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# Recent developments in the study of walks, polygons and the Ising model.

A. J. Guttmann, A. L. Owczarek, D. Bennett-Wood and T. Prellberg[a]

[a]Department of Mathematics, The University of Melbourne,
Parkville, Victoria 3052, Australia

In this paper we discuss some general developments in the study of self-avoiding walks and polygons in two dimensions, as well Ising models in both two- and three-dimensions, and then focus in greater detail on universal distance ratios for *interacting* self-avoiding walks.

## 1. Self-avoiding walk problems

In collaboration with I.G. Enting, one of us (AJG) has extended the square lattice polygon series to 70 steps. By direct enumeration we reach only 66 steps, but the knowledge of convex polygons allows the 68 step polygons to be enumerated, and the knowledge of "almost-convex" polygons allows the 70 step polygons to be enumerated. In enumerating the 66 step polygons, the use of differential approximants to predict the most significant digits, coupled with the enumeration program working in integer*2 modular arithmetic allows a saving in both time and space of about a factor of 2.

Also in collaboration with I.G. Enting a parallelised version of the counting algorithm has been developed for the honeycomb lattice. It is anticipated that this will permit enumerations of honeycomb polygons of about 100 steps.

For self-avoiding walks (SAW) on the square lattice, A.R. Conway has parallelised the algorithm we have previously used, and after judicious load balancing, has obtained 43 step SAW on the square lattice on an Intel Paragon (56 processor). Extension of the series to 47 or 51 steps requires the availability of a Paragon with 3GB or 10GB of memory respectively. Analysis of these extended series is still being undertaken.

## 2. Ising model problems

Developments of Ising model series have been achieved with I.G. Enting and I. Jensen. For the two-dimensional square lattice spin-1/2 Ising model, the low temperature series have been extended to $u^{38}$, while for the spin-1 Ising model, low-temperature series to $z^{79}$ have been obtained and analysed [1], where $u = e^{-4J/kT}$ and $z = e^{-J/kT}$. For the three-dimensional simple-cubic lattice Ising model, the high-temperature specific heat series has been obtained [2] to $v^{26}$, where $v = \tanh(J/kT)$.

## 3. Universal distance ratios for self-interacting polymers

One recent problem we have investigated [6] concerns a hypothesis about the ratio of size measures of interacting polymer models in two dimensions. The renormalisation 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. Importantly, one (linear) combination of amplitude ratios (with rational factors) has been calculated exactly [4,5] using conformal invariance for non-interacting SAW, and hence for polymers in a good solvent. Based on numerical work [6], we have recently claimed that this proposition can be extended to $\theta$-point polymers by suitably modifying the original prediction. To accomplish this we utilised a 29 term series for the quantities of interest for self-interacting self-avoiding walks (ISAW) on the square lattice. We have also tested this claim with two stochastic enumeration simulations.


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The quantities of concern are the average-square end-to-end distance $\langle R_e^2\rangle_N$, the ensemble average of the mean-square distance of a monomer from the endpoints $\langle R_m^2\rangle_N$, and the average radius-of-gyration $\langle R_g^2\rangle_N$. The finite-length amplitude ratios defined as

$$A_N = \frac{\langle R_g^2\rangle_N}{\langle R_e^2\rangle_N} \text{ and } B_N = \frac{\langle R_m^2\rangle_N}{\langle R_e^2\rangle_N} . \quad (1)$$

approach constants, $A_N \to A_\infty$ and $B_N \to B_\infty$, in the limit $N \to \infty$, and these are believed to be universal [7]. For ISAW, the limiting values should depend only on dimension and whether the temperature is above or at the $\theta$-point – above the $\theta$-point they should take on their SAW values.

For SAW, and hence ISAW at high temperatures, it was predicted [4,5] that

$$\frac{246}{91}A_\infty - 2B_\infty + \frac{1}{2} = 0 . \quad (2)$$

In the derivation [4] of this invariant the factor multiplying $A_\infty$ was given by $2 + y_t/y_h$, where $y_t = 4/3$ and $y_h = 91/48$ are the thermal and magnetic renormalisation 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 $\gamma/\nu = 2y_h - 2$.

We set out to test whether or not at the $\theta$-point of the interacting system the quantity

$$G_N = \frac{4B_N - 1}{2A_N} \quad (3)$$

behaves as

$$G_N \to 2 + y_t/y_h \text{ as } N \to \infty , \quad (4)$$

where $y_t$ and $y_h$ now take on their $\theta$-point values. To begin this investigation we first considered the canonical model of SAW interacting via nearest-neighbour attraction and generated series for $G_N(\omega)$, where $\omega$ is the Boltzmann weight for each interaction.

For ISAW at the $\theta$-point the critical exponents are now believed to take on the values predicted by Duplantier and Saleur [8]. These give $y_t = 7/4$ and $y_h = 2$ and hence $2 + y_t/y_h = 23/8 = 2.875$. Previous estimates of the critical temperature led us to use $\log\omega_\theta = 0.660(5)$ as our standard $\theta$-point. As mentioned above, we have generated SAW up to 29 steps on the square lattice counting interactions and calculating each of the size measures. We have formed the series $G_N(\omega)$ and extrapolated from this $G_\infty(\omega)$ for a range of values of $\omega$. The results of our analysis based upon differential approximants are shown in figure 1.

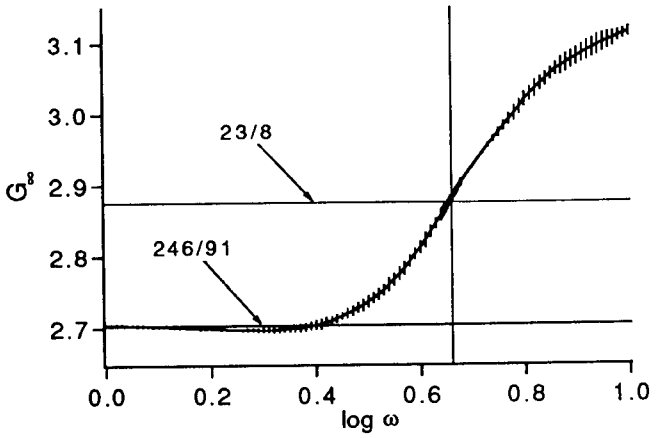


Figure 1. This shows estimates of $G_\infty$ obtained from a differential approximant analysis of products of $G_N$. The vertical line is the position of the $\theta$-temperature.

For repulsive interactions and mildly attractive interactions ($\log\omega \approx 0$) our estimates of $G_\infty$ are close to the predicted SAW value (246/91), as they should be. In addition, our estimates for amplitude ratios $A_\infty$ and $B_\infty$ in the non-interacting case are 0.14030(23) and 0.439669(6) respectively, using the same method. These are comparable to the best available Monte Carlo data [3] for these ratios. As the $\theta$-point is approached there is a rapid change in the estimates of $G_\infty(\omega)$ as $\omega$ is varied. At the currently accepted value $\omega_\theta$ of the $\theta$-point the estimate of $G_\infty$ is 2.88(1) which clearly encompasses our prediction.

We have also tested the hypothesis for ISAW on the Manhattan lattice. On this lattice the collapse transition is in a different universality class to that on regular lattices [9,10]. Here we car-

Table 1
Best estimates of the distance ratios for the collapse transition of interacting polymer models. The estimates of $G_\infty$ are to be compared with the values of $2 + y_t/y_h$ computed from the conjectured exact scaling dimensions of each of the models.

| $\theta$-point models | $\log \omega_\theta$ | $G_\infty$ | $2 + y_t/y_h$ |
|---|---|---|---|
| Square Lattice ISAW | 0.660(5) | 2.88(1) | 2.875 |
| Manhattan Lattice ISAW | $\log \sqrt{2}$ | 3.0000(16) | 3 |
| Square Lattice Interacting Trails | $\log 3$ | 3.000(16) | 3 |

ried out kinetic growth simulations for walks up to length $N = 65536$. For this problem $y_t = 7/4$ and $y_h = 7/4$ so $2+y_t/y_h = 3$. We have estimates of $A_N$ and $B_N$ for $N = 2^k, k = 7, ..., 16$. Being conservative with our estimated errors gives $A_\infty = 0.15740(5)$ and $B_\infty = 0.4861(1)$, and hence $G_\infty = 3.0000(16)$ which is in excellent agreement with the hypothesis.

A third model of polymer collapse is that of interacting trails on the square lattice. This problem is numerically complicated by the presence of multiplicative logarithmic corrections. Here it is believed [11] that $y_t = 2$ and $y_h = 2$ making $2 + y_t/y_h = 3$. Estimates of $A_N$ and $B_N$ for $N = 2^k, k = 7, ..., 16$ were taken. A simple minded extrapolation using a logarithmic scale gives $A_\infty = 0.1620(5)$ and $B_\infty = 0.493(1)$ and hence $G_\infty = 3.000(16)$, in agreement with the hypothesis.

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

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