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1994 J. Phys. A: Math. Gen. 27 L919

(http://iopscience.iop.org/0305-4470/27/24/003)

J. Phys. A: Math. Gen. 27 (1994) L919–L925. Printed in the UK

LETTER TO THE EDITOR

Universal distance ratios for interacting two-dimensional polymers

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Received 30 September 1994

Abstract. We present the hypothesis that at the θ-temperature of a single interacting polymer in two dimensions, a particular combination of universal distance amplitude ratios is given exactly by a simple formula in terms of critical indices only. This generalizes a similar claim for non-interacting self-avoiding walks, which was derived from conformal invariance considerations. We support our hypothesis with a series analysis of interacting self-avoiding walks on the square lattice, high-precision simulations of interacting self-avoiding walks on the Manhattan lattice at the exact θ-point and similar simulations of interacting trails on the square lattice.

A great deal of effort has been directed towards elucidating the properties of lattice models of the geometric features of large-molecular-weight linear polymers in solution. The canonical model is that of self-avoiding walks (SAW). The large-length asymptotic behaviour of SAW can be viewed as a critical phenomenon [1] and, hence, it is believed that there are universal properties of polymers that are independent of much of the microscopic detail of the system. For example, the critical exponents of the SAW model on any regular lattice should hold exactly for flexible linear polymers in so-called 'good' solvents. Much attention is often paid to the indices of the power-law behaviour that characterizes many of the quantities of interest. On the other hand, the renormalization group description of critical phenomena predicts that critical exponents are not the only universal features: certain ratios of critical amplitudes (multiplicative constants of the power laws) are also universal. There has been some interest in these amplitude ratios for SAW [2].

In two dimensions, conformal invariance, and the associated field-theoretic description of critical phenomena [3], provides a very powerful method of determining the critical behaviour of statistical mechanical systems. In particular, through the formal mapping of SAW to the $n \to 0$ O(n) magnetic model [1], conformal invariance [4] allows one to predict the critical indices for self-avoiding walks (these have also been found from the Coulomb gas [5]). There have also been recent calculations on amplitude ratios for SAW [6]. Importantly, one (linear) combination of amplitude ratios (with rational factors) has been calculated exactly [7, 8] using conformal invariance. This result, found from Zamolodchikov's c-theorem [9], holds for non-interacting SAW and, hence, for polymers in a good solvent. Based on numerical work, we claim that this proposition can be extended to θ-point polymers by suitably modifying the original prediction. Equivalently, we hypothesize that a particular combination of universal distance amplitude ratios is given exactly by a simple formula in terms of critical indices only.

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0305-4470/94/240919+07$19.50

We have tested this assertion first with an exact enumeration analysis for interacting SAW (ISAW) on the square lattice. This indicates that the quantity in question does indeed behave as we predict (with an error of 1 part in 200). In addition, we have simulational evidence for ISAW on the Manhattan lattice, where it proved to be correct within, at least, 1 part in 1000. Even for the model of interacting self-avoiding trails (ISAT) on the square lattice, where the presence of logarithmic corrections makes an analysis much more difficult, it proved to be correct to within 1 part in 100. Given the affirmative results from all three models, and especially the accuracy of the Manhattan data, we are confident that the Cardy–Saleur result is more widely applicable than previously thought.

We define any N-step path φ_N on a lattice by a sequence $r_0, r_1, \ldots, r_N$ of vector positions of the vertices of that path. For the interacting problems considered, the average of any quantity Q over the ensemble set $C(\varphi_N)$ of allowed paths φ_N of length N is given generically as

$$\langle Q \rangle = \frac{\sum_{C(\varphi_N)} Q(\varphi_N)\omega^m}{\sum_{C(\varphi_N)} \omega^m} \tag{1}$$

where m is the number of 'interactions' (being the number of nearest neighbours for walks and the number of contacts for trails). The Boltzmann weight $\omega = e^{\beta\varepsilon}$ is the usual function of the (inverse) temperature β and the energy ε associated with each interaction. We are interested in the average-square end-to-end distance

$$\langle R_e^2 \rangle_N = \langle r_N \cdot r_N \rangle \tag{2}$$

the ensemble average of the mean-square distance of a monomer from the endpoints

$$\langle R_m^2 \rangle_N = \frac{1}{N+1} \sum_{i=0}^{N} \langle r_i \cdot r_i \rangle \tag{3}$$

the average centre of mass

$$\langle R_c^2 \rangle_N = \frac{1}{(N+1)^2} \sum_{i=0}^{N} \sum_{j=0}^{N} \langle r_i \cdot r_j \rangle \tag{4}$$

and the average radius of gyration

$$\langle R_g^2 \rangle_N = \langle R_m^2 \rangle_N - \langle R_c^2 \rangle_N. \tag{5}$$

In the above formulae, we use $r_0 \equiv \mathbf{0}$.

Each of these measures of the size of the polymer is expected to scale as

$$\langle R^2 \rangle_N \sim C_R N^{2\nu} \tag{6}$$

where the amplitude C_R is non-univeral and temperature dependent, while ν is expected to be universal, depending only on the temperature in as much as its value is above, at, or below the θ-point. We define the finite-length amplitude ratios

$$A_N = \frac{\langle R_g^2 \rangle_N}{\langle R_e^2 \rangle_N} \qquad \text{and} \qquad B_N = \frac{\langle R_m^2 \rangle_N}{\langle R_e^2 \rangle_N}. \tag{7}$$

These approach

$$A_N \to A_\infty = \frac{C_{R_g}}{C_{R_e}} \qquad \text{and} \qquad B_N \to B_\infty = \frac{C_{R_m}}{C_{R_e}} \tag{8}$$

in the limit $N \to \infty$, and these *are* believed to be universal [10]. For ISAW, the limiting values should depend only on dimension and whether the temperature is above, or at, the θ-point—above the θ-point they should take on their SAW values.

For SAW, SAT and ISAW at high temperatures, and hence polymers in a good solvent, it was predicted [7, 8] that

$$\tfrac{246}{91} A_\infty - 2B_\infty + \tfrac{1}{2} = 0. \tag{9}$$

In the derivation [7] of this invariant, the factor multiplying A_∞ (let us call it λ) was given by

$$\lambda = 2 + \frac{y_t}{y_h} \tag{10}$$

where $y_t = \frac{4}{3}$ and $y_h = \frac{91}{48}$ are the thermal and magnetic renormalization-group eigenvalues, respectively, of the O(0) (SAW) model. These eigenvalues are related to the conformal scaling dimensions via $y = 2 - x$. They are also functions of the canonical exponents $\nu = 1/y_t$ and $\gamma/\nu = 2y_h - 2$. Rewriting the more general identity

$$\lambda A_\infty - 2B_\infty + \tfrac{1}{2} = 0 \tag{11}$$

simply gives the relation

$$\frac{4B_\infty - 1}{2A_\infty} = \lambda.$$

In other words, a particular combination of universal distance ratios is given in terms of critical indices. Cast in this fashion, the relation begs the question as to its wider applicability. It is not clear to us from the original argument [7, 8] that a suitably modified expression would not hold for ISAW at the collapse tricritical point.

Hence, we set out to test whether or not, at the θ-point of the interacting system, the quantity

$$G_N = \frac{4B_N - 1}{2A_N} \tag{13}$$

behaves as

$$G_N \to \lambda \qquad \text{as} \qquad N \to \infty \tag{14}$$

where again $\lambda = 2 + y_t/y_h$, and y_t and y_h now take on their θ-point values. To begin this investigation, we first considered the canonical model of SAW interacting via nearest-neighbour attraction and generated series for $G_N(w)$.

For ISAW at the θ-point, the critical exponents are now believed to take on the values predicted by Duplantier and Saleur [11]. These give $y_t = \frac{7}{4}$ and $y_h = 2$ and, hence, $\lambda = \frac{23}{8} = 2.875$. The critical temperature has been estimated by Meirovitch and Lim [12]

as $\beta\varepsilon = 0.658(4)$ from Monte Carlo simulations. Other estimates are around this value and we have used $\log\omega_\theta = 0.660(5)$ as our standard θ-point. We have generated SAW up to 29 steps, counting interactions and calculating each of the size measures. We have formed the series $G_N(\omega)$ and from this extrapolated $G_\infty(\omega)$ for a range of values of ω. As the series data show various irregularities (especially in the collapsed phase), we used differential approximants on a transformed series with coefficients $H_n = \Pi_{M=0}^{N} G_M$, which has $1/G_\infty$ as its critical point. This method is expected to give good results if the finite-size corrections are not stronger than $1/N$. For instance, if $G_N \sim G_\infty(1 + b/N)$, then $H_N \sim G_\infty^N \binom{N+b}{b}$ and the generating function behaves as $\sum H_N x^N \sim (1 - G_\infty x)^{-(b+1)}$. We note that even stronger corrections can be accommodated if they are alternating in sign. The results of this analysis are shown in figure 1.

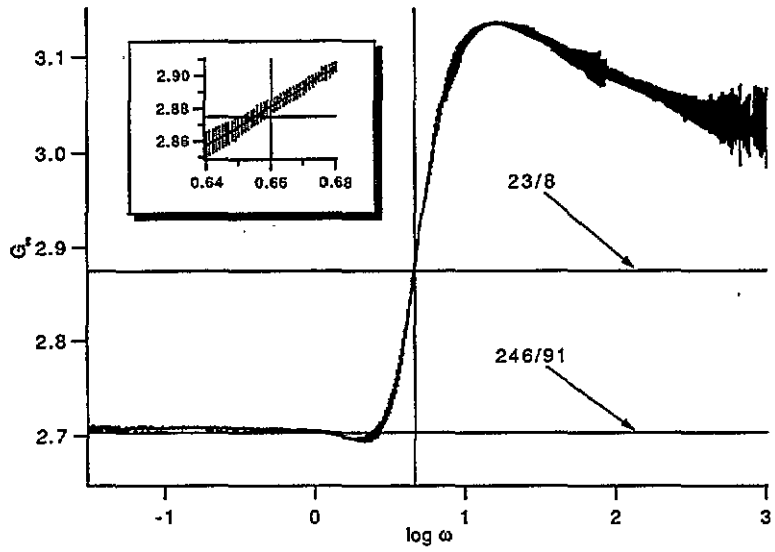

Figure 1. This shows estimates of G_∞ obtained from a differential approximant analysis of products of G_N. The G_N were calculated from series data of ISAW on the square lattice. The inset shows a magnified region around the θ-point.

For repulsive and mildly attractive interactions, our estimates of G_∞ are close to the predicted SAW value ($\frac{246}{91}$), as expected. In addition, our estimates for amplitude ratios A_∞ and B_∞ in the non-interacting case are 0.140 30(23) and 0.439 669(6), respectively, using the same method. These are comparable to the best available Monte Carlo data [2] for these ratios. As the θ-point is approached, there is a rapid change in the estimates of $G_\infty(\omega)$ as ω is varied. At the currently accepted value ω_θ of the θ-point, the estimate of G_∞ is 2.88(1). This value clearly encompasses our prediction. Furthermore, we can estimate the values $A_\infty = 0.180(1)$ and $B_\infty = 0.510(2)$. Alternatively, assuming the hypothesis' validity, one can estimate the θ-temperature utilizing the value of λ for G_∞ at the θ-point. This gives us $\log\omega = 0.655(5)$ and compares well with the Meirovitch and Lim value. As a comparison, we have plotted in figure 2 our (conventional) differential approximant analysis of the exponent ν, estimated from the radius of gyration series. Now, using the believed value of $\nu = \frac{4}{7}$ to estimate the critical temperature, gives $\log\omega = 0.665(5)$. There are some corrections-to-scaling obviously to be taken into account, but this shows that, up

to the accuracy of the present analysis, that determinations of the critical temperature from G_N and exponent estimates, such as ν_N, are comparable. The low-temperature behaviour is difficult to ascertain, with very low temperatures unreliable because of corrections-to-scaling, and temperatures close to the θ-point similarly unreliable because of crossover effects.

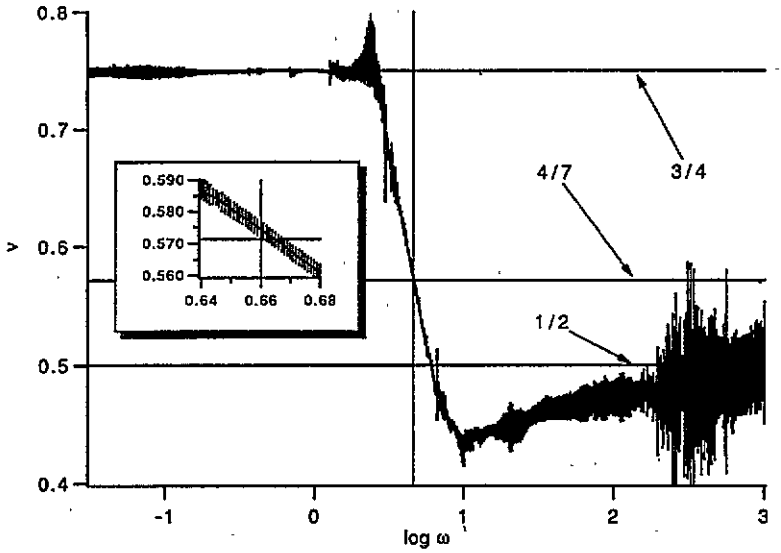

Figure 2. This shows estimates of the exponent ν obtained from a differential approximant analysis of the series for $\langle R_g^2 \rangle_N$. This is given as a comparison for figure 1. Note that the high- and θ-temperature values are accurately given, while at low temperatures the presence of strong corrections-to-scaling induces a systematic error in the analysis. The inset shows a magnified region around the θ-point.

Bradley [13] showed that kinetic growth loops on the Manhattan lattice could be mapped exactly onto the θ-point of closed ISAW on that lattice. Recently, kinetic growth simulations of SAW on the Manhattan lattice [14] have proven relatively successful in calculating the critical properties of Manhattan ISAW. In fact, there is an exactly solvable vertex model equivalent to this problem [14, 15]. The critical nature of the θ-point on the Manhattan lattice is similar to, but not exactly the same as, that of regular lattices [14, 15]. Regardless, it seemed natural to test our hypothesis on Manhattan ISAW at the θ-point. The simulations were carried out on the isomorphic problem of trails on the L-lattice, for trails up to length $N = 65\,536$. For this problem, $y_t = \frac{7}{4}$ and $y_h = \frac{7}{4}$, so $\lambda = 3$. We have estimates of A_N and B_N for $N = 2^k$, $k = 7, \ldots, 16$. These are plotted in figure 3 against $1/N$. The corrections-to-scaling are unknown but these plots are reasonably consistent, with the dominant corrections being of the $1/N$ type. Being therefore conservative with our estimated errors, gives $A_\infty = 0.157\,40(5)$ and $B_\infty = 0.4861(1)$ and, hence, $G_\infty = 3.0000(16)$. This then is a precise verification of the proposition at hand.

Interacting trails on the square lattice at the collapse temperature have also been found to be equivalent to kinetic growth trails on that lattice [16]. However, this problem is numerically complicated by the presence of multiplicative logarithmic corrections. Here it is believed [16] that $y_t = 2$ and $y_h = 2$, making $\lambda = 3$. Our simulations and analysis paralleled that of the L-lattice case. Estimates of A_N and B_N for $N = 2^k$, $k = 7, \ldots, 16$ were taken.

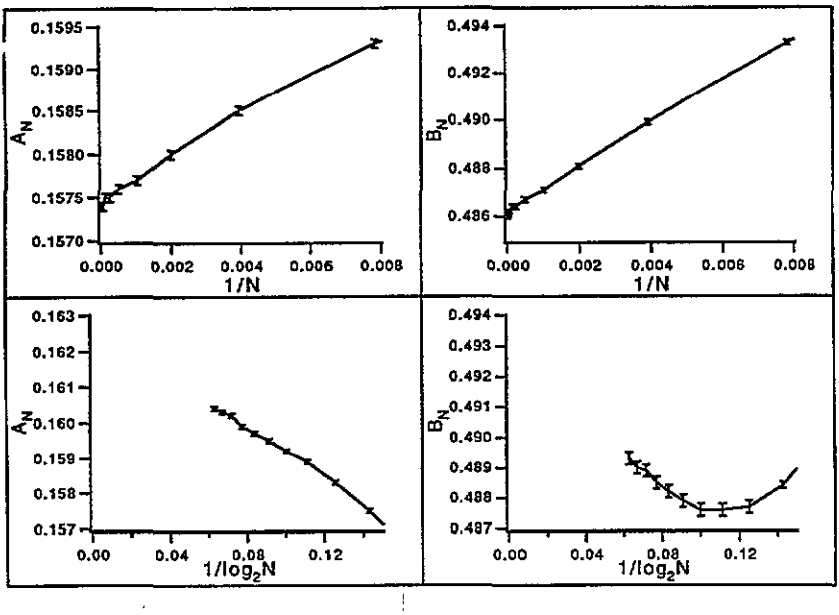

Figure 3. The top two graphs show the simulational data for A_N and B_N for interacting L-lattice trails (equivalent to Manhattan lattice ISAW) and the bottom two graphs show the simulational data for A_N and B_N for interacting square lattice trails. The L-lattice values are plotted against $1/N$, while the square lattice data is plotted against $1/(\log N)$ in accordance with known evidence of the corrections-to-scaling in the two cases.

These are plotted in figure 3 against $1/\log N$. There are clear strong corrections-to-scaling left in the estimates. However, a simple minded extrapolation using the logarithmic scale gives $A_\infty = 0.1620(5)$ and $B_\infty = 0.493(1)$ and, hence, $G_\infty = 3.000(16)$. Once again, our estimate is in excellent agreement with the supposition $G_\infty = \lambda$.

We have concentrated on the θ-point since it is generally believed to be a critical point. However, it may also be the case that G_∞ takes on a simple constant value in the collapsed phase. If so, that value would be near 3.0 according to our extrapolations, which is consistent with the pseudo-critical exponents $\nu = \frac{1}{2}$ and $\eta = 0$. However, our data is not accurate enough to verify or refute this additional prediction.

In conclusion, we have series and simulational evidence that a suitably modified Cardy–Saleur–Caracciolo–Pelissetto–Sokal invaraint should exist for θ-point polymers. Our numerical findings are summarized in table 1. It would, of course, be desirable if this invariant could be derived from conformal invariance arguments, as was the original prediction.

Table 1. Best estimates of the distance ratios for the collapse transition of interacting walk models. The estimates of G_∞ are to be compared with the values of λ computed from the conjectured exact scaling dimensions.

θ-point models	$\log \omega_\theta$	A_∞	B_∞	G_∞	y_t	h_h	λ
ISAW	0.660(5)	0.180(1)	0.510(2)	2.88(1)	$\frac{7}{4}$	2	2.875
Manhattan ISAW	$\log\sqrt{2}$	0.157 40(5)	0.4861(1)	3.0000(16)	$\frac{7}{4}$	$\frac{7}{4}$	3
ISAT	$\log 3$	0.1620(5)	0.493(1)	3.000(16)	2	2	3

The authors thank R Brak for carefully reading the manuscript and making several useful suggestions. We have benefitted from correspondence with J L Cardy and A D Sokal. We are grateful to the Australian Research Council for financial support and D B-W thanks the Graduate school of the University of Melbourne for a studentship.

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