

## Reply to comment "On self-avoiding walks in critical dimensions"

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COMMENT

## Reply to comment 'On self-avoiding walks in critical dimensions'

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**Abstract.** We show that the logical basis of using a different renormalization scheme is flawed compared to standard renormalization group predictions.

In the comment [1], Chirikov criticizes the use of standard renormalization group predictions [2, 3] in our analysis of high statistics simulations of four-dimensional self-avoiding walks (SAWs) [4]. Instead, he suggests a simple ansatz for logarithmic corrections obtained by Flory type arguments. More precisely, he predicts that the average end-to-end distance scales asymptotically as

$$R_N^2 \sim AN[\ln N]^{1/3} \quad (1)$$

in contrast to the field theoretic result

$$R_N^2 \sim AN[\ln N]^{1/4}. \quad (2)$$

It is true that our comparison with the standard theory was 'a tricky task', since equation (2) by itself is not sufficient and higher order corrections are essential. But we should stress that the next-to-leading terms are uniquely predicted by theory, and that the agreement is perfect when taking them into account as fully as possible. Of course there are ambiguities in very high order terms, but we have no reason to suspect that they are anomalously large.

Nevertheless, it is puzzling that *without these corrections* equation (1) provides a much better fit to our Monte Carlo data than equation (2), and extrapolations of the field theoretic results *including* all known corrections suggest that equation (1) will provide a very good fit up to  $N \approx 10^6$ .

Equation (1) is derived in [1] from the assumption that the correlation between two steps in a SAW is only a function of their distance along the chain, and independent of the total chain length:

$$\langle \mathbf{a}_{n_1} \cdot \mathbf{a}_{n_2} \rangle (\cdots)_N = c(n_2 - n_1) \quad (3)$$

where  $\mathbf{a}_n$  is the step from the  $n$ th monomer to the  $(n + 1)$ st. Furthermore, it is assumed that  $c(m)$  is a linear function of the average monomer density corresponding to a chain of  $m$  steps,

$$c(m) = b \frac{m}{R_m^d}. \quad (4)$$

Using the fact that the end-to-end distance of a walk with correlations described by equation (3) is given by  $d^2 R_N^2/dN^2 = 2c(N)$ , one derives from these assumptions for  $d < 4$  Flory's result  $R_N \sim N^\nu$  with  $\nu = 3/(2+d)$ , and for  $d = 4$  one obtains equation (1).

The main criticism of this derivation is that equation (3) is well known to be much too naive. The step-step correlation is actually a complicated function of all three arguments  $n_1, n_2$  and  $N$  [5]. Also, it is not immediately clear why  $c$  should be proportional to the monomer density.

Nevertheless, we can consider the above as a new derivation of Flory's result for  $d < 4$ , and as a very reasonable first step for estimating logarithmic corrections in  $d = 4$ . Since it is still very badly understood why Flory theory works so well, any new argument which could shed new light on it should be welcome.

This is particularly highlighted by extending the above argument to  $\theta$ -polymers. There we expect that  $c(m)$  should depend quadratically on the monomer density, since the  $\theta$  point is characterized by the absence of two-body forces. From

$$\frac{d^2 R_N^2}{dN^2} = 2c(N) = 2b \left[ \frac{N}{R_N^d} \right]^2 \quad (5)$$

we indeed obtain the Flory result  $\nu = 2/(1+d)$  for  $d < 3$ . We find the correct critical dimension  $d_c = 3$ , and there we obtain logarithmic corrections, using arguments analogous to those of [1],

$$R_N^2 \sim AN[\ln N]^{1/4}. \quad (6)$$

This is to be compared to the field theoretic prediction [6]

$$R_N^2 \sim AN \left[ 1 - \frac{37}{363 \ln N} + \dots \right] \quad (7)$$

which is *much* smaller for presently available values of  $N$  ( $\sim 10^2$ – $10^4$ ). But simulations [7] show that the deviations from  $R_N^2/N = \text{constant}$  are much larger—by at least one order of magnitude—than the field theoretic prediction. Indeed, equation (6) provides a reasonable fit to the data of [7], provided we take into account the uncertainty implied by the imprecise location of the  $\theta$  point.

Of course, we should expect that here also the agreement between simulations and field theory should improve if higher order corrections are included. But since their computation is highly non-trivial, even the next terms in equation (7) have not yet been calculated.

In summary, we can say that the arguments given in [1] cannot claim to be exact, and cannot invalidate the field theoretic predictions tested in [4]. But they provide very easy and not too wrong heuristic estimates which, in the case of  $\theta$ -polymers, are dramatically better than the best currently available predictions from field theory. This is so in spite of the fact that the latter has a sound theoretical foundation, while the logical basis of the assumptions involved in [1] is dubious and remains to be understood.

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