Lattice trees with a restricted number of branch points

1983 J. Phys. A: Math. Gen. 16 3119

(http://iopscience.iop.org/0305-4470/16/13/036)

J. Phys. A: Math. Gen. 16 (1983) 3119–3125. Printed in Great Britain

Lattice trees with a restricted number of branch points

J E G Lipson and S G Whittington

Department of Chemistry, University of Toronto, Toronto, Ontario, Canada

Received 14 March 1983

Abstract. We investigate the asymptotic behaviour of the number of trees having n vertices, weakly embeddable in the d-dimensional hypercubic lattice, with restrictions on the number (n^+) of vertices with degree greater than two. We show rigorously that if $n^+ = o(n/\log n)$ the growth constant is equal to the corresponding quantity for self-avoiding walks. For n^+ increasing linearly with n we show that the growth constant still exists and present arguments indicating that it is strictly greater than that for self-avoiding walks.

1. Introduction

The configurational behaviour of linear polymers, in dilute solution in a good solvent, has been modelled using the statistics of self-avoiding walks on regular lattices (Barber and Ninham 1970). In spite of the apparent simplicity of this model there are few rigorous results. If the number, per lattice site, of self-avoiding walks with n edges is c_n then Hammersley and Morton (1954) have shown that

$$0 < \lim_{n\to\infty} n^{-1} \log c_n = \inf_{n>0} n^{-1} \log c_n \equiv \log \mu < \infty \tag{1.1}$$

where the value of μ, the 'effective coordination number', depends on the detailed structure of the lattice. In the polymer problem $\log \mu$ plays the role of the limiting entropy per monomer.

In a similar way branched polymers have been modelled as lattice animals (Lubensky and Isaacson 1979). Several groups have investigated the importance of cycles in determining the lattice statistics of these graphs (Lubensky and Isaacson 1979, Redner 1979, Family 1980, Whittington *et al* 1983) and it has been shown that the growth constant (analogous to μ in (1.1)) exists for animals (Klarner 1967) and for animals with a restricted number of cycles (Whittington *et al* 1983). A case of particular interest is when no cycles are allowed (a tree), and there is evidence that critical exponents are the same for trees and for unrestricted animals (Seitz and Klein 1981, Duarte and Ruskin 1981, Gaunt *et al* 1982, Lubensky and Isaacson 1979).

Simple chains (undirected self-avoiding walks) are trees with no branch points. In this paper we investigate the behaviour of the growth constant as we allow increasing numbers of branch points but no cycles. Defining $t(n; n_3, n_4, \ldots, n_{2d})$ to be the number, per lattice site, of trees with n vertices, n_3 of degree 3, n_4 of degree 4, etc, weakly embeddable in the d-dimensional hypercubic lattice, we show that

$$\lim_{n\to\infty} n^{-1} \log t(n; n_3, n_4, \ldots, n_{2d}) = \log \mu \tag{1.2}$$

when n_3, $n_4, \ldots$ are fixed, and with μ given by (1.1). This implies that the limiting entropy per monomer is independent of the number of branch points, provided that this number remains finite as n goes to infinity. It is interesting to consider the behaviour of the corresponding limit when $n_3, n_4, \ldots$ are allowed to increase with n. We show that the value of the limit remains unchanged provided that $n_k = o(n/\log n)$ for all k greater than two.

We also consider the situation in which $n_3, n_4, \ldots, n_{2d}$ are not fixed but subject to the restriction $\Sigma_{k>2} n_k \leq \alpha n$ for $\alpha > 0$. We show that the corresponding limit exists and is *strictly* greater than $\log \mu$, and less than or equal to $\log \lambda_0$, where λ_0 is the growth constant for weakly embeddable trees (Klein 1981).

Previous work on valence restrictions has been of two types. Daoud and Cotton (1982) have considered star-shaped polymers with excluded volume, which are trees having a single vertex of degree s, s vertices of unit degree, and all other vertices of degree 2. Using scaling arguments they investigated the dimensions of these polymers. Although there is an extensive literature on star-shaped polymers (see e.g. Mansfield and Stockmayer 1980) excluded volume effects have been largely ignored.

Gaunt *et al* (1980) have studied lattice animals with the restriction that no vertex has valence greater than v. They found that the growth constant depended on v but that the critical exponent was independent of v for v greater than two; the case $v = 2$ corresponds to no branch points.

2. Existence of the growth constant for trees with valence restrictions

In this section we shall show rigorously that the growth constant for the set of trees, weakly embeddable in a simple hypercubic lattice and having a fixed number of vertices with degree between three and $2d$, is equal to that for self-avoiding walks. This proof can be extended to other types of lattices.

The vertices of a d-dimensional hypercubic lattice are the integer points in a d-dimensional Euclidean space with coordinates $(x_1, x_2, \ldots, x_d)$. The edges of the lattice join vertices which differ by unity in a single coordinate.

Suppose the tree under consideration consists of a set S_0 of vertices. The top (bottom) vertex is defined as follows. First, construct the subset $S_1 \subset S_0$ such that the coordinate x_1 of every vertex in S_1 has the maximum (minimum) value over all coordinates in S_0. Then recursively construct $S_k \subset S_{k-1}$ such that the coordinate x_k of every vertex in S_k has the maximum (minimum) value over all vertices in S_{k-1}. Continue this process until the jth subset (S_j) has been constructed where j is the smallest integer such that S_j has only one member. We shall call the vertex in S_j the top (bottom) vertex v_t (v_b) of S_0. v_t is joined to one or more other vertices, the coordinates of each differing from those of v_t by unity in exactly one coordinate. The top edge, e_t, is that which joins v_t to the vertex differing from it in the coordinate of highest number; this vertex is labelled v_e.

We are interested in the set of trees $T(n; n_3, n_4, \ldots, n_{2d})$ each member having $m = n - 1$ edges where n is the total number of vertices, n_3 being of degree 3, n_4 of degree 4 and so on, up to the coordination number of the lattice and let the cardinality (per lattice site) of this set be $t(n; n_3, n_4, \ldots, n_{2d})$. (A vertex of degree i has i incident edges.) The number n_1 of vertices of degree 1 is determined by the numbers of vertices with degree $3, 4, \ldots,$ as

$$n_1 = 2 + n_3 + 2n_4 + \ldots + (2d-2)n_{2d} \tag{2.1}$$

a result which follows from Euler's theorem applied to trees. Knowing n, n_3, n_4, and so on, therefore, determines both n_1 and n_2.

Consider a tree $g \in T(n; n_3, n_4, \ldots, n_k, \ldots, n_{2d})$. We now construct from each such graph, g, a tree with an additional vertex of degree k. Let the top vertex of g be v_t, with coordinates $(x_1^t, \ldots, x_d^t)$. Define the unit vectors $\hat{u}_1 = (1, 0, 0, \ldots, 0)$, $\hat{u}_2 = (0, 1, 0, \ldots, 0), \ldots, \hat{u}_d = (0, 0, 0, \ldots, 1)$. If v_t is of unit degree and $k \leq d+1$, add the vertices $v_t' = v_t + \hat{u}_1$, $v_1 = v_t' + \hat{u}_1$, $v_2 = v_t' + \hat{u}_2, \ldots, v_{k-1} = v_t' + \hat{u}_{k-1}$, and the edges $(v_t - v_t')$, $(v_t' - v_1)$, $(v_t' - v_2), \ldots, (v_t' - v_{k-1})$. If $k > d+1$, add the vertices v_t', $v_1, v_2, \ldots, v_d$ together with the additional vertices $v_{d+1} = v_t' - \hat{u}_2, \ldots, v_{k-1} = v_t' - \hat{u}_{k-d}$, and the edges $(v_t - v_t'), (v_t' - v_1), \ldots, (v_t' - v_d), \ldots, (v_t' - v_{k-1})$. The resulting graph is a tree with $(m+k)$ edges, $n_k + 1$ vertices of degree k, $n_2 + 1$ of degree 2 and $n_1 + k - 2$ of degree 1, the numbers of vertices of all other degrees being unchanged.

If v_t is of degree greater than one, we construct a new graph as follows: delete the top edge e_t, adding the vertices $v_t' = v_t + \hat{u}_1$ and $v_e' = v_e + \hat{u}_1$, and the edges $(v_t - v_t')$, $(v_e - v_e')$ and $(v_e' - v_t')$. The resulting graph is connected and is still a tree. Now add $k-2$ additional vertices (and appropriate edges) in a manner similar to that described above (i.e. for the case when v_t is of unit degree) so that v_t' in the resulting graph is of degree k (see figure 1 for an example in two dimensions). This construction yields, as before, a tree with $m+k$ edges, $n_k + 1$ vertices of degree k, $n_2 + 1$ of degree 2 and $n_1 + k - 2$ of degree 1, the numbers of vertices of all other degrees being unchanged.

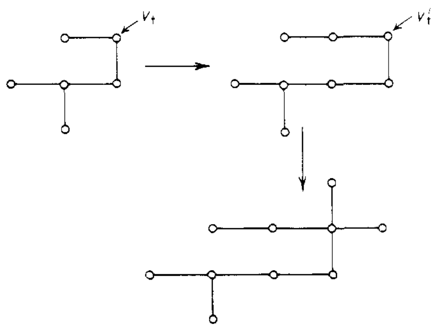

Figure 1. Construction of a tree with an additional vertex of degree $k = 4$, for the square lattice.

Therefore, for all such trees with m edges and n_k vertices of degree k we can uniquely construct a new tree with $m+k$ edges and $n_k + 1$ vertices of degree k. Since this defines an injection from $T(n; n_3, n_4, \ldots, n_k, \ldots, n_{2d})$ to $T(n+k; n_3, \ldots, n_k + 1, \ldots, n_{2d})$, we have the inequality

$$t(n+k; n_3, \ldots, n_k + 1, \ldots, n_{2d}) \geq t(n; n_3, \ldots, n_k, \ldots, n_{2d}). \tag{2.2}$$

Setting $n_3 = n_4 = \ldots = n_{2d} = 0$ the resulting graphs are simple chains, so that (Hammersley and Morton 1954)

$$0 < \lim_{n\to\infty} n^{-1} \log t(n; 0, 0, \ldots, 0) = \log \mu < \infty. \tag{2.3}$$

Then by induction on $n_3, n_4, \ldots$ etc we have, using (2.2) and (2.3),

$$\liminf_{n\to\infty} n^{-1} \log t(n; n_3, n_4, \ldots, n_{2d}) \geq \log \mu. \tag{2.4}$$

To obtain an upper bound on the number of such trees we consider a tree with n_3 vertices of degree 3, n_4 of degree 4, etc. This tree will contain N simple chains, where

$$N=(2d-1)n_{2d}+(2d-2)n_{2d-1}+\ldots+2n_3+1. \tag{2.5}$$

To construct the number of embeddings of these trees, we first require the number of (homeomorphically irreducible) trees on n_1 vertices of degree 1, n_3 of degree 3, n_4 of degree 4, ..., n_{2d} of degree $2d$. The total number of vertices in this tree is

$$n^*=n-n_2 \tag{2.6}$$

and an upper bound on the number of ways of connecting these n^* vertices to form such a tree is given by a result of Cayley's (1889) that the number of trees on n^* labelled vertices is $n^{*(n^*-2)}$.

The edges in this tree are now replaced by N simple chains having a total of m edges. We need to count the number of ways of distributing the edges among these chains, such that each chain has between one and $m-(N-1)$ edges, and then consider the number of ways in which these chains can be embedded in the d-dimensional lattice. From equation (1.1) the number of embeddings of a simple chain of m edges is $\exp[mk+o(m)]$, where $k=\log\mu$. Using the above it is now possible to bound the number of trees which can be constructed from the given set of vertices and edges as

$$t(n;n_3,n_4,\ldots,n_{2d})\leqslant n^{*(n^*-2)}\sum_{m_1}\sum_{m_2}\ldots\sum_{m_N}\exp[m_1k+o(m_1)+m_2k+o(m_2)+\ldots] \tag{2.7}$$

where m_l is the number of edges in the lth simple chain and the sums are taken over $\{m_l\}$ subject to the conditions

$$m_l>0 \qquad \sum_{l=1}^{N}m_l\equiv m=n-1. \tag{2.8}$$

The sum on the right-hand side of (2.7) includes configurations with self-avoiding but not mutually-avoiding chains.

From (2.7), performing the summations, and noticing that $m_l\leqslant m$ for all l, gives

$$t(n;n_3,n_4,\ldots,n_{2d})\leqslant n^{*(n^*-2)}m^N\exp[mk+o(m)] \tag{2.9}$$

and from (2.5), (2.6) and (2.9)

$$t(n;n_3,n_4,\ldots,n_{2d})\leqslant\exp[nk+o(n)] \tag{2.10}$$

when $n_3,n_4,\ldots,n_{2d}$ are fixed.

Then from (2.4) and (2.10)

$$\lim_{n\to\infty}n^{-1}\log t(n;n_3,n_4,\ldots,n_{2d})=k\equiv\log\mu. \tag{2.11}$$

We now investigate how rapidly $n_3,n_4,\ldots,n_{2d}$ can increase as $n\to\infty$, such that the value of the limit in (2.11) is unchanged. From (2.5) and (2.9) we obtain

$$\begin{aligned}t(n;n_3,n_4,\ldots,n_{2d})&\leqslant[2d(1+n^+)]^{2dn^+}n^{2d(1+n^+)}\exp[nk+o(n)]\\&\leqslant(2dn)^{4d(1+n^+)}\exp[nk+o(n)]\end{aligned} \tag{2.12}$$

where

$$n^+=n_3+\ldots+n_{2d}=n^*-n_1. \tag{2.13}$$

We note that

$$\limsup_{n\to\infty} n^{-1}\log t(n; n_3, n_4, \ldots, n_{2d}) \leq \log \mu \tag{2.14}$$

if

$$(2dn)^{4d(1+n^+)} = \exp[o(n)] \tag{2.15}$$

or, equivalently, if

$$n^+ = o(n/\log n). \tag{2.16}$$

In addition the arguments leading to (2.4) are valid under this restriction on n^+ so that (2.16) is a sufficient condition for the value of the limit in (2.11) to remain unchanged. In particular, the case of

$$n^+ < n^\beta \tag{2.17}$$

for $\beta < 1$ satisfies (2.16).

We now examine the situation in which n^+ can increase linearly with n, and we consider trees with the restriction

$$n^+ \leq \alpha n \tag{2.18}$$

with $\alpha > 0$. Let the number of such weakly embeddable trees be $t(n;\alpha)$, per site of the d-dimensional hypercubic lattice. We shall show that the limit $\lim_{n\to\infty} n^{-1}\log t(n;\alpha)$ exists for positive α. Assuming that the asymptotic form for $t(n;\alpha)$ is

$$t(n;\alpha) \sim n^{-\theta(\alpha)}\lambda(\alpha)^n, \tag{2.19}$$

we also show that

$$\lambda(\alpha) > \mu \tag{2.20}$$

for all positive α.

Let $T(n;\alpha)$ be the set of trees with n vertices having at most αn vertices of degree greater than two. For any pair of graphs $g \in T(n;\alpha)$ and $g' \in T(m;\alpha)$, $m \neq n$, we construct a graph $g'' \in T(n+m+q(\alpha);\alpha)$, as follows. Let v_t be the top vertex of g and let v_b be the bottom vertex of g'. Let v_t have coordinates $(x_1^t, x_2^t, \ldots, x_d^t)$ and translate g' so that the coordinates of v_b are $(x_1^t+q+1, x_2^t, x_3^t, \ldots, x_d^t)$. We now add the vertices $v_1 = (x_1^t+1, x_2^t, \ldots, x_d^t)$, $v_2 = (x_1^t+2, x_2^t, \ldots, x_d^t), \ldots, v_q = (x_1^t+q, x_2^t, \ldots, x_d^t)$ and the edges $(v_t - v_1), (v_1 - v_2), \ldots, (v_q - v_b)$. The resulting graph g'' is a tree with $n+m+q$ vertices and at most $n\alpha + m\alpha + 2$ vertices with degree greater than two. Therefore, choosing q to be the smallest integer greater than or equal to $2/\alpha$ ensures that $g'' \in T(n+m+q;\alpha)$. This construction produces a unique g'' for each pair g and g' but not all members of $T(n+m+q;\alpha)$ can be obtained in this fashion. Therefore,

$$t(n;\alpha)t(m;\alpha) \leq t(n+m+q;\alpha). \tag{2.21}$$

Since $T(n;\alpha)$ is a subset of the set of animals and the nth root of the number of animals with n vertices is bounded above (Klarner 1967), $t(n;\alpha)^{1/n}$ is bounded above. Hence (Wilker and Whittington 1979) there exists a positive constant $\lambda(\alpha)$ such that

$$\lim_{n\to\infty} n^{-1}\log t(n;\alpha) = \log\lambda(\alpha) < \infty \tag{2.22}$$

and

$$\log t(n;\alpha) \leqslant (n + q(\alpha)) \log \lambda(\alpha). \tag{2.23}$$

Assuming the expected asymptotic behaviour

$$t(n;\alpha) \sim n^{-\theta(\alpha)} \lambda(\alpha)^n \tag{2.19}$$

(2.23) implies that $\theta(\alpha) \geqslant 0$.

We now wish to argue that

$$\lambda_0 \geqslant \lambda(\alpha) > \mu \tag{2.24}$$

for all $\alpha > 0$. Since (undirected) self-avoiding walks are a proper subset of $T(n;\alpha)$ which, in turn, is a subset of the set of unrestricted trees with cardinality $t(n)$ and growth constant λ_0,

$$\tfrac{1}{2}c_n < t(n;\alpha) \leqslant t(n) \tag{2.25}$$

and it follows that

$$\mu \leqslant \lambda(\alpha) \leqslant \lambda_0. \tag{2.26}$$

To show that the first inequality in (2.26) is strict we assume the contrary, that $\mu = \lambda(\alpha)$. The expected asymptotic form for c_n is

$$c_n \sim n^{\phi} \mu^n \tag{2.27}$$

with $\phi > 0$. Then (2.19), (2.25), (2.27) together with the assumption that $\mu = \lambda(\alpha)$, $\alpha > 0$, imply that $\phi \leqslant -\theta(\alpha)$. Since this is impossible, μ is strictly less than $\lambda(\alpha)$, $\alpha > 0$.

3. Discussion

We have investigated the dominant asymptotic behaviour of the number of lattice trees having restrictions on the fraction of vertices with degree greater than two. If the number (n^+) of such vertices increases as $o(n/\log n)$ then the dominant asymptotic behaviour is the same as that of self-avoiding walks.

When n^+ is, at most, a linear function of n, we have shown that the connective constant exists; with some formal assumptions on the subdominant asymptotic behaviour, this connective constant is strictly greater than the value of the corresponding limit for self-avoiding walks.

In the context of the branched polymer problem this implies that the limiting entropy per monomer of a branched polymer with a vanishingly small fraction of branch points is identical to that of a linear polymer. If the number of branch points is allowed to increase linearly with the degree of polymerisation then the limiting entropy per monomer is strictly greater than that for a linear polymer.

Acknowledgments

JEGL gratefully acknowledges financial support in the form of an Ontario Graduate Fellowship. The authors appreciate the hospitality of the Institute for Mathematics and its Applications, Minneapolis, USA, where some of this research was carried out.

References

Barber M N and Ninham B W 1970 *Random and Restricted Walks* (New York: Gordon and Breach) ch 9
Cayley A 1889 *Quart. J. Math.* **23** 376
Daoud M and Cotton J P 1982 *J. Physique* **43** 531
Duarte J A M S and Ruskin H J 1981 *J. Physique* **42** 1585
Family F 1980 *J. Phys. A: Math. Gen.* **13** L325
Gaunt D S, Martin J L, Ord G, Torrie G M and Whittington S G 1980 *J. Phys. A: Math. Gen.* **13** 1791
Gaunt D S, Sykes M F, Torrie G M and Whittington S G 1982 *J. Phys. A: Math. Gen.* **15** 3209
Hammersley J M and Morton K W 1954 *J. R. Stat. Soc.* **B16** 23
Klarner D A 1967 *Can. J. Math.* **19** 851
Klein D J 1981 *J. Chem. Phys.* **75** 5186
Lubensky T C and Isaacson J 1979 *Phys. Rev.* A **20** 2130
Mansfield M L and Stockmayer W H 1980 *Macromolecules* **13** 1713
Redner S 1979 *J. Phys. A: Math. Gen.* **12** L239
Seitz W A and Klein D J 1981 *J. Chem. Phys.* **75** 5190
Whittington S G, Torrie G M and Gaunt D S 1983 *J. Phys. A: Math. Gen.* **16** 1695
Wilker J B and Whittington S G 1979 *J. Phys. A: Math. Gen.* **12** L245