# Low-temperature 2D polymer partition function scaling: series analysis results



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LETTER TO THE EDITOR

# Low-temperature 2D polymer partition function scaling: series analysis results

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**Abstract.** By utilizing newly extended series for self-avoiding walks and polygons with nearest-neighbour interactions on the square lattice we have examined the validity of a recent conjecture on the scaling of their partition functions at low temperatures. The ratio of the walk to polygon partition functions should have a length-dependent power law singularity, $n^{\gamma^D}$, at all temperatures. At low temperatures we find $\gamma^D$ is $0.92 \pm 0.09$ in distinction to the conjectured value of $19/16 = 1.1875$, though we find agreement at high temperatures and at the $\theta$-temperatures with the conjectured values there.

The collapse transition of a dilute polymer solution is a subset of perennial interest [1–3]. Much work has been accomplished on lattice models such as interacting self-avoiding walks to elucidate this phenomenon. The lattice models possess a critical point as a function of temperature which is identified as the $\theta$-point for polymers. This point can be viewed as a type of tricritical point in the appropriate thermodynamic space. The critical phenomena analogy arises from the 'formal' mapping [4–6] of polymer configurations to those of the magnetic $O(n)$ model in the $n \to 0$ limit. The study of a single polymer has focused on two cases. The high temperature or good solvent regime has been studied extensively, as has been the region around the $\theta$-point. Much less has been attempted at low temperatures (that is, in a poor solvent) with some work at zero temperatures [7]. In the above works the polymer density is zero. The subject of dense polymer networks has also been active [8–11]. In a system of finite polymer density, at low temperatures, the solution phase-separates into a dense phase and a dilute one. Recently, this dilute low temperature phase, modelled by a single self-avoiding walk with strong effective monomer–monomer attraction, has become the subject of several conjectures.

At high temperatures and at the $\theta$-point the partition function for a walk is believed to scale as

$$Z_n \sim Z \mu^n n^{\gamma - 1} \tag{1}$$

where $\gamma$ is some universal exponent that takes on one value at high temperatures and another at the $\theta$-temperature. Here, $\mu$ is related to the temperature dependent bulk

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free energy. ($Z$ is also temperature dependent.) At these temperatures the walk has zero average internal density with the radius of gyration and end-to-end distance scaling as

$$\langle R_n \rangle \sim R n^{\nu} \tag{2}$$

with $\nu > 1/d$, where $d$ is the dimension of the system.

At temperatures below the $\theta$-point a single walk is, on average, in a collapsed state with a finite internal monomer density. The radius of gyration and end-to-end distance scale with the exponent $\nu = 1/d$. Taking account of this observation, it has been conjectured [12, 13] that at low temperatures the above scaling (1) for the partition function should be replaced by

$$Z_n \sim Z \mu_0^n \mu_1^{n^\sigma} n^{\gamma - 1} \tag{3}$$

where $\sigma$ is most likely to have the value $(d-1)/d$ and so $\mu_1$ is related to a temperature dependent surface free energy. Again, $Z$ is temperature dependent. The rationale for such a conjecture arises from the posited generic singularity structure of first order transitions [14]. This conjecture was supported by work on interacting *partially-directed* self-avoiding walks, first numerically [15], and then by exact calculation [16] in two dimensions.

This work was extended by Duplantier [17] who pointed out that because the walk is internally dense at low temperatures it may be possible to adapt work on dense polymer networks where the partition function scaling form above has occurred in a different context. He further suggested that previous work on Hamiltonian walks on the Manhattan lattice [9, 10] was applicable and conjectured values for the $\gamma$ exponent for open and closed polymers in two dimensions. We note that the connection between Hamiltonian walks and the $T=0$ limit of the collapse problem has been suggested previously [18]. However, it is not clear, firstly, whether the dense analogy is truly applicable because of (unseen) subtleties with the surface configurations and, secondly, whether the Manhattan lattice imposes a relevant constraint that changes these values [19]. To attempt to answer these questions we have utilized newly extended series for interacting self-avoiding walks and polygons on the square lattice.

The series for interacting self-avoiding walks has been extended using direct enumeration on an Intel Paragon supercomputer [20] up to length $n=29$. The values of the walk partition function $Z_n^w(\omega)$ can be found for any $\omega$ as

$$Z_n^w(\omega) = \sum_m c_n(m) \omega^m \tag{4}$$

where $\omega$ is the Boltzmann weight associated with each interaction, related to the temperature and coupling constant $J$ as $\omega = \exp(\beta J)$, and $c_n(m)$ is the number of configurations of length $n$ with $m$ interactions. The series for interacting self-avoiding polygons has also been extended up to $n=42$ by using the finite lattice method [21]. The partition function is similarly defined as

$$Z_n^l(\omega) = \sum_m p_n(m) \omega^m \tag{5}$$

with $p_n(m)$ being the number of rooted polygons (loops) of length $n$ with $m$ interactions.

The scaling form (3) contains four unknown parameters, even assuming that $\sigma = 1/2$, and it would be very difficult to extract a reasonable value of $\gamma$ without knowing $\mu_0(\omega)$ and $\mu_1(\omega)$. To ameliorate this problem we have concentrated our study to the ratio of walk $Z_n^w$ to polygon $Z_n^l$ partition functions, which we denote as $Q_n(\omega)$. This

**Table 1.** Partition functions at high temperature ($\omega = 1.000$).

| $n$ | $Z_n^w$ | $Z_n^l$ | $Q_n$ |
|---|---|---|---|
| 4 | 2.50000000e+01 | 4.00000000e+00 | 6.25000000 |
| 6 | 1.95000000e+02 | 1.20000000e+01 | 16.25000000 |
| 8 | 1.47900000e+03 | 5.60000000e+01 | 26.41071429 |
| 10 | 1.10250000e+04 | 2.80000000e+02 | 39.37500000 |
| 12 | 8.12330000e+04 | 1.48800000e+03 | 54.59206989 |
| 14 | 5.93611000e+05 | 8.23200000e+03 | 72.11017979 |
| 16 | 4.31133300e+06 | 4.70080000e+04 | 91.71487832 |
| 18 | 3.11646830e+07 | 2.74824000e+05 | 113.39869520 |
| 20 | 2.24424291e+08 | 1.63652000e+06 | 137.13507380 |
| 22 | 1.61114012e+09 | 9.89058400e+06 | 162.89635890 |
| 24 | 1.15365993e+10 | 6.05104800e+07 | 190.65456640 |
| 26 | 8.24281966e+10 | 3.74019776e+08 | 220.38459420 |
| 28 | 5.87844646e+11 | 2.33213187e+09 | 252.06320990 |
| 30 | 4.18548949(1)e+12 | 1.46515358e+10 | 285.66899280(1) |
| 32 | 2.9758749(8)e+13 | 9.26538451e+10 | 321.182023(8) |
| 34 | 2.11319768(1)e+14 | 5.89317729e+11 | 358.58376070(1) |
| 36 | 1.4989351(4)e+15 | 3.76752338e+12 | 397.85688(1) |
| 38 | 1.0621688(5)e+16 | 2.41960061e+13 | 438.98515(2) |
| 40 | 7.5199558(6)e+16 | 1.56030800e+14 | 481.95329(4) |
| 42 | 5.3196749(7)e+17 | 1.00991100e+15 | 526.74690(7) |

function should have the scaling form

$$Z_n^w/Z_n^l \equiv Q_n(\omega) \sim Q n^{\gamma^D} \tag{6}$$

where

$$\gamma^D = \gamma_{\text{walks}} - \gamma_{\text{loops}}. \tag{7}$$

Note that at high and $\theta$- temperatures the $\gamma$-like exponent for loops is usually denoted as $\alpha - 1$. This form should be valid at all temperatures with $\gamma^D$ assuming different values at high, $\theta$- and low temperatures. The conjecture of Duplantier [17] determined from dense walks on the Manhattan lattice is that

$$\gamma^D = 19/16 = 1.1875 \tag{8}$$

for low temperatures (that is, large $\omega$).

Because of the differing lengths of the interacting walk and polygon series (29 steps and 42 steps respectively), we have used the method of differential approximants to extend the walk series at the required temperatures. In this technique, a number—typically 12—of inhomogeneous differential approximants are constructed that utilize all the available terms (29). Such approximants implicitly provide estimates of all future terms. We have explicitly evaluated the next 13 terms, taking as our estimates the mean of the values given by the differential approximants, and taking as the error the standard deviation. The results are given in tables 1–3, where it can be clearly seen that the error increases with $\omega$, and also, of course with the order of the estimated term. For $\omega = 1$, the first unknown term can be estimated with an error better than 1 part in $10^9$, while for $\omega = 3$, the 13th unknown term can only be estimated with an error of 1 part in $10^4$. Nevertheless, even this worst case is sufficient for our subsequent analysis. This method

**Table 2.** Partition functions at estimated $\theta$-temperature ($\omega = 1.931$).

| $n$ | $Z_n^w$ | $Z_n^l$ | $Q_n$ |
|---|---|---|---|
| 4 | 3.24480000e+01 | 4.00000000e+00 | 8.11200000 |
| 6 | 3.41904352e+02 | 2.31720000e+01 | 14.75506439 |
| 8 | 3.63072388e+03 | 1.86980528e+02 | 19.41765767 |
| 10 | 3.83575893e+04 | 1.47052275e+03 | 26.08432227 |
| 12 | 4.02490162e+05 | 1.21589867e+04 | 33.10227845 |
| 14 | 4.21534104e+06 | 1.05680646e+05 | 39.88754059 |
| 16 | 4.40962830e+07 | 9.38597465e+05 | 46.98103779 |
| 18 | 4.60529811e+08 | 8.44895530e+06 | 54.50730830 |
| 20 | 4.80407121e+09 | 7.71556406e+07 | 62.26467919 |
| 22 | 5.00724526e+10 | 7.13294615e+08 | 70.19883730 |
| 24 | 5.21524402e+11 | 6.65768863e+09 | 78.33415331 |
| 26 | 5.42842404e+12 | 6.26306464e+10 | 86.67360699 |
| 28 | 5.64721081e+13 | 5.93226873e+11 | 95.19479080 |
| 30 | 5.872026(4)e+14 | 5.65234291e+12 | 103.88658(8) |
| 32 | 6.10326(2)e+15 | 5.41333920e+13 | 112.7448(3) |
| 34 | 6.34126(4)e+16 | 5.20783699e+14 | 121.7637(7) |
| 36 | 6.58634(7)e+17 | 5.03015913e+15 | 130.937(1) |
| 38 | 6.8389(1)e+18 | 4.87586020e+16 | 140.261(3) |
| 40 | 7.0994(2)e+19 | 4.74141858e+17 | 149.731(5) |
| 42 | 7.3677(3)e+20 | 4.62400596e+18 | 159.337(6) |

**Table 3.** Partition functions at low temperature ($\omega = 3.000$).

| $n$ | $Z_n^w$ | $Z_n^l$ | $Q_n$ |
|---|---|---|---|
| 4 | 4.10000000e+01 | 4.00000000e+00 | 10.25000000 |
| 6 | 5.79000000e+02 | 3.60000000e+01 | 16.08333333 |
| 8 | 8.87100000e+03 | 4.40000000e+02 | 20.16136364 |
| 10 | 1.38665000e+05 | 5.12000000e+03 | 27.08300781 |
| 12 | 2.17828100e+06 | 6.63840000e+04 | 32.81334358 |
| 14 | 3.50760430e+07 | 9.32400000e+05 | 37.61909374 |
| 16 | 5.73158285e+08 | 1.33023040e+07 | 43.08714378 |
| 18 | 9.44831607e+09 | 1.94372280e+08 | 48.60938024 |
| 20 | 1.57375376e+11 | 2.92281812e+09 | 53.84371149 |
| 22 | 2.64701687e+12 | 4.49030413e+10 | 58.94961226 |
| 24 | 4.48810534e+13 | 7.00275379e+11 | 64.09057745 |
| 26 | 7.66350539e+14 | 1.10665766e+13 | 69.24910627 |
| 28 | 1.31684515e+16 | 1.77135867e+14 | 74.34096604 |
| 30 | 2.27581(5)e+17 | 2.86704279e+15 | 79.378(2) |
| 32 | 3.9539(3)e+18 | 4.68568795e+16 | 84.383(6) |
| 34 | 6.903(1)e+19 | 7.72373830e+17 | 89.37(2) |
| 36 | 1.2109(5)e+21 | 1.28297713e+19 | 94.39(4) |
| 38 | 2.132(1)e+22 | 2.14625630e+20 | 99.34(6) |
| 40 | 3.766(3)e+23 | 3.61388474e+21 | 104.20(9) |
| 42 | 6.682(8)e+24 | 6.12166211e+22 | 109.2(1) |

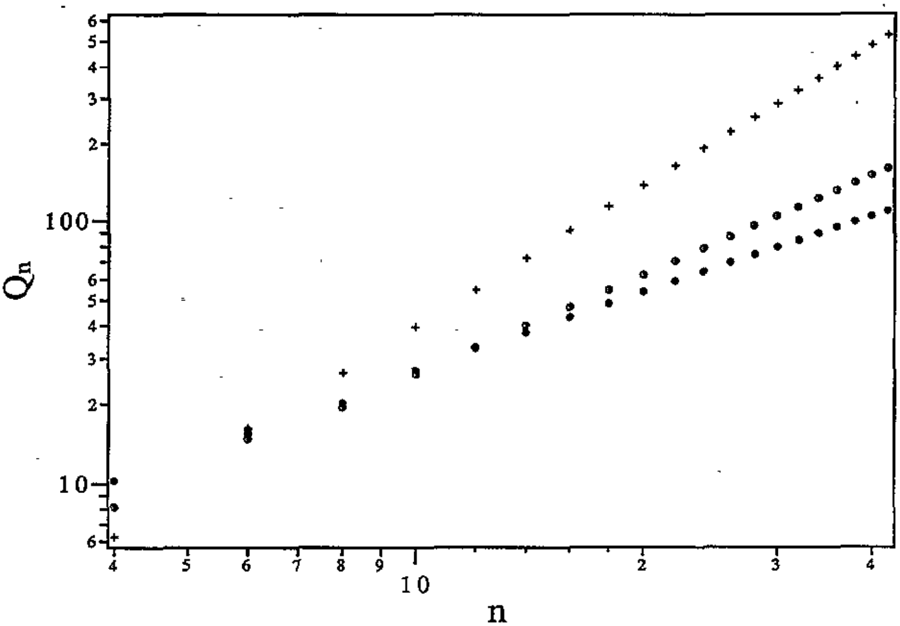


**Figure 1.** This graph is a log–log plot of the ratio of partition functions $Q_n(\omega)$ against length $n$ for three temperatures. The Boltzmann weights chosen $w=1.0$, 1.913, 3.0 represent high (infinite), critical and low temperatures respectively. The crosses are high temperature values, the open circles are $\theta$-temperature values and the full circles are the low temperature values.

of coefficient prediction was justified to some extent in previous work [22] in which a coefficient predicted to 10 digit accuracy was found to be correct to all claimed digits.

We have evaluated the partition functions at three specific temperatures: one high, one low and one at an estimated $\theta$-temperature. The estimated values of the exponent $\gamma^D$ at high and $\theta$-temperatures can be compared with well regarded (but non-rigorous) theoretical exact values to help establish the accuracy of our method. The high temperature was simply chosen as $\omega=1.0$ (that is, infinite temperature) to minimize unwanted thermal corrections and the estimated exponent extracted ($1.847\pm0.032$) compared well with the exact value of $59/32=1.843\,75$. The $\theta$-temperature was taken from a recent estimate [23] as $\omega_\theta=\exp(0.658\pm0.004)=1.931\pm0.008$ and the estimated exponent ($1.298\pm0.028$) also compared well with the exact value of $9/7\approx1.2857$. We note in passing that the uncertainty in the critical point naturally increases the error in the estimation of the value of $\gamma^D$ at this point, as there is a drift of the estimated exponent value with the assumed critical temperature. This can be utilized for an estimation of the $\theta$-temperature assuming that the conjectured value of $\gamma^D=9/7$ is correct and yields the estimate $\omega_\theta=\exp(0.663\pm0.016)=1.94\pm0.03$.

The choice of a suitable low temperature was difficult as one had to balance the concerns of being far enough away from the $\theta$-point to avoid crossover effects while not being at too low a temperature where parity effects (due to certain polygon sizes permitting significantly more interactions) make it impossible to extrapolate series meaningfully. By examining the partition function ratio over a range of temperatures we decided upon $\omega=3.0$ as a value where exponent estimates could be usefully extrapolated while crossover curvature in the estimates seemed to be small. Given these considerations, our result at this low temperature for $\gamma^D$, $0.921\pm0.088$, excludes the

**Table 4.** $\gamma^D$ extrapolations and conjectured values in all three regimes.

| | $\omega = 1.000$ | $\omega = 1.931$ | $\omega = 3.000$ |
|---|---|---|---|
| $n$ | $\gamma_n^D$ local slopes | | |
| 5 | 2.35658118 | 1.47544613 | 1.11108410 |
| 7 | 1.68824168 | 0.95451366 | 0.78553572 |
| 9 | 1.78970588 | 1.32269838 | 1.32263930 |
| 11 | 1.79220461 | 1.30685403 | 1.05269360 |
| 13 | 1.80541916 | 1.20960799 | 0.88664211 |
| 15 | 1.80099516 | 1.22577962 | 1.01633727 |
| 17 | 1.80183222 | 1.26156301 | 1.02384742 |
| 19 | 1.80386831 | 1.26289746 | 0.97065867 |
| 21 | 1.80618465 | 1.25839056 | 0.95055357 |
| 23 | 1.80837356 | 1.26020239 | 0.96095831 |
| 25 | 1.81042024 | 1.26389686 | 0.96714474 |
| 27 | 1.81229778 | 1.26539426 | 0.95741279 |
| 29 | 1.81401183(1) | 1.26642(1) | 0.9503(3) |
| 31 | 1.8155706(4) | 1.26787(4) | 0.947(1) |
| 33 | 1.8169889(4) | 1.2694(1) | 0.947(4) |
| 35 | 1.8182812(5) | 1.2708(2) | 0.955(8) |
| 37 | 1.819462(1) | 1.2723(4) | 0.947(14) |
| 39 | 1.820542(2) | 1.2737(8) | 0.931(21) |
| 41 | 1.821534(3) | 1.274(1) | 0.951(29) |
| | extrapolations to $\infty$ | | |
| | 1.85 | 1.29 | 0.95 |
| | extrapolations from DAs | | |
| | 1.847(32) | 1.298(28) | 0.921(88) |
| | $\gamma^D$ conjectured values | | |
| | $59/32 = 1.84375$ | $9/7 \approx 1.2857$ | $19/16 = 1.1875$ |

conjectured value of $19/16 = 1.1875$. The values of the two partition functions and their ratio are given in tables 1, 2, and 3 for these three temperatures. Figure 1 is a plot of the ratio of partition functions $Q_n$. It can be seen that these are smooth on a graphical scale in this log–log plot.

In order to estimate exponent values, we used two different methods. Firstly, we performed a differential approximant analysis [24]. At all temperatures we used approximants with critical points biased at 1.0 with and without assumed confluent exponents. The approximants giving the best results were the ones utilizing all available coefficients and covering all possible combinations of approximants in the range of [1..3, 1..3, 1..3, 1..3; −1..2] with assumed confluent exponents. Averaging over these approximants after discarding defective ones we get the results presented in table 4. Secondly, we computed the local slopes from the log–log plot and estimated their limiting values using a suite of extrapolation methods [24], thereby confirming the results obtained from the differential approximant analysis.

Table 4 gives the list of local slopes extracted from the $Q_n$ and figure 2 plots these against $1/n$ to illustrate the data. They show graphically the answers given by differential approximant analysis.

In conclusion, the differential approximant analysis gives answers consistent with the believed exact results at high ($59/32 = 1.84375$) and $\theta$- ($9/7 \approx 1.2857$) temperatures

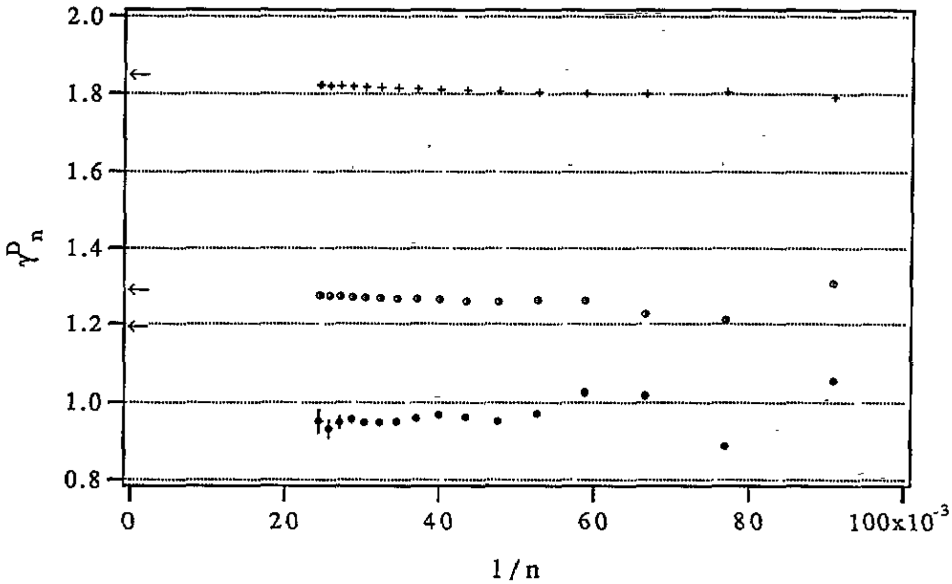


**Figure 2.** This graph is a plot of local estimates of the exponent $\gamma^D$ against $1/n$ for the three temperatures. The crosses are high temperatures values, the open circles are $\theta$-temperature values and the full circles are the low temperature values. The arrows indicate the conjectured results. At low temperatures the estimates are more erratic than at high temperatures though they still settle to a value well away from the conjectured 19/16.

but the value extracted at low temperatures ($0.921 \pm 0.088$) excludes the recent conjecture ($19/16 = 1.1875$).

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