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LETTER TO THE EDITOR

Polygons and stars in a slit geometry

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Abstract. We consider self-avoiding polygons, uniform 3-stars and uniform 4-stars, weakly embeddable in the square lattice and confined between two parallel lines, $y = 0$ and $y = L$. We show rigorously that the connective constants of these three structures (provided that the corresponding limits exist) are all strictly less than the connective constant $\kappa(L)$ of self-avoiding walks with the same geometrical constraint. We also derive lower bounds on the connective constants of uniform 3-stars and 4-stars. These bounds appear to be strong, at least for small L.

The numbers of self-avoiding walks, polygons and uniform stars with f branches, weakly embeddable in the d-dimensional hypercubic lattice, are all known to grow exponentially with the total number of edges in the graph and to have the same connective constant (Hammersley 1962, Wilkinson *et al* 1986). These structures are interesting models of linear, ring and star polymers and studies of the effects of various geometrical constraints on their behaviour have provided useful information about polymers confined in slits, slabs and tubes (Daoud and de Gennes 1977, Wall *et al* 1977, Wall and Klein 1979, Klein 1980, Hammersley and Whittington 1985, Chee and Whittington 1987).

We first state some results on the d-dimensional hypercubic lattice. This is the set of integer points, with coordinates $(x, \ldots, y)$, in R^d and the set of edges joining pairs of points unit distance apart. Let $c_n(L)$, $p_n(L)$ and $s_n(f, L)$ be the numbers of n-edge self-avoiding walks, n-edge (unrooted) polygons and uniform f-stars with n edges in each branch, weakly embeddable in the d-dimensional hypercubic lattice, confined to lie between or in the $(d$-$1)$-dimensional hyperplanes $y = 0$ and $y = L$. Two configurations are counted as distinct if they differ by translation in the y direction and as the same if they differ only by translation in any other coordinate directions.

For $d > 2$, the connective constant for any f-star, defined by

$$\lim_{n\to\infty} (nf)^{-1} \log s_n(f, L) = \kappa(f, L) \tag{1}$$

is independent of f and so equal to that $(\kappa(L))$ for a self-avoiding walk (Chee and Whittington 1987). The connective constant for a polygon, defined by

$$\lim_{n\to\infty} n^{-1} \log p_n(L) = \kappa_0(L) \tag{2}$$

can be shown to be equal to that for a walk, using arguments along the lines of those in Hammersley (1962).

When $d = 2$ the situation appears to be quite different. Klein (1980) has calculated $\kappa(L)$ and $\kappa_0(L)$ explicitly for $L \leq 6$, using transfer matrix methods, and it appears that $\kappa_0(L) < \kappa(L)$. Similarly Chee and Whittington (1987) have calculated $\kappa(3, 1)$ and this is less than $\kappa(1)$. Although the existence of the limits defined by equation (1) for $d = 2$ has not been shown rigorously, these results suggest that $\kappa(3, L)$ and $\kappa(4, L)$ (if the limits exist) as well as $\kappa_0(L)$ are all strictly less than $\kappa(L)$, for all L. In this letter we give a short proof of this.

We first show that the connective constant $\kappa_0(L)$ *exists* for polygons in a slit of width L. To do this we define the top (bottom) vertex of a polygon as the vertex having largest (smallest) y coordinate in the subset of vertices of the polygon having largest (smallest) x coordinate. We take each m-gon and each n-gon and translate in the x direction so that the top vertex, with coordinates (x_t, y_t), of the m-gon, is three lattice spacings to the left of the bottom vertex, with coordinates (x_b, y_b), of the n-gon, i.e. $x_b = x_t + 3$. We delete the edges (x_t, y_t)-$(x_t, y_t - 1)$ and (x_b, y_b)-$(x_b, y_b + 1)$. (By the definitions of top and bottom vertices, these edges clearly exist.) We now join the two polygons using a rectangular 'pad' as shown in figure 1. The resulting polygon has $m + n + 2(L + 1)$ edges and each pair of m- and n-gons gives a distinct $(m + n + 2(L + 1))$-gon, so that

$$p_m(L)p_n(L) \leq p_{m+n+2(L+1)}(L). \tag{3}$$

In addition, by deleting an edge it is clear that

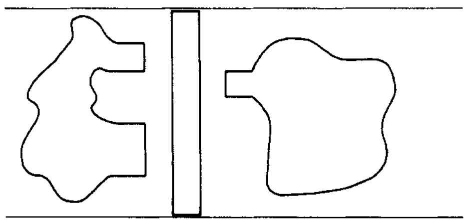
$$p_n(L) \leq c_{n-1}(L) \tag{4}$$

and, since

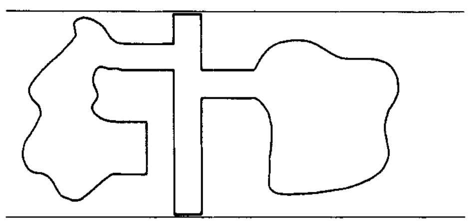
$$\lim_{n\to\infty} n^{-1} \log c_n(L) = \kappa(L) \tag{5}$$

is known to exist (Whittington 1983), equations (3)-(5) imply (Wilker and Whittington 1979) that

$$\lim_{n\to\infty} n^{-1} \log p_n(L) = \kappa_0(L) \tag{6}$$



(*a*)



(*b*)

Figure 1. The concatenation of two polygons through a rectangular pad.

exists with $\kappa_0(L) \leq \kappa(L)$. (Since the number of edges in a polygon is necessarily even n goes to infinity in equation (6) through only even values.)

For each polygon, with bottom vertex at (x_b, y_b) and top vertex at (x_t, y_t), we construct a rectangle (R) with vertices at $(x_b-1, -\frac{1}{2})$, $(x_b-1, L+\frac{1}{2})$, $(x_t+1, L+\frac{1}{2})$, $(x_t+1, -\frac{1}{2})$. We delete the two edges (x_b, y_b)-(x_b, y_b+1) and (x_t, y_t)-(x_t, y_t-1) and add the edges (x_b, y_b)-(x_b-1, y_b), (x_b, y_b+1)-(x_b-1, y_b+1), (x_t, y_t)-(x_t+1, y_t) and (x_t, y_t-1)-(x_t+1, y_t-1). This yields two self- and mutually avoiding walks w_1 and w_2 with their endpoints embedded in the boundary of the rectangle R. We take w_1 to be the walk joining (x_b-1, y_b+1) and (x_t+1, y_t). w_1 is a simple polygonal arc (homeomorphic to a 1-ball) with its endpoints properly embedded in the boundary of R, which is a polygonal Jordan curve (homeomorphic to a 1-sphere). Hence w_1 separates R (i.e. $R-w_1$ is not connected) and w_2 lies entirely in one of these two regions of R (see, for example, Stillwell 1980). All points on the line $y=L$ between (x_b-1, L) and (x_t+1, L) lie above or on w_1 so that w_2 lies entirely below this line and is confined between or in $y=0$ and $y=L-1$. A similar argument establishes that w_1 also lies entirely in a slit of width $L-1$.

w_1 and w_2 are self-avoiding walks whose leftmost and rightmost vertices are of unit degree and whose first and last edges are horizontal. Let $b_m(L)$ be the number of such 'unfolded' walks with m edges confined in a slit of width L. The above construction establishes that

$$p_n(L) \leq \sum_m b_m(L-1)b_{n+2-m}(L-1). \tag{7}$$

These unfolded walks can be concatenated in pairs to form unfolded walks with L additional steps (using a construction on the lines of that described by Whittington (1983)) so that

$$b_m(L)b_{n-m}(L) \leq b_{n+L}(L). \tag{8}$$

Hence

$$p_n(L) \leq nb_{n+L+1}(L-1). \tag{9}$$

Unfolded walks in a slit of width L have the same connective constant, $\kappa(L)$, as self-avoiding walks in a slit of width L (Whittington 1983) so that equation (9) gives $\kappa_0(L) \leq \kappa(L-1)$. But $\kappa(L)$ is a strictly monotone increasing function of L (Hammersley and Whittington 1985). Hence

$$\kappa_0(L) < \kappa(L). \tag{10}$$

The corresponding proof for a star is similar. We give the argument for $f=4$ but this can be easily adapted to the case $f=3$.

We consider a 4-star with n edges in each branch, confined to lie in or between $y=0$ and $y=L$. We can define the top and bottom vertices of a star in exactly the same way as for a polygon. Let the top vertex have coordinates (x_t, y_t) and the bottom vertex have coordinates (x_b, y_b). The star lies in, or in the boundary of, the rectangle R with vertices $(x_b, -\frac{1}{2})$, $(x_b, L+\frac{1}{2})$, $(x_t, L+\frac{1}{2})$, $(x_t, -\frac{1}{2})$. There is a self-avoiding walk w, which is a subgraph of the union of at most two branches of the star, from (x_b, y_b) to (x_t, y_t), and there is a subwalk (w') of w which has two vertices of degree one in ∂R but no edge in ∂R. $\partial w'$ is properly embedded in ∂R and $R-w'$ is not connected. Hence there are at least two branches of the star, each of which must lie in a component of $R-w'$ (though both may be in the same component). By arguments analogous to those given for the polygon case, both of these lie in a slit of width $L-1$ and we have the inequality

$$s_n(4, L) \leqslant c_n(L)^2 c_n(L-1)^2 \tag{11}$$

so that

$$\limsup_{n\to\infty} (4n)^{-1} \log s_n(4, L) \leqslant \tfrac{1}{2}(\kappa(L)+\kappa(L-1)) < \kappa(L). \tag{12}$$

Therefore, provided that $\kappa(4, L)$ exists, it is strictly less than $\kappa(L)$.

The corresponding result for a 3-star is

$$\limsup_{n\to\infty} (3n)^{-1} \log s_n(3, L) \leqslant \tfrac{1}{3}\kappa(L-1)+\tfrac{2}{3}\kappa(L) < \kappa(L). \tag{13}$$

Using the approach of Chee and Whittington (1987) it is easy to establish corresponding lower bounds. A subset of the 3-stars can be obtained by concatenating an unfolded walk with n edges and a polygon with $2(n-L)$ edges, using a rectangular 'pad' of $2L+2$ edges, similar to that shown in figure 1. The resulting graph is a tadpole with $2n+2$ edges in the circuit and n edges in the tail. We now delete two edges from the circuit to give a uniform 3-star. This construction establishes that

$$\liminf_{n\to\infty} (3n)^{-1} \log s_n(3, L) \geqslant \tfrac{1}{3}\kappa(L)+\tfrac{2}{3}\kappa_0(L). \tag{14}$$

A corresponding construction concatenating a pair of polygons gives

$$\liminf_{n\to\infty} (4n)^{-1} \log s_n(4, L) \geqslant \kappa_0(L). \tag{15}$$

These bounds are compared to the numerical estimates of $\kappa(3, L)$ and $\kappa(4, L)$ obtained by Chee and Whittington (1987) in table 1. The numerical values of the bounds were evaluated using results for $\kappa(L)$ and $\kappa_0(L)$ from a transfer matrix calculation by Klein (1980). For $f=3$ the lower bound at $L=3$ is greater than the numerical estimate. The error bound quoted for the numerical estimate is only approximate and hence, in this instance, presumably too small. At least for small L the lower bound for $f=3$ is remarkably close to the numerical estimate. It is tempting to conjecture that this bound is the best possible and additional numerical results for larger values of L would be informative.

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Table 1. Numerical estimates and bounds for $\kappa(3, L)$ and $\kappa(4, K)$.

	$f=3$			$f=4$		
L	Lower bound	Numerical estimate	Upper bound	Lower bound	Numerical estimate	Upper bound
1	0.1604	0.1604	0.3208	—	—	—
2	0.4474	0.44 ± 0.01	0.5932	0.3466	0.36 ± 0.01	0.5652
3	0.5919	0.57 ± 0.01	0.707	0.5199	0.55 ± 0.01	0.69255
4	0.6775	0.68 ± 0.01	0.7706	0.6222	—	0.7620
5	0.7337	—	0.8109	0.6893	—	0.8052

References

Chee M N and Whittington S G 1987 *J. Phys. A: Math. Gen.* **20** 4915
Daoud M and de Gennes P G 1977 *J. Physique* **38** 85
Hammersley J M 1962 *Proc. Camb. Phil. Soc.* **58** 235
Hammersley J M and Whittington S G 1985 *J. Phys. A: Math. Gen.* **18** 101
Klein D J 1980 *J. Stat. Phys.* **23** 561
Stillwell J 1980 *Classical Topology and Combinatorial Group Theory* (Berlin: Springer)
Wall F T and Klein D J 1979 *Proc. Natl Acad. Sci. USA* **76** 1529
Wall F T, Seitz W A, Chin J C and Mandel F 1977 *J. Chem. Phys.* **67** 434
Whittington S G 1983 *J. Stat. Phys.* **30** 449
Wilker J B and Whittington S G 1979 *J. Phys. A: Math. Gen.* **12** L245
Wilkinson M K, Gaunt D S, Lipson J E G and Whittington S G 1986 *J. Phys. A: Math. Gen.* **19** 789