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Two-dimensional lattice embeddings of connected graphs of cyclomatic index two

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Abstract. This paper is concerned with the numbers of figure eights, dumbells and theta graphs, weakly embeddable in a two-dimensional lattice. We show rigorously that, for the square lattice, the dominant limiting behaviour of the numbers of dumbells and theta graphs is the same as the limiting behaviour of the number of self-avoiding walks and that the total number of figure eights is less than or equal to the number of rooted polygons. We present numerical data to suggest that this bound may be best possible. Estimates of critical exponents for dumbells and theta graphs are also obtained.

1. Introduction

Exact enumeration work on the number of self-avoiding walks has been influenced in an important way by a counting theorem, due to Sykes (1961), which relates the numbers of self-avoiding walks, polygons, figure eights, dumbells and theta graphs. Hammersley's work (Hammersley and Morton 1954, Hammersley 1961) on the limiting behaviour of polygons and self-avoiding walks, has been extended to include tadpoles (Whittington *et al* 1975) and figure eights (Whittington *et al* 1977). However, no rigorous results have appeared on the numbers of theta graphs or dumbells. Apart from their importance in Sykes' counting theorem, the numbers of these graphs are of interest both in that they contribute to expansions of the Ising model and in view of their influence on the general question of the effects of various kinds of constraints on the behaviour of self-avoiding walks.

In this paper we present results on all the closed connected graphs of cyclomatic index two, i.e. figure eights, dumbells and theta graphs. In § 2 we show (rigorously) that there exist limits for dumbells and theta graphs, equal to the connective constant for self-avoiding walks, while in § 3 we obtain an upper bound on the total number of figure eights, weakly embeddable in the square lattice. Section 4 is concerned with some restrictions on the generating functions of these graphs which arise from their interrelation through Sykes' counting theorem. In § 5 we analyse some exact enumeration data to estimate critical exponents for these graphs, while § 6 comprises a discussion and conclusion.

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2. Limiting behaviour of the numbers of dumbells and theta graphs on the square lattice

In this section we discuss the existence of limits for the numbers of dumbells and theta graphs on the square lattice which establish that the dominant term in their asymptotic behaviour is the same as for self-avoiding walks.

We first define some notation concerning the numbers of undirected, unrooted graphs. Let the numbers of simple chains (undirected self-avoiding walks) and polygons, having n edges, weakly embeddable in the square lattice, per site of the lattice, be $(n)_c$ and $(n)_o$. Hammersley (1961) has established that

$$\lim_{n\to\infty} n^{-1} \ln (n)_c = \lim_{n\to\infty} n^{-1} \ln(n)_o \equiv \ln \mu \tag{2.1}$$

where μ is the 'effective coordination number' of the lattice, that is, the exponential of the connective constant, Let the corresponding number of theta graphs having l, m and n edges in the three chains joining the two vertices of degree three be $(l, m, n)_\theta$ and let the number of dumbells with l edges in the simple chain joining the vertices of degree three and m and n edges in the two circuits, be $(n, l, m)_{o\text{—}o}$. In addition, define the numbers of theta graphs and dumbells with a total of n edges as $(n)_t$ and $(n)_d$ respectively.

The top (bottom) vertex of a graph will be defined to be the rightmost (leftmost) vertex in the top (bottom) row of vertices, while the top (bottom) edge joins the top (bottom) vertex to the vertex on its immediate left (right). Consider each polygon with $n-3$ edges. To the top edge add three edges to form a $(n-4, 1, 3)$ theta graph (see figure 1). Each polygon gives rise to a unique theta graph so that

$$(n-4, 1, 3)_\theta \geq (n-3)_o \tag{2.2}$$

and since

$$(n)_t \geq (n-4, 1, 3)_\theta \tag{2.3}$$

it follows that

$$\liminf_{n\to\infty} n^{-1} \ln (n)_t \geq \ln \mu\dagger. \tag{2.4}$$

To obtain an upper bound, for each (n, l, m) theta graph, delete an edge from each of two of the chains to form a simple chain with two less edges (see figure 2). Since each

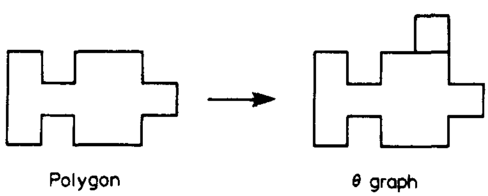

Figure 1. Transformation of a $(n-3)$-edge polygon to a $(n-4, 1, 3)$ theta graph, as described above (2.2).

† A slightly stronger version of this result has been proved by D S K Ng and J B Wilker (1977, private communication).

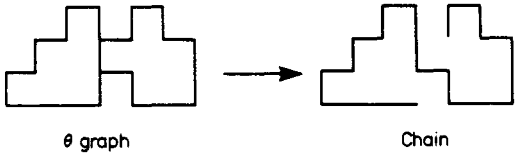

Figure 2. Transformation of an (n, l, m) theta graph to a $(n+l+m-2)$-edge chain, as described above (2.5).

theta graph gives a distinct simple chain we have

$$(n, l, m)_\theta \leq (n+l+m-2)_c. \tag{2.5}$$

From (2.1), (2.4) and (2.5) we have

$$\lim_{n\to\infty} n^{-1} \ln (n)_t = \ln \mu. \tag{2.6}$$

To establish the existence of the corresponding limit for dumbells we first consider the subset of n-edge simple chains with top and bottom vertices of degree one. Let there be $(n)_{c'}$ of these. Clearly

$$(n)_{c'} \leq (n)_c. \tag{2.7}$$

Each polygon can be considered as a pair of c′-chains which are mutually avoiding except that they meet at their top and bottom vertices. Hence

$$(n)_o \leq \sum_m (n-m)_{c'}(m)_{c'}. \tag{2.8}$$

If two c′-chains are joined so that the bottom vertex of one coincides with the top vertex of the other, the result is a new c′-chain so that

$$(n-m)_{c'}(m)_{c'} \leq (n)_{c'}. \tag{2.9}$$

From (2.7), (2.8) and (2.9) we have

$$\sup_{n>0} n^{-1} \ln(n)_{c'} = \lim_{n\to\infty} n^{-1} \ln(n)_{c'} = \ln \mu. \tag{2.10}$$

Now consider joining the top vertex of an m-gon to the bottom vertex of an l-edge c′-chain and the top vertex of the c′-chain to the bottom vertex of an n-gon. The result is a dumbell and each triple of two polygons and a c′-chain gives a distinct dumbell so that

$$(n)_o(l)_{c'}(m)_o \leq (n, l, m)_{o\text{—}o}. \tag{2.11}$$

To obtain an upper bound delete an edge from each circuit, adjacent to a vertex of degree three to give a simple chain, yielding

$$(n, l, m)_{o\text{—}o} \leq (n+l+m-2)_c. \tag{2.12}$$

From (2.1), (2.11) and (2.12) we have

$$\lim_{n+l+m\to\infty} (n+l+m)^{-1} \ln(n, l, m)_{o\text{—}o} = \ln \mu \tag{2.13}$$

and, since

$$(n)_d = \sum_{l,m} (n-l-m, l, m)_{\text{O——O}} \tag{2.14}$$

then

$$\lim_{n\to\infty} n^{-1} \ln(n)_d = \ln \mu. \tag{2.15}$$

These arguments can be extended to other lattices with no great difficulty.

3. An upper bound on the total number of figure eights on the square lattice

In this section we shall show that the numbers of n-edge figure eights, weakly embeddable in the square lattice, $(n)_E$ is bounded above by the number of rooted polygons. Each figure eight has an articulation point, O, joined to four other adjacent vertices which we label (clockwise) N, E, S and W, in an obvious notation. We shall say that the figure eight belongs to class A if vertices N and E are connected by a path not passing through O, and to class B otherwise. It is clear that class B figure eights have a path joining vertices N and W without passing through O. We explicitly consider only class A figure eights but an exactly analogous argument can be constructed for those in class B.

Consider a particular class A figure eight, e, say which is rooted at O. We define an operation T_A on the edges ON and OW. The edges ON and OW are removed and replaced by edges O'N and O'W as shown in figure 3. If O' is a new vertex, not already present in e, then the graph T_Ae is a rooted n-edge polygon. Alternatively O' may already be a vertex of e. In this case T_Ae may contain a double edge, i.e. two vertices joined by two different edges. If these two edges are deleted the resulting graph is a rooted $(n-2)$-edge polygon. The only other possibility is that O' already exists in e but T_Ae contains no double edge; then T_Ae is a *class A* figure eight, with articulation point O' and root O.

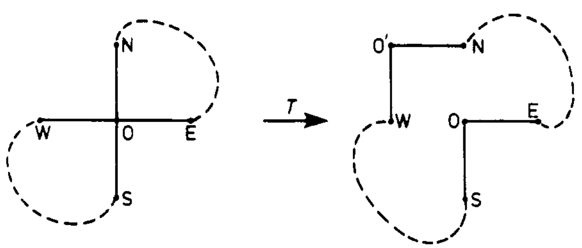

Figure 3. Transformation of a class A figure eight by moving vertices ON and OW as shown.

For each class A figure eight we successively apply the transformation T_A until a rooted n-gon or $(n-2)$-gon is produced. It is clear that, if figure eights are produced, the further application of T_A will eventually produce a polygon since, at each transformation, the root remains invariant and the articulation point moves through a lattice diagonal in a north-westerly direction and would otherwise eventually leave the original figure eight. Moreover, the (rooted) polygon eventually produced from each original figure eight is unique since the final vertex O′, when the polygon is produced, is on a line at 45° to WO (i.e. running in a north-westerly direction from O). Since each figure eight is eventually converted either into an n-gon or an $(n-2)$-gon we have

$$(n)_e \leq n(n)_0 + (n-2)(n-2)_0 \leq 2n(n)_0 \tag{3.1}$$

which is a significant improvement on the previous best upper bound (Whittington *et al* 1977).

4. Restrictions on the critical exponents

In this section we derive certain restrictions on the generating functions of chains, polygons, dumbells, theta graphs and figure eights. These follow, in the main, from the counting theorem introduced by Sykes (1961), which may be stated as follows:

$$(n+1)_c - 2(q-1)(n)_c + (q-1)^2(n-1)_c$$
$$= n(n)_0 - (n+1)(n+1)_0 + 4(n+1)_d + 4(n+1)_e + 6(n+1)_\theta \tag{4.1}$$

where q is the coordination number of the underlying lattice. Multiplying (4.1) by x^n, where x is a dummy variable, and summing $\Sigma_{n+1=0}^{\infty}$, we obtain

$$[1-(q-1)x]^2 C(x) = x(x-1)P'(x) + 4D(x) + 6\theta(x) + 4E(x) \tag{4.2}$$

where

$$\sum_{n=0}^{\infty} (n)_c x^n = C(x), \qquad ((-1)_c = (-2)_c = 0);$$
$$\sum_{n=0}^{\infty} (n)_0 x^n = P(x), \qquad ((-1)_0 = 0); \tag{4.3}$$
$$\sum_{n=0}^{\infty} (n)_d x^n = D(x); \qquad \sum_{n=0}^{\infty} (n)_e x^n = E(x); \qquad \sum_{n=0}^{\infty} (n)_\theta x^n = \theta(x).$$

From previous results, both those proved here and elsewhere, it is known that the generating functions defined in (4.3) are all non-analytic at the same point $x = 1/\mu$, where μ is the 'effective coordination number'. If asymptotically

$$\begin{aligned} C(x) &\sim A(1-\mu x)^{-\gamma} \\ P(x) &\sim B(1-\mu x)^{1-\alpha} \\ D(x) &\sim C(1-\mu x)^{-\beta} \\ \theta(x) &\sim D(1-\mu x)^{-\delta} \\ E(x) &\sim E(1-\mu x)^{-\epsilon} \end{aligned} \tag{4.4}$$

it immediately follows from (4.2) and (4.3) that

$$\gamma \leq \max\{\alpha, \beta, \delta, \epsilon\} \tag{4.5}$$

provided that $\mu \neq 1$ and $\mu \neq q-1$. These last conditions are satisfied for all non-trivial lattices. That is, at least one of the generating functions $P(x)$, $D(x)$, $\theta(x)$ and $E(x)$

must diverge with the same exponent as the chain generating function $C(x)$. The inequality arises from the possibility of cancellation occurring between two terms on the right-hand side of equation (4.2).

For any regular lattice we have studied, the coefficients of all non-zero generating functions are monotone increasing functions of n, for sufficiently large n. Therefore the amplitudes of these generating functions are all positive, which precludes any cancellation. Thus for all non-pathological lattices, it is immediately clear that the inequality in (4.5) may be replaced by an equality.

Further, for any lattice with coordination number 3, we can say that at least one of the generating functions $P(x)$, $D(x)$ and $\theta(x)$ must diverge with the same exponent as $C(x)$, since $E(x)=0$ for these lattices.

5. Numerical results

The polygon generating function has been extensively studied by several authors, and it is generally accepted that $\alpha \approx -0{\cdot}5$ in two dimensions. Similarly, the chain generating function has also been extensively investigated (Sykes *et al* 1972, Watts 1975) and the generally accepted result is $\gamma \approx \frac{4}{3}$ for all two-dimensional lattices.

For other generating functions there are no corresponding results in the literature, and we have studied these here. For the dumbell generating function we have terms to order x^{17} on the triangular lattice. The available coefficients have been studied by the usual techniques of series analysis (Gaunt and Guttmann 1974) and yield consistent results. Assuming that, close to the singularity, the generating function can be represented as $\sum_{n=0}^{\infty} (n)_{\rm d} x^n \sim C(1-\mu x)^{-\beta}$ it follows that

$$r_n = \frac{(n)_{\rm d}}{(n-1)_{\rm d}} \sim \mu\left[1 + \frac{\beta - 1}{n} + \mathrm{O}\left(\frac{1}{n^2}\right)\right]. \tag{5.1}$$

So that $t_n = (r_n/\mu - 1)n$ should approach $\beta - 1$ as $n \to \infty$. The rate of convergence of the sequence $\{t_n\}$ is typically hastened by forming linear and quadratic extrapolants of the sequence $\{t_n\}$—corresponding to the sequences $\{\delta_n\}$ and $\{\epsilon_n\}$, where $\delta_n = nt_n - (n-1)t_{n-1}$ and $\epsilon_n = n^2\delta_n^a - (n-1)^2\delta_{n-1}/(2n-1)$. In table 1 we show the sequences for the triangular lattice dumbell generating functions. From this table we conclude that $\beta - 1 < 0{\cdot}36$ and that $\beta - 1 \approx 0{\cdot}30 \pm 0{\cdot}05$, so that $\beta = 1{\cdot}30 \pm 0{\cdot}05$.

Table 1. Ratio method analysis of $D(x)$ for the triangular lattice ($\mu = 4{\cdot}1517$).

n	$r_n = \frac{(n+7)_{\rm d}}{(n+6)_{\rm d}}$	$t_n = n(r_n/\mu - 1)$	$\delta_n = nt_n - (n-1)t_{n-1}$	$\epsilon_n = \frac{n^2\delta_n - (n-1)^2\delta_{n-1}}{2n-1}$
2	5·7545	0·7721	2·514	
3	5·1137	0·6952	0·541	−1·037
4	4·8276	0·6512	0·519	0·491
5	4·6605	0·6127	0·459	0·351
6	4·5565	0·5850	0·447	0·420
7	4·4849	0·5619	0·423	0·356
8	4·4332	0·5425	0·407	0·355
9	4·3945	0·5262	0·397	0·358
10	4·3643	0·5122	0·385	0·338

Since $\gamma \approx \frac{4}{3}$, it appears plausible that $\beta = \gamma$. Subsequent analysis supports this conclusion. For the (loose-packed) square lattice, the corresponding results are not as regular as those for the triangular lattice, but are entirely consistent with the above numerical estimate of β.

From the rigorous inequalities on the number of figure eights derived in § 3 and elsewhere (Whittington *et al* 1972), $(n-4)_0 \leq (n)_e \leq 2n(n)_0$, it follows from the definitions (4.4) that $\alpha \geq \epsilon \geq \alpha - 1$. From the numerical evidence cited earlier from α, these inequalities yield

$$0{\cdot}5 \leq -\epsilon \leq 1{\cdot}5 \tag{5.2}$$

in two dimensions. Thus we see immediately that neither the polygon nor the figure eight generating functions have an exponent remotely near that of the chain generating function. Similar analyses to those performed on the dumbell generating function have been applied to the figure eight generating function. We show just one set of results, the linear and quadratic extrapolents of the sequence $\{t_n\}$, defined immediately following (5.1), for the triangular lattice figure eight generating function. These results are shown in table 2, from which we conclude that $\epsilon = -0{\cdot}45 \pm 0{\cdot}05$. Combining this with (5.2) suggests $\epsilon = -0{\cdot}5$ exactly. This result implies that our upper bound $(n)_e \leq 2n(n)_0$ is best possible. As observed for the dumbell generating function, the square lattice results are less regular than, but consistent with, the triangular lattice estimate.

Table 2. Ratio method analysis of $E(x)$ for the triangular lattice ($\mu = 4{\cdot}1517$).

n	$r_n = \frac{(n+5)_e}{(n+4)_e}$	$t_n = n(r_n/\mu - 1)$	$\delta_n = nt_n - (n-1)t_{n-1}$	$\epsilon_n = \frac{n^2\delta_n - (n-1)^2\delta_{n-1}}{2n-1}$
3	3·1333	−0·7359	−1·098	−1·831
4	3·2766	−0·8431	−1·165	−1·251
5	3·3506	−0·9647	−1·451	−1·960
6	3·4331	−1·0384	−1·407	−1·307
7	3·5010	−1·0971	−1·449	−1·566
8	3·5559	−1·1481	−1·505	−1·687
9	3·6052	−1·1847	−1·478	−1·374
10	3·6472	−1·2151	−1·489	−1·538
11	3·6838	−1·2396	−1·484	−1·462
12	3·7159	−1·2592	−1·478	−1·446

For theta graphs our results are less precise. The results of a standard ratio method analysis for the triangular lattice are shown in table 3. These are not converging as well as the corresponding results for the other classes of graphs considered, but we can estimate $(n)_\theta \sim n^{-\nu}\mu^n$ where ν is between 1·2 and 1·5. Forming Padé approximants to

$$(x - x_c)\frac{\mathrm{d}}{\mathrm{d}x} \ln \theta(x)|_{x=x_c}$$

gives slightly better converged results (not shown), suggesting $\nu \approx 1{\cdot}35$. We therefore summarise these results as $\nu = 1{\cdot}35 \pm 0{\cdot}15$, from which it follows that $\delta =$

Table 3. Ratio method analysis of $\theta(x)$ for the triangular lattice ($\mu = 4{\cdot}1517$).

n	$r_n = (n+5)_\theta/(n+4)_\theta$	$t_n = n(r_n/\mu - 1)$	$\delta_n = nt_n - (n-1)t_{n-1}$
3	3·9286	−0·1612	0·144
4	3·6909	−0·4440	−1·292
5	3·7488	−0·4853	−0·650
6	3·7898	−0·5231	−0·712
7	3·7868	−0·6153	−1·169
8	3·8138	−0·6510	−0·901
9	3·8278	−0·7022	−1·112
10	3·8427	−0·7442	−1·121
11	3·8568	−0·7813	−1·153
12	3·8703	−0·8134	−1·166

$-0{\cdot}35 \pm 0{\cdot}15$. We have also studied the exponent δ for the square lattice, for which we obtain results which are consistent with those obtained for the triangular lattice.

In summary, we find that $P'(x)$, $\theta(x)$ and $E(x)$ display cusp-like singularities as $x \to 1/\mu$. Only $D(x)$ displays a divergent singularity. It then follows from (4.5) that $\gamma = \beta$. This is supported by our numerical estimates of β, which are close to the value $\frac{4}{3}$, which is a generally accepted mnemonic for γ.

As part of our numerical investigation of those graphs which contribute to the chain generating function, we are able to confirm numerically a widely held belief concerning the presence of a singularity on the negative real axis for the chain generating function on loose-packed lattices. This belief is that the chain generating function has a singularity at $x = -1/\mu$ if it has a singularity at $x = 1/\mu$. This seems to have first appeared in print in Guttmann (1972). It is clear that the polygon and figure eight generating functions, being even functions of x, are singular at $x = -1/\mu$ if they are singular at $x = 1/\mu$. Thus for the square lattice our earlier investigations suggest

$$P(x) \sim (1+\mu x)^{1\frac{1}{2}}, \qquad E(x) \sim (1+\mu x)^{\frac{1}{2}}$$

as $x \to -1/\mu$. This observation coupled with Sykes' chain counting theorem (4.2) is not sufficient evidence to prove the existence of a singularity at $x = -1/\mu$, since it is *possible* that a singularity in the theta graph and/or dumbell generating function precisely cancels the singularities in the polygon and figure eight generating functions. Our numerical studies of the dumbell and theta graph generating functions by Padé approximants (we formed Padé approximants to $(x - x_c)\mathrm{d}(\ln f(x))/\mathrm{d}x$ with $x_c = -1/\mu$ and $f(x) = D(x)$ and $\theta(x)$) and also a study of the generating functions by standard ratio and Neville table methods, suggest that any non-analyticity at $x = -1/\mu$ in those generating functions is extremely weak. More precisely, the available evidence suggests that any singularity at $x = -1/\mu$ is considerably weaker than the square root cusp singularity of both the figure eight generating functions and the derivative of the polygon generating function.

Thus we conclude that, for the square lattice, the figure eight generating function and polygon generating function jointly dominate the chain generating function at $x = -1/\mu$, from which it follows that $C(x)$ has a singularity at $x = -1/\mu$ corresponding to the singularity at $x = 1/\mu$. This is, of course, the analogue of the antiferromagnetic singularity of the Ising model, which is known to be characteristic of loose-packed lattices.

6. Discussion

The primary rigorous results obtained here are the existence and identification of the limits (2.6) and (2.15) for theta graphs and dumbells and the upper bound, (3.1), on the number of figure eights. The interesting question which is raised by the first two results is: for what class of graphs is the corresponding limit equal to the self-avoiding walk limit? That is, if we classify graphs by topologies, for which topologies is the connective constant invariant? Assuming plausible forms for the asymptotic dependence of the generating functions we have also obtained several exponent inequalities (e.g. (4.5)) and that concerning figure eights and polygons seems likely to be best possible.

The numerical estimates of the exponents are the first which have been obtained for dumbells and theta graphs and while the theta graph estimates leave much to be desired in the way of accuracy, the estimates for figure eights and dumbells are very satisfactory.

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