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LETTER TO THE EDITOR

Scaling in the collapsed polymer phase: exact results

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Abstract. We derive an exact scaling form for the low temperature partition function in a model of polymer collapse. This confirms recent series work and so gives the exponents $\sigma=1/2$, $\gamma_-=1/4$ and $\chi=3/4$ exactly. The model considered is a variant of the self-interacting partially directed self-avoiding walk in two dimensions.

The asymptotic scaling form, in the length L of the chain, of the partition function, Q_L, for models of polymer collapse (θ-point) has usually been assumed to take the following form [1]:

$$Q_L \sim q_0 \mu^L L^{\gamma-1} \tag{1}$$

where $\log\mu(\beta)$ is proportional to the temperature (β^{-1}) dependent free energy. The exponent γ takes on a different value at the θ-temperature to that at high temperatures. Evidence has recently [2] been given that in one model of polymer collapse in two dimensions the *low* temperature scaling form is markedly different. Following fluid analogies, a Fisher droplet model type scaling has been suggested [2], which gives

$$Q_L \sim q_0 \mu_0^L \mu_1^{L^\sigma} L^{\gamma_- -1} \tag{2}$$

where σ and $\gamma-$ are expected to be universal exponents. Series work [2, 3] on the self-interacting partially directed self-avoiding walks (IPDSAW) at low temperatures strongly suggests that this scaling form is indeed correct and that the values of σ and γ_- are close to 1/2 and 1/4 respectively. In this letter, these exponents are derived exactly for a semi-continuous version (ICPDSAW) of this model. We note that all the exponents previously derived for the IPDSAW and ICPDSAW have been identical and so we expect this property to hold for σ and γ (in fact, σ may well be 1/2 for isotropic interacting walks).

For both the original discrete [4] and the variant [5], where the length is a continuous variable, a generating function approach has yielded exact expressions for

$$G(\alpha,\beta) = \int_0^\infty e^{-\alpha L} Q_L(\beta)\, \mathrm{d}L \tag{3}$$

(the integral becomes a sum in the discrete case). The generating function converges for small $e^{-\alpha}$ and I shall use $e^{-\alpha_c}$ to denote the radius of convergence of the generating function. The radius of convergence is pivotal in determining the mathematical

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properties of the model. Firstly, the function $\alpha_c(\beta)$ is directly related to the thermodynamic (infinite L) free energy and secondly, because the partition function is determined by an inverse Laplace transform which can be computed by summing over the poles of G, the singularity at the radius of convergence determines the large L behaviour of the partial function. For temperatures $\beta \leqslant \beta_\theta$ these generating functions can easily be used to extract the scaling form of the partition function. This is because the generating function has a simple pole or power law type singularity at its radius of convergence; that is, the form (1) is equivalent to the following behaviour in the generating function:

$$G(\alpha, \beta) \sim (\alpha - \alpha_c)^{-\gamma}. \tag{4}$$

Hence, one needs only to find the asymptotics of G on approaching α_c to deduce the form (1). However, at low temperatues an infinite accumulation of poles produces an essential singularity at the radius of convergence. As a consequence one is effectivly forced to invert the Laplace transform explicitly and hence the partition function scaling has not previously been derived. In this letter I shall derive the asymptotic expression for large L of the partition function for the ICPDSAW by summing over the residues at this accumulation.

The configurations of the IPDSAW are partially directed walks on a square lattice, which are self-avoiding walks that are restricted from growing in the negative x-direction. An energy is assigned to each (non-consecutive), nearest neighbour pair of monomers (steps) to introduce a temperature. However, the generating function [4] contains q-hypergeometric series about which little asymptotic analysis is known. A slight modification considers partially directed walks where the length of each vertical segment is allowed to assume real values. (One still has the discrete character in the horizontal direction.) These are the configurations of the ICPDSAW. An energy $U(r_1, \ldots, r_N)$ is assigned to each configuration of length L and number of vertical segments N, where each vertical segment, $i = 1, \ldots, N$, has length r_i measured in the positive y direction giving $L = \Sigma_{i=1}^{N} |r_i|$. This energy is

$$U(r_1, \ldots, r_N) = -J \sum_{i=1}^{N-1} \min(|r_i|, |r_{i+1}|) \mathcal{H}(-r_i r_{i+1}) \tag{5}$$

where $\mathcal{H}(r)$ is the Heaviside step function. The energy is then proportional to the overlap of successive segments (as in the discrete case). We are interested in attractive interactions and so set $J = 1$ for convenience. The thermodynamics can be deduced from the canonical partition function

$$Q_L(\omega) = \sum_{N=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}r_1 \ldots \int_{-\infty}^{\infty} \mathrm{d}r_N \delta(\Sigma_{i=1}^{N} |r_i| - L)\, e^{-\beta U(r_1, \ldots, r_N)} \tag{6}$$

where the Dirac delta function restricts the 'counting' to fixed length (equal to L) walks. By interchanging the summation and integration the generating function $G(\alpha, \beta)$ defined via (3) can be rewritten as

$$G(\alpha, \beta) = \sum_{N=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}r_1 \ldots \int_{-\infty}^{\infty} \mathrm{d}r_N \exp\left(-\alpha \sum_{i=1}^{N} |r_i| + \beta \sum_{i=1}^{N-1} \min(|r_i|, r_{i+1}|) \mathcal{H}(-r_i r_{i+1}) \right). \tag{7}$$

It has been shown (a detailed account can be found in [5]) that one can calculate the generationg function by considering a slightly more general function $\mathcal{G}(z, x; \alpha, \beta)$, given as

$$\mathcal{G}(z, x; \alpha, \beta) = \sum_{N=1}^{\infty} x^N \mathfrak{X}_N(z; \alpha, \beta) \tag{8}$$

where

$$\mathfrak{X}_N(z; \alpha, \beta) = \int_{-\infty}^{\infty} \mathrm{d}t \exp(-\alpha|t| + \beta \min(|t|, |z|) \mathcal{H}(-tz)) \, \mathfrak{X}_{N-1}(t; \alpha, \beta) \tag{9}$$

and

$$\mathfrak{X}_0(z; \alpha, \beta) = 1. \tag{10}$$

One can view $\mathcal{G}(z, x; \alpha, \beta)$ as being the generating function for continuous walks where the first vertical segment is of length z and a fugacity x has been assigned to horizontal steps. It is important to see that the generating function is related to $\mathcal{G}$ by

$$G(\alpha, \beta) = \mathcal{G}(0, 1; \alpha, \beta). \tag{11}$$

Now, an integral equation which $\mathcal{G}$ satisfies is found by substituting the recursive formula for $\mathfrak{X}_N$ into the equation for $\mathcal{G}$. The integral equation can be reduced (with loss of boundary condition) to a differential equation. The solution to the differential equation is then substituted back into the integral equation to fix the constants of the differential equation's general solution. The method is closely related to the solution of the discrete case. The differential equation so produced can be converted to an inhomogeneous form of Bessel's differential equation. The solution and hence the generating function is given in terms of Bessel functions.

In the continuous model then the generating function is given [5] as a ratio of Bessel functions:

$$1 + G(\alpha, \beta) = \varepsilon^{-1} \frac{J_\nu(\varepsilon\nu)}{J'_\nu(\varepsilon\nu)} \tag{12}$$

where

$$\varepsilon = \left(\frac{4}{\beta}\right)^{1/2} \tag{13}$$

and

$$\nu = \frac{\beta}{\alpha - \beta}. \tag{14}$$

(The coupling constant for nearest neighbour interactions has been set to 1 for convenience). The critical value of β is $\beta_\theta = 4$ and for low temperatures, $\beta > \beta_\theta$, the radius of convergence is simply given by $\alpha_c = \beta$. A plot of $\alpha_c(\beta)$ is given in figure 1. These results can be understood by realising that the poles of G occur at the zeros of

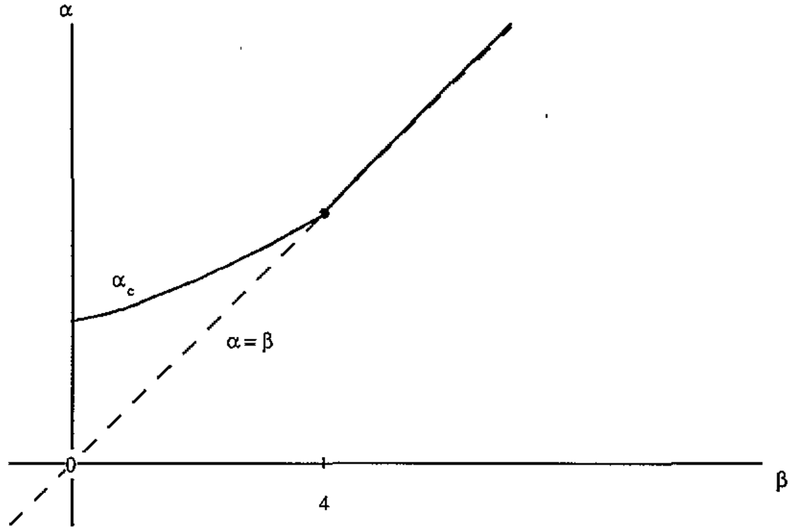

Figure 1. This graph illustrates (schematically) the function $\alpha_c(\beta)$ (which is essentially related to the radius of convergence of the generating function). The dashed line is $\alpha=\beta$; for $\beta>4$ this line coincides with $\alpha_c(\beta)$. The generating function converges everywhere above the curve $\alpha_c(\beta)$ and $\alpha_c(0)\approx 0.8526$.

the denominator of (12) and knowing the asymptotics of Bessel functions of large order and argument [6]. There exist solutions of

$$J'_\nu(\varepsilon\nu)=0 \tag{15}$$

for positive ν provided $\varepsilon>1$. The radius of convergence $\alpha_c>\beta$, and there exists an isolated pole at α_c. As ε approaches 1 then $\alpha_c\to\beta$ and at $\varepsilon=1$ the asymptotics of the generating function can be deduced from standard results [6] with $\gamma=1/3$. For $\varepsilon<1$ (15) has only solutions for negative ν and always for arbitrarily large $|\nu|$. This leads naturally to introduce the parameter $\eta=\alpha-\beta=\beta/\nu$. Figure 2 illustrates the pole structure of the generating function in the complex η plane—all the poles lie on the real axis. Interest then lies in finding

$$Q_L(\beta)=\frac{e^{\beta L}}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{\eta L}G(\beta+\eta,\beta)\,\mathrm{d}\eta \tag{16}$$

for $\beta>4$ (we can take any $c>0$). Despite the large amount that has been written about ratios of Bessel functions, the required information is apparently not in the literature [7] (so that an inverse transform valid for all L has not been found). However, in recent work [8, 9] on the bubble model of correlations similar (though not identical) expressions arise, and similar information is required. Asymptotics for large L can be found [9] by using a transformation from ν to $-\nu$.

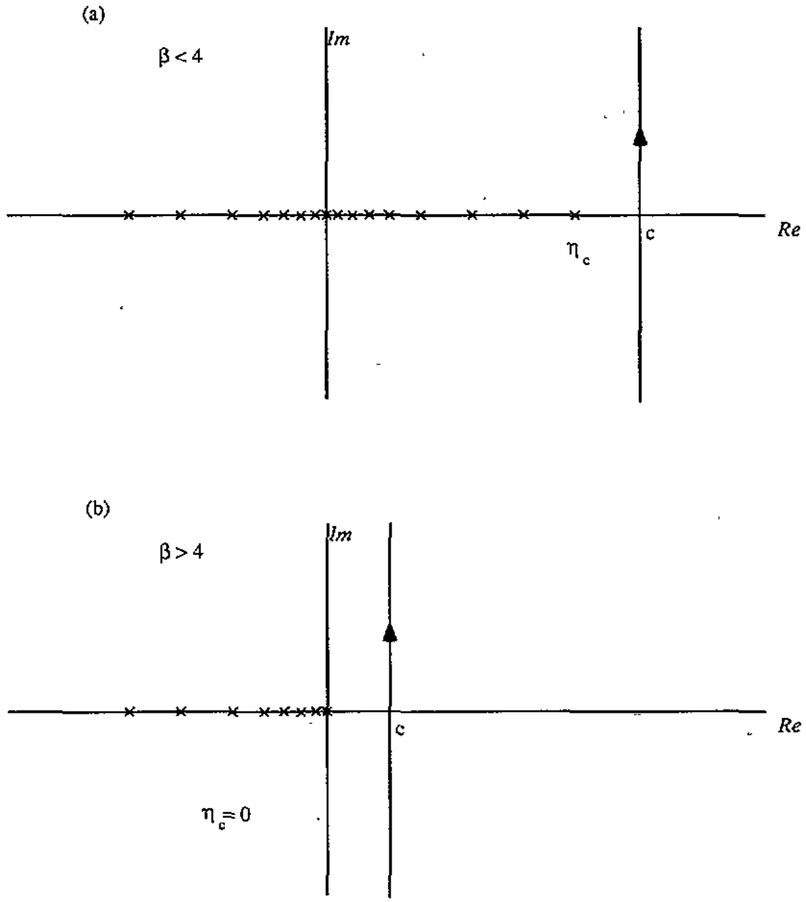

Figure 2. The two schematic diagrams show the positions of the poles of the generating function in the complex η plane for high temperatures (a) and low temperatures (b). The crosses mark these positions; near the origin there is, in fact, an accumulation of poles in both diagrams. The necessary contour for the inversion of the Laplace transform is also shown, where c (the real part of the contour) is chosen so that $c > \eta_c$.

Let the zeros of (15) be labelled as $\eta_j < 0$ so that $\eta_{j+1} > \eta_j$ (that is $|\nu_{j+1}| > |\nu_j|$) beginning at $j = 1$. There exists an infinite number of η_j such that $\lim_{j\to\infty} \eta_j = 0$. This can be deduced from the results of [10]. So by Cauchy's theorem we have

$$Q_L(\beta) = e^{\beta L} \sum_j e^{\eta_j L} R_j \tag{17}$$

where R_j are the residues of $G(\beta + \eta, \beta)$ at η_j. Our problem is two fold: first to find the residues R_j and the values η_j at which poles occur, and then to compute the above sum for large L.

Now the residues fo G at ν_j can be found in the following way: We use the transformation

$$J_{-u}(z) = J_u(z) \cos(\pi u) - Y_u(z) \sin(\pi u) \tag{18}$$

and the recurrence relations [10, 6] amongst J_u, $J_{u\pm1}$ and J'_u (and similarly for Y_u). One can then deduce that the solutions of (15) occur at

$$\tan(\pi u)=\frac{J'_u(\varepsilon u)}{Y'_u(\varepsilon u)} \tag{19}$$

where $\nu=-u$. Given that

$$Y'_u(\varepsilon u)\sim\left(\frac{2g}{\pi u}\right)^{1/2}e^{fu} \tag{20}$$

and

$$J'_u(\varepsilon u)\sim\left(\frac{g}{2\pi u\varepsilon^2}\right)^{1/2}e^{-fu} \tag{21}$$

with

$$g=(1-\varepsilon^2)^{1/2}>0 \tag{22}$$

and

$$f=\log\left(\frac{1+g}{\varepsilon}\right)-g>0 \tag{23}$$

it is clear that for large u

$$u_j\approx j. \tag{24}$$

Again using the transformation from positive to negative order in the generating function and recalling how η is related to u, the residues at $\eta_j=-\beta/u_j$ are found to be

$$R_j=\text{Residue of } G \text{ at } \eta_j\sim\frac{\beta}{\pi g}\,\frac{e^{-2fu_j}}{u_j^2}. \tag{25}$$

The Wronskian identity

$$J_{u+1}(z)Y_u(z)-J_u(z)Y_{u+1}(z)=\frac{2}{\pi z} \tag{26}$$

is useful here. Substituting (24) into (25) gives us a sum for the partition function as

$$Q_L(\beta)\sim\frac{\beta}{\pi g}e^{\beta L}\sum_{j=1}^{\infty}j^{-2}e^{-2fj-\beta L/j}. \tag{27}$$

Now the sum,

$$S(a,b)=\sum_{j=1}^{\infty}j^{-2}e^{-aj-b/j} \tag{28}$$

can be shown to behave as

$$S(a,b)\sim\left(\frac{\pi a}{b}\right)^{1/2}\frac{e^{-2(ab)^{1/2}}}{(ab)^{1/4}} \tag{29}$$

using a steepest descent method. Substituting the relevant expressions for a and b into this formula gives us the partition function scaling form, and therefore we have

$$Q_L(\beta) \sim A_1 e^{\beta L} e^{-A_2 L^{1/2}} L^{-3/4} \tag{30}$$

with

$$A_1(\beta) = \left(\frac{2\beta f}{\pi^2 g^4}\right)^{1/4} \tag{31}$$

and

$$A_2(\beta) = (8\beta f)^{1/2} \tag{32}$$

where $f(b)$ and $g(\beta)$ are given via (23), (22) and (13). We can then compare this directly with the conjectured form (2) to give our major results that $\sigma = 1/2$ and $\gamma_- = 1/4$.

The exponent χ, defined by

$$|1 - \mu_1(\beta)| \sim \text{const}\,|\beta - \beta_\theta|^\chi \tag{33}$$

as $\beta \to \beta_\theta$, can be simply extracted from the coefficient A_2. By simple expansions $\chi = 3/4$, which confirms both the series analysis of [2] and the scaling theory of [11].

In conclusion, the form of the length scaling for the partition function of the (continuous) interacting partially directed SAW model at low temperatures has been extracted from the generating function by explicitly inverting the Laplace transform involved. The essential singularity in the generating function at low temperatures destroys the scaling form (1) and indeed gives the form (2). The exponents are found to have the values previously inferred from series analysis.

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