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High resolution Monte Carlo study of the Domb-Joyce model

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Abstract. We study the Domb-Joyce model of weakly self-avoiding walks on the simple cubic lattice via Monte Carlo simulations. We determine to excellent accuracy the value for the interaction parameter which results in an improved model for which the leading correction-to-scaling term has zero amplitude.

1. Introduction

The Domb-Joyce model of weakly self-avoiding walks has a long history [1]. It consists of the set of random walks on the simple cubic lattice \mathbb{Z}^3 , with walks starting at the origin and taking steps to adjacent neighbors, where there is a contact interaction which introduces an energy penalty of w for each pair of visits to the same lattice site. A walk of N steps may be defined as a mapping ω from the integers $0, 1, \dots, N$ to sites on \mathbb{Z}^3 , with $|\omega(i+1) - \omega(i)| = 1 \forall i \in [0, N-1]$, and $\omega(i) \neq \omega(j) \forall i \neq j$, and the energy due to overlaps of a walk ω is then given by

$$E(\omega) = w \sum_{i < j} \delta_{\omega(i), \omega(j)}. \quad (1)$$

Note that if a walk visits a particular site exactly k times, then the associated weight for that site will be equivalent to $\binom{k}{2}$ pairwise interactions. We then define the partition function as

$$Z_N = \sum_{|\omega|=N} e^{-E(\omega)}, \quad (2)$$

and the expectation of an observable A is computed over the set of all simple random walks of length N as follows:

$$\langle A \rangle_N = \frac{1}{Z_N} \sum_{|\omega|=N} A(\omega) e^{-E(\omega)}. \quad (3)$$

The Domb-Joyce model interpolates between simple random walks when $w = 0$, and self-avoiding walks when $w = +\infty$.

Here we perform Monte Carlo simulations of Domb-Joyce walks via the pivot algorithm [2, 3] using a recent implementation [4, 5] (which improved on earlier work by Kennedy [6]).



We calculated the expected value of the two most common measures of size, the squared end-to-end distance, R_E^2 , and the squared radius of gyration, R_G^2 , which are defined as:

$$R_E^2 = |\omega(N) - \omega(0)|^2; \quad (4)$$

$$R_G^2 = \frac{1}{2(N+1)^2} \sum_{i,j} |\omega(i) - \omega(j)|^2. \quad (5)$$

For any positive w the Domb-Joyce model is in the same universality class as self-avoiding walks, and the asymptotic behavior of these observables for large N is given by

$$\langle R_E^2 \rangle = D_E(w) N^{2\nu} \left(1 + \frac{a_E(w)}{N^{\Delta_1}} + \dots \right), \quad (6)$$

$$\langle R_G^2 \rangle = D_G(w) N^{2\nu} \left(1 + \frac{a_G(w)}{N^{\Delta_1}} + \dots \right). \quad (7)$$

The critical exponent ν , known as the Flory exponent, is a universal quantity with value $\nu = 0.58759700(40)$ [7]. The leading correction-to-scaling exponent Δ_1 is also universal, and the best estimate for it is $\Delta_1 = 0.528(8)$. The amplitudes $D_E(w)$, $D_G(w)$, $a_E(w)$, and $a_G(w)$ are non-universal quantities which depend on the details of the model, including the value of the weight w and the lattice type. But, crucially for the present study, the amplitude ratios $D_E(w)/D_G(w) = 6.253531(10)$ [7] and $a_E(w)/a_G(w)$ are universal quantities which are independent of w .

A key reason for the continuing interest in the Domb-Joyce model is the observation that the addition of the interaction parameter w allows for the possibility of tuning it to a value such that the leading correction-to-scaling terms have negligible amplitude. As $a_E(w)/a_G(w)$ is universal, if there is a value $w = w^*$ such that $a_E(w^*) = 0$, then $a_G(w^*) = 0$ also. Thus, if w^* can be found to good accuracy it will ensure that the leading correction-to-scaling term for each observable will have small amplitude, thus enhancing convergence in the large- N limit. The Domb-Joyce model with $w = w^*$ is called an ‘‘improved’’ model due to this feature.

Previously, Belohorec [8] estimated that $w^* = 0.506$ for the Domb-Joyce model, and Caracciolo et al. [9] found that $w^* = 0.48(2)$ when studying virial coefficients for the self-avoiding walk universality class. More recently, Adamo and Pelissetto [10] made a detailed study of the Domb-Joyce model in the presence of hard spheres, and obtained an estimate of $w^* = 0.486 \pm 0.003 \pm 0.005$, where the first error is statistical, and the second comes from varying parameters which were used to bias their fits.

Here we seek to build on earlier work and obtain an accurate estimate of w^* to facilitate future Monte Carlo studies of properties of the self-avoiding walk universality class.

2. Monte Carlo simulation

We sampled self-avoiding walks on \mathbb{Z}^3 over a range of lengths from one thousand to ten million steps, for weights $e^{-w} = 0.50, 0.54, 0.57, 0.59, 0.60, 0.61, 0.63, 0.66$, and 0.70 ($w = 0.6931, 0.6162, 0.5621, 0.5276, 0.5108, 0.4943, 0.4620, 0.4155$, and 0.3567 respectively). We used a variant of the SAW-tree implementation of the pivot algorithm as described in [4] to collect data for the observables $\langle R_E^2 \rangle$ and $\langle R_G^2 \rangle$.

The SAW-tree implementation was adapted to count the number of intersections created when a pivot move is performed, whereas for self-avoiding walks one only needs to know if an intersection occurs. To initialize the system we used a variant of the `pseudo_dimerize` procedure, and to eliminate any initialization bias we then performed approximately $20N$ successful pivots before collecting any data.

We sampled pivot sites uniformly at random along the chain, and with the pivot symmetry operations sampled uniformly at random from amongst the 47 lattice symmetries of \mathbb{Z}^3 that do not correspond to the identity.

After initialization, we started collecting data for our observables for each time step, and aggregated the results in batches of 10^8 .

The computer experiment was run for 130 thousand CPU hours on Dell PowerEdge FC630 machines with Intel Xeon E5-2680 CPUs. (Run in hyperthreaded mode, so in fact 260 thousand thread hours were used.) In total there were 5.7×10^5 batches of 10^8 attempted pivots, and thus there were a grand total of 5.7×10^{13} attempted pivots across all walk sizes and values of the parameter w .

Our data for $\langle R_E^2 \rangle$, $\langle R_G^2 \rangle$, and $\langle R_E^2 \rangle / \langle R_G^2 \rangle$ for different values of w are collected in Tables A1–A9 of [11].

3. Analysis

Finding a good method to analyze our data and obtain an accurate estimate for w^* is a difficult problem. The heart of the difficulty is that we have conflicting goals that need to be accommodated, namely we wish to reduce the influence of unfitted corrections to scaling and thus go to the large- N limit, and we wish to study the Domb-Joyce model in the vicinity of $w \approx w^*$, but at the same time we want a large signal for the leading-correction-to-scaling term, which necessitates collecting data for intermediate values of N , and for values of w which are quite far from w^* .

The most robust and accurate method we could devise involves the use of information about the value of $D_E/D_G = 6.253531(10)$ from simulations of SAWs in the large- N limit [7]. For fixed N , we found the value of $w(N)$ such that $\langle R_E^2 \rangle_N / \langle R_G^2 \rangle_N = D_E/D_G$ via a quartic fit. These fits are perfect, in the sense that the reduced χ^2 value for the fits are approximately one indicating that the model accurately describes the data, and so we are confident that the resulting estimates for $w(N)$ are reliable. We found that the error bars for $w(N)$ became too large to be useful for $N \geq 10^6$. One can see the reason for this in Fig. 1: as N increases, $N^{-\Delta_1}$ decreases, the amplitude of deviations from the limiting value of D_E/D_G become smaller, and so errors on the estimates for $w(N)$ increase.

To gain an understanding of the convergence behavior of our estimates $w(N)$ we examine the equation we are solving when the next correction-to-scaling term with exponent -1 is included. The expected asymptotic form for the ratio $\langle R_E^2 \rangle_N / \langle R_G^2 \rangle_N$ is

$$\frac{\langle R_E^2 \rangle_N}{\langle R_G^2 \rangle_N} = \frac{D_E}{D_G} \left(1 + \frac{f(w)}{N^{\Delta_1}} + \frac{g(w)}{N} + \dots \right). \quad (8)$$

By solving $\langle R_E^2 \rangle_N / \langle R_G^2 \rangle_N = D_E/D_G$ at finite N , we find the value of w which forces the correction-to-scaling terms to be zero in aggregate, i.e. we are solving

$$\frac{f(w)}{N^{\Delta_1}} + \frac{g(w)}{N} = 0, \quad (9)$$

neglecting higher order corrections. Now, N is large, and we expect the solution for w to be close to w^* , and so we take $w = w^* + \Delta w$, and drop subleading terms:

$$f(w^* + \Delta w) = -g(w^* + \Delta w)N^{\Delta_1-1}, \quad (10)$$

$$f(w^*) + \Delta w f'(w^*) = -g(w^*)N^{\Delta_1-1}, \quad (11)$$

$$\Delta w = -\frac{g(w^*)}{f'(w^*)}N^{\Delta_1-1}. \quad (12)$$

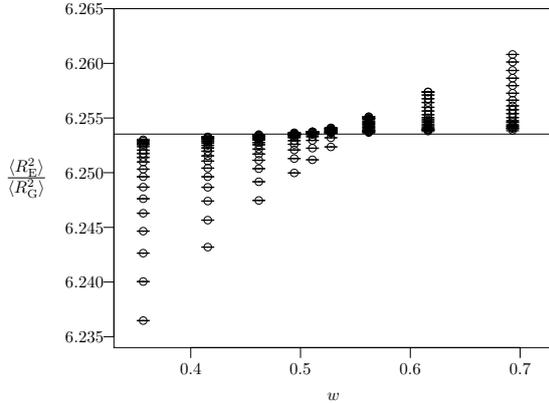


Figure 1. $\langle R_E^2 \rangle / \langle R_G^2 \rangle$ as a function of w for $1000 \leq N \leq 10^7$. The smaller values of N have larger corrections to scaling, and so deviate to a greater extent from the limiting value. We show a horizontal line for the best estimate of $D_E/D_G = 6.253531$.

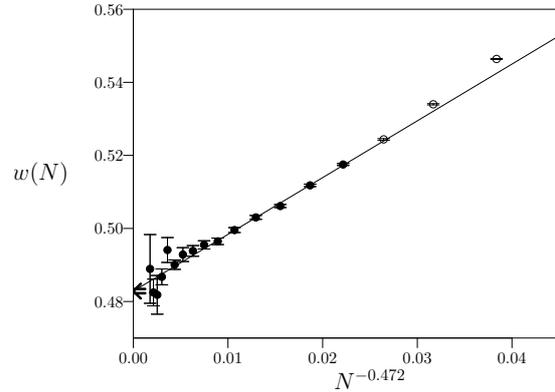


Figure 2. Estimates for $w(N)$ for $1000 \leq N \leq 680000$ plotted against N^{Δ_1-1} with $\Delta_1 = 0.528$. The estimate for $w^* = 0.48284(58)$, which is obtained by performing a linear fit of the solid data points, is shown on the vertical axis.

Thus we expect the deviation of our estimates $w(N)$ from the limiting value w^* to be $\Delta w = O(N^{\Delta_1-1})$. One quite significant issue with this assumption is that there are competing next-to-leading correction terms, namely the analytic $O(N^{-1})$ correction term, the $O(N^{-2\Delta_1})$ correction term, and a further non-analytic correction term $O(N^{-\Delta_2})$ for which it is believed that $\Delta_2 \approx 1$. We will assume for now that the deviation is well described by $\Delta w = O(N^{\Delta_1-1})$, but will touch on this point again later in Sec. 4.

Now that we have $w(N)$, we plot the estimates against N^{Δ_1-1} with $\Delta_1 = 0.528$ in Fig. 2. We performed linear fits of these data, finding that the fit is excellent for N in the range $3200 \leq N \leq 680000$, with reduced χ^2 approximately one. The resulting estimate of $w^* = 0.48284(58)$ is shown in the plot on the vertical axis. Note that the estimates here for $w(N)$ are independent of each other, and hence it makes sense to perform fits and then derive a statistical error estimate for w^* , in contrast to, say, estimates of Δ_1 in Fig. 10 of [7] which form a correlated sequence for which a linear fit no longer gives a meaningful statistical error.

Our estimate for w^* is biased via the choice of values for D_E/D_G and Δ_1 . Although we have only shown estimates in Fig. 2 which are biased with the central values of estimates for D_E/D_G and Δ_1 , we have varied these values within their confidence intervals. We find that varying $D_E/D_G = 6.253531(10)$ within the confidence interval ± 0.000010 causes a variation in the estimate of w^* of ± 0.0011 . Varying $\Delta_1 = 0.528(8)$ within the confidence interval ± 0.008 causes a variation in the estimate of w^* of ± 0.00034 . Thus the largest source of error comes from our earlier estimate of D_E/D_G .

We combine the statistical error of 0.00058 with the errors due to biasing as if they were statistically independent sources of error, giving $\sigma(w^*) = \sqrt{0.00058^2 + 0.0011^2 + 0.00034^2} = 0.0013$. Thus our final estimate, incorporating all known sources of error, is $w^* = 0.4828(13)$.

Finally, we note that for the analysis we essentially have to take 2 limits, $N \rightarrow \infty$, and $w \rightarrow w^*$. The previously described method involves first solving for $w(N)$ (taking the limit $w \rightarrow w^*$ at finite N), and then taking the limit $w^* = \lim_{N \rightarrow \infty} w(N)$. We also tried taking the limit in the reverse order as follows. We fitted data for $\langle R_E^2 \rangle$ and $\langle R_G^2 \rangle$ with biased values for ν and Δ_1 , obtaining sequences of estimates for $a_E(w)$ and $a_G(w)$ which were their limiting (large N) values. We then solved the equations $a_E(w^*) = 0$ and $a_G(w^*) = 0$ for w^* . Unfortunately, we found that this process gave significantly larger error bars, and so we will not report the details.

4. Discussion and conclusion

We hope that an ingenious method of analysis may yet be found which can extract more information from the data given in Tables A1–A9 of [11]. We note that a more accurate value for D_E/D_G would result in a correspondingly more accurate estimate for w^* ; it may be the case that such an improved estimate comes from a simulation of the Domb-Joyce model with the value for w^* reported in this paper!

As mentioned in the previous section, the error bar for our estimate of w^* relies on the fact that the next-to-leading correction term is well approximated by a single $O(N^{-1})$ term, despite the fact that there may be competing terms. The observation that the data in Fig. 2 is well described by a straight line gives us some confirmation that this is true, but nonetheless we are mindful that the competing terms may result in a subtle error that could be larger than our reported confidence interval for w^* . The only way we can think of to mitigate this possible source of error is to obtain better data for larger N , which would allow for easier extrapolation. But, this is a hard problem: statistical errors are relatively larger for large N , so it is unclear how much the situation would be improved by doing this.

The use of the improved version of the Domb-Joyce model is undoubtedly an attractive choice for many problems in polymer physics as it allows for faster convergence. We note that there is another alternative to improve convergence for particular observables by reducing the amplitude of the leading correction-to-scaling term. This has been done for the Ising model [12, 13], and more recently for self-avoiding walks [7, 14]. The manner in which the amplitude of the leading correction-to-scaling term is reduced is independent between the two methods, and so in fact it is possible to use both methods simultaneously and compound the effect. Thus, a study of the Domb-Joyce model at $w = w^*$ for the improved observable $R_{\text{imp}}^2 = R_E^2 - 4.478R_G^2$ [7] would be expected to have a completely negligible leading correction-to-scaling term.

Finally, we give our best estimate for the value of w which gives an improved model as $w^* = 0.4828(13)$; we hope that it proves useful in future studies of the venerable Domb-Joyce model.

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