chi^2_5 = 2.0$	$\chi^2_4 = 1.9$	$\chi^2_3 = 1.2$	$\chi^2_2 = 0.6$	$\chi^2_1 = 0.4$
0.20	<b>0.500 73</b>	<b>0.500 78</b>	<b>0.500 77</b>	<b>0.500 72</b>	<b>0.500 57</b>	<b>0.500 34</b>	<b>0.499 96</b>
	$\chi^2_7 = 3.4$	$\chi^2_6 = 2.5$	$\chi^2_5 = 2.4$	$\chi^2_4 = 2.2$	$\chi^2_3 = 1.3$	$\chi^2_2 = 0.6$	$\chi^2_1 = 0.4$
0.23	0.501 04	0.501 05	0.501 01	0.500 93	0.500 76	0.500 52	0.500 09
	$\chi^2_7 = 3.4$	$\chi^2_6 = 3.4$	$\chi^2_5 = 3.1$	$\chi^2_4 = 2.5$	$\chi^2_3 = 1.4$	$\chi^2_2 = 0.6$	$\chi^2_1 = 0.4$
$\Delta\nu$	0.000 20	0.000 25	0.000 32	0.000 41	0.000 56	0.000 79	0.001 31

$N_{\min}$  decreasing strongly from 0.525 towards the expected value of  $\frac{1}{2}$  (see table 9), a clear signal of the presence of sizeable corrections to simple scaling.

To conclude, we analysed the radius of gyration. By using the expected logarithmic form of the corrections to scaling we can estimate

$$0.5003 \pm 0.0010 \pm 0.0002. \quad (48)$$

Results are collected in table 10. It appears that the results of [1] are also well confirmed for simple random walks.

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