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A note on the corrections-to-scaling for the number of nearest neighbour contacts in self-avoiding walks

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Abstract. Recently, an exhaustive study has been made of the corrections-to-scaling for the number of, and various size measures (eg. radius of gyration) of, self-avoiding walks on the various two-dimensional lattices. This study gave compelling evidence that the first non-analytic correction-to-scaling has exponent $\Delta_1 = 3/2$. However, there also exist predictions in the literature for the corrections-to-scaling of the number of nearest neighbour contacts of self-avoiding walks. These are partially based on the analysis of relatively short series. Here we demonstrate that the form for the scaling of the number of self-avoiding walks recently proposed, and some standard scaling assumptions, implies that this older conjecture on the corrections-to-scaling for the number of nearest neighbour contacts is unlikely to hold. We consolidate this claim by the analysis of Monte Carlo data for both two and three dimensional self-avoiding walks. This work also shows that the often standard assumption that all quantities have the same corrections-to-scaling is misleading.

Recently, an exhaustive study [1] by Caracciolo, Guttmann, Jensen, Pelissetto, Rogers and Sokal of the corrections-to-scaling for various quantities of self-avoiding walks (SAW) on the square and triangular lattice has been made. In particular, they analysed the number of walks, the mean-square end-to-end distance, the mean-square radius of gyration and the mean-square distance of a monomer from its endpoints. Actually, the complete endpoint distribution was calculated. Series analysis of enumerations up to length 59 on the square and 40 steps on the triangular lattice were consider as well as Monte Carlo data up to length 8000. A careful theoretical discussion of field theoretic aspects of the problems led to refined scaling predictions for each of the measured quantities. The analyses gave compelling evidence that the first non-analytic correction-to-scaling has exponent $\Delta_1 = 3/2$.

In this paper I want to focus on their prediction for the number of self-avoiding walks. They conjectured that the number, c_n, of n-step SAW in two dimensions scales as

$$\begin{aligned} c_n \sim \; & \mu^n n^{11/32} \left[A_1 + \tfrac{A_2}{n} + \tfrac{B_1}{n^{3/2}} + \tfrac{A_3}{n^2} + \cdots\right] \\ & + (-\mu)^n n^{-3/2} \left[D_1 + \tfrac{D_2}{n} + \tfrac{D_3}{n^2} + \cdots\right] \end{aligned} \tag{1}$$

where they estimated the values of the constants A_j, B_j and D_j with accuracy of between 7 and 3 significant figures. Let us concentrate on the leading corrections, which are non-oscillatory, and rewrite this result in more general form

$$c_n \sim \mu^n n^{\gamma-1} \left[A_1 + \frac{A_2}{n} + \frac{B_1}{n^{\Delta_1}} + \cdots\right] \tag{2}$$

on the assumption that $0 < \Delta_1 < 2$.

Let us now consider the problem of *interacting* self-avoiding walks momentarily. These are self-avoiding walks with a Boltzmann weight $\omega = e^{\epsilon}$ associated with pairs of vertices along the walk which are nearest neighbours on the lattice but do not lie consecutively along the walk. The partition function $Z_n(\epsilon)$ is given by

$$Z_n(\epsilon) = \sum_{\phi \in \Omega_n} e^{m(\phi)\epsilon} \tag{3}$$

given that Ω_n is the set of self-avoiding walks of length n and $m(\phi)$ is the number of nearest neighbour interaction pairs as described above. The average number of nearest neighbour interaction pairs $m_n \equiv \langle m \rangle(n)$ is clearly

$$m_n = \frac{\sum_{\phi \in \Omega_n} m(\phi) e^{m(\phi)\epsilon}}{Z_n(\epsilon)} = \frac{d \log(Z_n(\epsilon))}{d\epsilon} \tag{4}$$

We note immediately that when $\epsilon = 0$ the partition function is simply equal to the number of self-avoiding walks: that is, $Z_n(0) = c_n$.

It is well known (though not proven rigorously) that for $\epsilon < \epsilon_\theta$, where $\epsilon_\theta > 0$, the universality class of *interacting* self-avoiding walks is unchanged and is therefore that of the non-interacting case of self-avoiding walks as studied in [1]. Let us begin by assuming that the scaling of the partition function follows that of c_n when $\epsilon < \epsilon_\theta$ except that the 'constants' μ, A_j and B_j now depend upon ϵ:

$$Z_n \sim e^{\kappa(\epsilon)n} n^{\gamma-1} \left[A_1(\epsilon) + \frac{A_2(\epsilon)}{n} + \frac{B_1(\epsilon)}{n^{\Delta_1}} + \cdots \right] \tag{5}$$

Making the mild assumption that the asymptotic expansion (5) can be differentiated we conclude that for $\epsilon < \epsilon_\theta$, including $\epsilon = 0$, that

$$m_n \sim E(\epsilon) n \left(1 + \frac{d_1(\epsilon)}{n} + \frac{d_2(\epsilon)}{n^2} + \frac{g_1(\epsilon)}{n^{\Delta_1+1}} + \cdots \right) \tag{6}$$

where $\Delta_1 + 1 = 5/2$ in two dimensions, and $E(\epsilon)$ is the internal energy. We note immediately that the first non-analytic correction-to-scaling for the thermodynamic observable internal energy is $5/2$ in two dimensions. This means such corrections are even smaller than for the raw observable of the partition function. We note here that the standard assumption (see the opening paragraph of [1]) that all global observables have the same corrections-to-scaling, excepting special symmetry considerations, can be misleading.

On the other hand, the introduction of interactions could give rise to other corrections-to-scaling which would be visible in the scaling of the partition function at values of ϵ other than zero. For example, it has been established that the exponent $11/16$ arises as a correction-to-scaling exponent for self-avoiding trails and walks on the Manhattan lattice (see [1] for a review), which are accepted to be in the self-avoiding walk universality class. In any case, the corrections-to-scaling exponent, $1 + \Delta_1$, for the number of contacts must be greater than one, and this is the crucial conclusion of this paper (here we consider Δ_1 simply as the smallest non-analytic corrections-to-scaling exponent for the partition function, whether it be $3/2$ or something else).

If there arises no other corrections-to-scaling from the interactions themselves, and if we use the estimated value of $\Delta_1 \approx 0.56(3)$ [2] for three dimensions, it follows for self-avoiding walks in three dimensions

$$m_n \sim En \left(1 + \frac{d_1}{n} + \frac{d_2}{n^2} + \frac{g_1}{n^{1.56}} + \cdots \right) \tag{7}$$

However, in the literature there exist other predictions for both the two and three dimensional results [3] by Douglas and Ishinabe. Their starting point was the result noted by Domb [4, 5, 6] that for pure random walks the number of self-intersections s_n scaled as

$$s_n \sim S_0 n + S_1 n^{\phi} + S_2 \tag{8}$$

where $\phi = (4-d)/2$ for d-dimensional random walks. This led Domb [4, 5, 6] to predict

$$m_n \sim En(1 + \frac{g_1}{n^\delta} + \frac{d_1}{n}) \tag{9}$$

where $\delta \approx 1/2$ in two dimensions and $\delta \approx 2/3$ in three dimensions. Douglas and Ishinabe tested this prediction using direct enumeration of self-avoiding walks and $1/d$ expansions. On the square and simple cubic lattice they utilised direct enumerations up to lengths 22 and 16 respectively. They estimated

$$\delta(d=2) = 0.75^{+0.05}_{-0.10} \qquad \text{and} \qquad \delta(d=3) = 0.85^{+0.05}_{-0.05} \tag{10}$$

Now it is clear that these are wildly inconsistent with the predictions from the arguments presented above based on the work of Caracciolo, Guttmann, Jensen, Pelissetto, Rogers and Sokal [1] which implies

$$\delta(d=2) = 2.5 \qquad \text{and} \qquad \delta(d=3) = 1.56(3) \tag{11}$$

Let us assume for a moment that the predictions of Domb or Douglas and Ishinabe were true with $0 < \delta < 1$ and so the scaling for m_n is given by equation (9) rather than equation (6). Now, let us consider the scaling form for Z_n that would be required to imply equation (9) with $0 < \delta < 1$ using the same simple differentiation argument we used in going from equation (5) to equation (6). One can see that the addition of a factor of a growing exponential $e^{hn^{1-\delta}}$, with $1-\delta > 0$, to the right-hand side of equation (5) would be sufficient to imply equation (9) and keep μ and γ unchanged in the scaling of the partition function. Now, it is clear from all previous series analysis work including [1] that this additional factor does not appear in the scaling form of the partition function. Hence it is very unlikely that the predictions of Domb or Douglas and Ishinabe are true.

So to check on this numerical discrepancy we have calculated Monte Carlo estimates of m_n for lengths up to 8192 for non-interacting self-avoiding walks on the square and simple cubic lattices. In two dimensions the longest length data did not prove useful for analysis, due to statistical uncertainties. Let us consider $u_n = m_n/n$. So we want to consider the scaling form

$$u_n \sim U_0 + \frac{U_1}{n^\delta} + \frac{U_2}{n} \tag{12}$$

as the statistical uncertainties in our data would not allow for an estimate of the next correction. If we fix $\delta = 0.75$ in two dimensions, or $\delta = 0.85$ in three dimensions, and estimate U_j it is clear that U_1 is much smaller than estimated by Douglas and Ishinabe. On the square lattice fitting to data from lengths 384 to 4096 we find the coefficient $U_1 \approx 0.002$ while Douglas and Ishinabe estimated 0.18. If on the other hand we try an iterative non-linear fit (one with some plausible starting values) and start δ at 0.75 (or 0.85 respectively for the cubic lattice) then δ moves slowly to 1. On the square lattice a fit from 384 to 4096 gives an effective δ of 0.94: this of course is just picking up the error in finding U_2 and the next correction-to-scaling which is presumably of order n^{-2}. Thirdly, if we consider $n(u_n - u_{2n})$ then this scales as

$$n(u_n - u_{2n}) \sim H_0 n^{1-\delta} + H_1 \tag{13}$$

given (12) holds. When this quantity is plotted there is no evidence in either two or three dimensions that this quantities diverges (as it would if $\delta < 1$). In two dimensions it is essentially constant within error while in three dimensions (see Figure 1) one can see that a plot against $1/n^{1/2}$ is roughly straight (as one would expect if δ was about 1.56). All three analyses then indicate that there is no evidence for a correction to scaling exponent δ less than 1. It would be interesting to do careful series analysis on extended enumerations for m_n to find the actual correction-to-scaling exponent and to analyse the partition function of interacting self-avoiding walks so as to test the relationship suggestion above.

We conclude that the scaling conjectures presented in [1] and some scaling arguments together can be used to conjecture the scaling form for the number of nearest neighbour contacts in self-avoiding

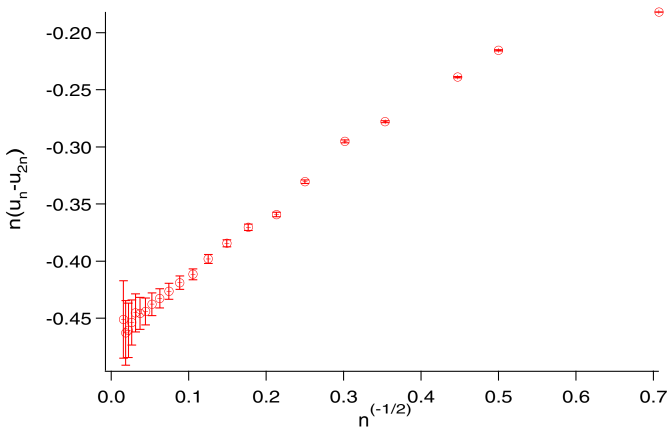

Figure 1. A plot of $n(u_n - u_{2n})$ with error bars as indicated against $1/\sqrt{n}$ showing a fairly straight line and the convergence to a finite value of this quantity in three dimensions.

walks. Furthermore, these contradict earlier predictions [4, 5, 6, 3] of the scaling forms which are almost certainly incorrect. This conclusion has been verified by the analysis of Monte Carlo data. We reiterate that the standard assumption (see the opening paragraph of [1]) that all global observables have the same corrections-to-scaling, excepting special symmetry considerations, can be misleading — rather they may also differ by one.

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