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LETTER TO THE EDITOR

Branched polymers attached in a wedge geometry

S A Colby†, D S Gaunt, G M Torrie‡ and S G Whittington§

† Department of Physics, King's College, Strand, London WC2R 2LS, UK
‡ Department of Mathematics and Computer Science, Royal Military College, Kingston, K7L 2W3 Canada
§ Department of Chemistry, University of Toronto, Toronto, M5S 1A1 Canada

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Abstract. We use exact enumeration and Monte Carlo techniques to test some recent predictions by Duplantier and Saleur of the values of the critical exponent γ for uniform star-branched polymers in a wedge geometry in two dimensions. Our results support their predictions.

We have also estimated the exponent ν and amplitude governing the n dependence of the mean square radius of gyration and the mean square end-to-end branch length. In some cases the branches are distinguished and have different mean lengths but the exponent ν is equal to the bulk self-avoiding walk value in every case.

The excluded volume effect in branched polymer molecules has attracted considerable attention over the last few years. The particular case of uniform star-branched polymers has been considered in detail (Daoud and Cotton 1982, Miyake and Freed 1983, Wilkinson *et al* 1986, Whittington *et al* 1986). The statistics, in particular, have been investigated by renormalisation group (Miyake and Freed 1983) and by exact enumeration and Monte Carlo methods (Wilkinson *et al* 1986).

If the number of uniform f-stars with n vertices in each of the f branches is $s_n(f)$, one expects that

$$s_n(f) \sim n^{\gamma(f)-1}\lambda(f)^n \tag{1}$$

where $\lambda(f)$ has been shown (Wilkinson *et al* 1986) to be μ^f, where μ is the growth constant of self-avoiding walks. The exponent $\gamma(f)$ has been estimated numerically (Wilkinson *et al* 1986) for small f, and by renormalisation group methods (Miyake and Freed 1983). Recently Duplantier (1986) has made use of conformal invariance arguments to preduct values of $\gamma(f)$ in two dimensions. These predictions are in quite good agreement with the numerical estimates.

Duplantier and Saleur (1986) have now generalised these results to stars in a wedge of angle α, with the f-star being attached at the apex of the wedge either by a vertex of degree 1 or f.

For all f the number of stars attached by a vertex at the wedge apex is expected to have an asymptotic behaviour analogous to (1). Using the methods of Hammersley and Whittington (1985) and Chee and Whittington (1987), it is easy to prove that $\lambda(f)=\mu^f$ for a wide class of situations including all those considered in this paper.

The particular case $f=1$ corresponds to self-avoiding walks which have been investigated for $\alpha=\pi$ by Barber *et al* (1978) and for $\alpha=\pi/2$ and $\pi/4$ by Guttmann and Torrie (1984). The agreement between these numerical results and the predictions of Duplantier and Saleur is excellent.

For $f>1$ we have tested the theoretical predictions for a variety of cases and present here results for the situations shown in figure 1. These include two modes of attachment for a 3-star in a half-space, and a 2-star in a wedge of angle α for $\alpha=\pi/2$, $2\pi/3$ and π.

In table 1 we present exact enumeration data for 2-stars on the square and triangular lattices for three values of α. We have analysed these data by standard ratio methods (Gaunt and Guttmann 1974) and give typical plots in figure 2. The series are converged

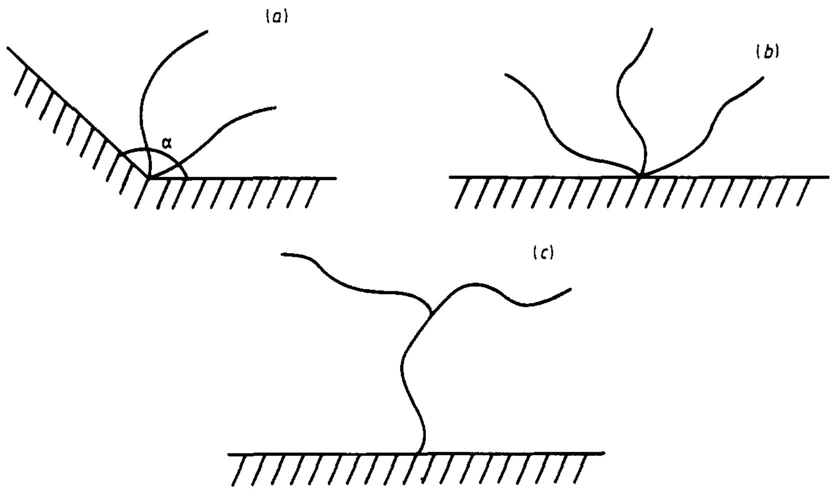

Figure 1. (*a*) 2-star in a wedge of angle α, (*b*) and (*c*) two modes of attachment for a 3-star in a half-space.

Table 1. Exact enumeration data for 2-stars in a wedge of angle $\alpha=\pi/2$, $2\pi/3$, π on the square and triangular lattices.

	Square		Triangular		
n	$\pi/2$	π	$\pi/2$	$2\pi/3$	π
1	1	3	1	3	6
2	3	14	5	22	66
3	10	76	43	248	919
4	51	482	467	3 164	13 645
5	250	3 002	5 365	42 136	206 391
6	1 356	19 130	66 179	582 024	3 193 827
7	7 164	121 580	850 323	8 303 686	50 236 630
8	39 990	788 430	11 338 710	121 174 262	799 178 388
9	224 859	5 124 180	155 539 357	1800 174 204	
10	1 301 942	33 625 482	2179 959 661		
11	7 597 242	221 243 104			
12	45 115 150	1464 558 768			
13	269 987 850				
14	1635 631 662				

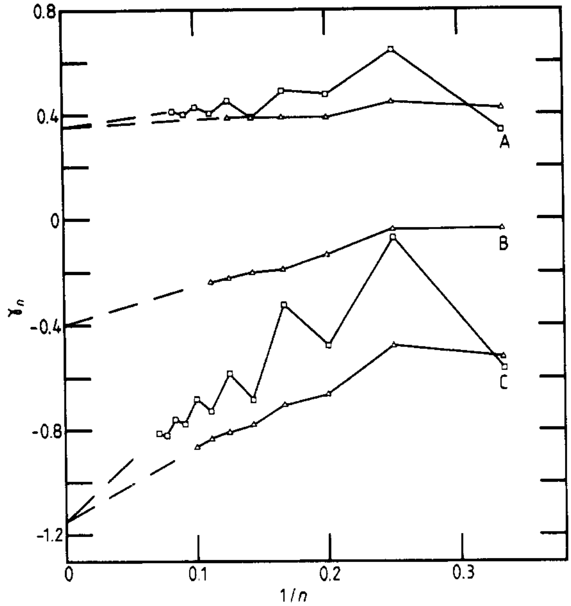

Figure 2. Ratio estimates of γ as calculated from $\gamma_n = 1 + n[(s_n/s_{n-1}\mu^2) - 1]$ for 2-stars on the square (□) and triangular (△) lattices. Plots (A), (B) and (C) correspond to $\alpha = \pi$, $2\pi/3$ and $\pi/2$, respectively.

and we estimate

$$\gamma_{2,2}(\pi/2) = -1.15 \pm 0.05 \qquad [-1\tfrac{5}{32} = -1.156\,25] \tag{2}$$

$$\gamma_{2,2}(2\pi/3) = -0.40 \pm 0.05 \qquad [-\tfrac{13}{32} = -0.406\,25] \tag{3}$$

$$\gamma_{2,2}(\pi) = 0.35 \pm 0.05 \qquad [\tfrac{11}{32} = 0.343\,75] \tag{4}$$

where the first subscript on γ indicates the functionality of the stars and the second indicates the degree of the apicial vertex. The predictions of Duplantier and Saleur are given in square brackets for comparison.

The analogous series which we have derived for 3-stars are too short to allow reliable extrapolation. This has led us to estimate the numbers of 3-stars (as well as 2-stars) on the triangular and square lattices, using an inversely restricted Monte Carlo approach (Rosenbluth and Rosenbluth 1955) with sample sizes up to 2×10^7. If $s_n(f)$ behaves as in (1), we note that a plot of $\ln[s_n(f)/\mu^{nf}]/\ln(nf)$ against $1/\ln(nf)$ will approach $\gamma - 1$ linearly as $n \to \infty$. In figure 3 we present corresponding plots for the topologies and modes of attachment shown in figure 1. For each of the cases of 2-stars, the values of γ estimated from this graph are in good agreement with the series estimates given in (2)-(4). We are therefore confident that this method of analysing the Monte Carlo data can give reliable results.

For the two modes of attachment of 3-stars we estimate

$$\gamma_{3,1}(\pi) = 0.68 \pm 0.05 \qquad [\tfrac{43}{64} = 0.671\ldots] \tag{5}$$

$$\gamma_{3,3}(\pi) = -0.82 \pm 0.05 \qquad [-\tfrac{53}{64} = -0.828\ldots]. \tag{6}$$

In all cases which we have considered (see (2)-(6)), the values of Duplantier and Saleur lie within our estimated error bars and we believe that this provides strong support for the general validity of their predictions.

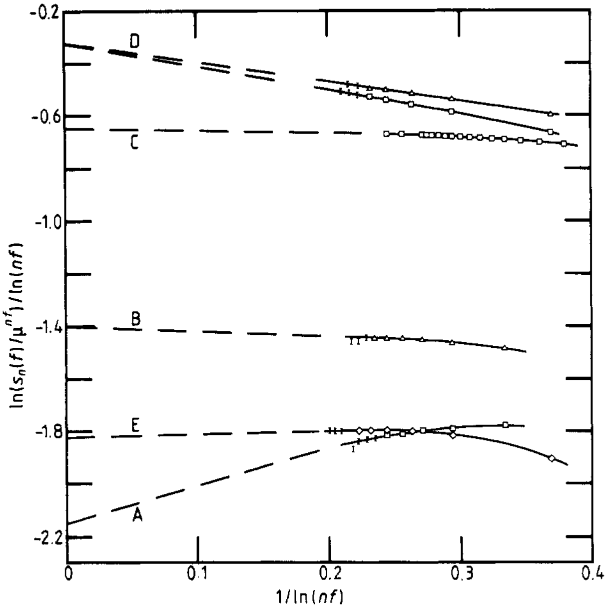

Figure 3. Monte Carlo estimates of $\gamma-1$ for the square (□ and ◇) and triangular (△) lattices. 2-stars for (A) $\alpha=\pi/2$, (B) $\alpha=2\pi/3$, (C) $\alpha=\pi$; 3-stars in a half-space with the modes of attachment shown in (D) figure 1(c), and (E) figure 1(b).

We now turn to consider the dimensions of the branches of these attached stars. We have generated Monte Carlo data for the mean square lengths of the branches, $\langle R_n^2\rangle$, and estimated the exponent ν, assuming that

$$\langle R_n^2\rangle \sim Bn^{2\nu}. \tag{7}$$

In each case the evidence suggests that $\nu=\frac{3}{4}$, the value for a self-avoiding walk (Nienhuis 1982) and for unconfined stars (Whittington *et al* 1986). However, we would expect the amplitude (B) to reflect the confining geometry and the mode of attachment. Indeed, in some cases, different branches in the same star should be expanded by different amounts (e.g. figure 1(c)).

In figure 4 we plot $\langle R_n^2\rangle/n^{1.5}$ against n for 2-stars in a half-space and for both types of branches for the 3-star shown in figure 1(c). For comparison, we include results for a self-avoiding walk in a half-space (Guttmann *et al* 1978). The branches of a 2-star in a half-space are noticeably more expanded than for a self-avoiding walk in a half-space, reflecting the interference between the branches. In the case of the 3-star (figure 1(c)) the branch containing the attaching vertex is more expanded than the 'free' branches, more expanded than an attached self-avoiding walk and, less obviously, more expanded than the branches of a 2-star in a half-space. The 'free' branches have dimensions very similar to those of unconstrained 3-stars (Whittington *et al* 1986). For small n, the unconstrained case is slightly less expanded while for larger n the opposite is true. For large n the expansion of the 'attached' branch leads to less interference between the 'free' branches, while at small n the interaction of the 'free' branches with the surface still seems to be important. In addition, the 'free' branches of the 3-star are slightly more expanded than a self-avoiding walk in a half-space, although the limiting amplitudes are clearly very similar.

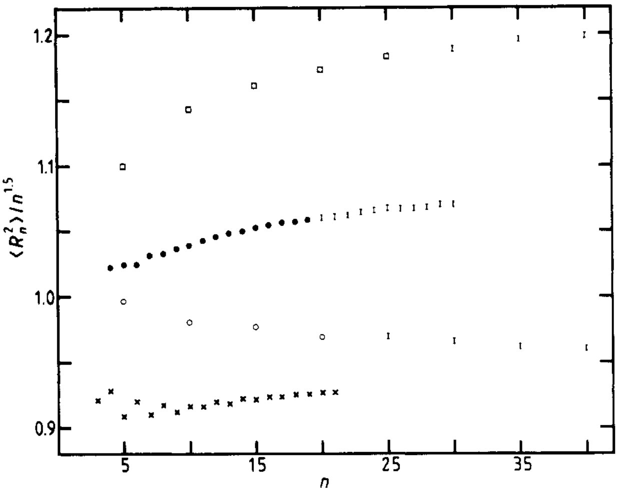

Figure 4. Mean square end-to-end length of a branch scaled by $n^{1.5}$ as a function of the branch length n for the square lattice. Exact enumeration data ($\times$) for a self-avoiding walk in a half-space, together with Monte Carlo data for a 2-star in a half-space (●) and for the 'attached' (□) and 'free' (○) branches of the 3-star in figure 1(c).

Finally, we have calculated the mean square radius of gyration $\langle S_N^2 \rangle$, where $N = 1 + nf$, for several of the cases discussed above. The most interesting is probably the 3-star in figure 1(c) where one branch is expanded relative to the unconstrained 3-star and, for large n, the other branches are slightly less expanded. We have estimated the amplitude (A) in

$$\langle S_N^2 \rangle \sim A N^{1.5} \tag{8}$$

and find $A = 0.077 \pm 0.001$. This is larger than the value for an unconstrained 3-star, $A = 0.074 \pm 0.001$ (Whittington *et al* 1986), so that the expansion of the attached branch, noted above, leads to an increase in $\langle S_N^2 \rangle$ relative to the unconstrained star.

In summary, we have presented the first numerical estimates of the exponent γ for uniform stars confined to a wedge geometry. Our results support the predictions of Duplantier and Saleur (1987) for these cases and suggest the validity of their more general predictions. We have also investigated the dimensions of the branches of these confined stars and discussed their sensitivity to the geometry and mode of attachment.

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