KNOTS IN GRAPHS IN SUBSETS OF Z^3

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Abstract. The probability that an embedding of a graph in Z^3 is knotted is investigated. For any given graph (embeddable in Z^3) without cut edges, it is shown that this probability approaches 1 at an exponential rate as the number of edges in the embedding goes to infinity. Furthermore, at least for a subset of these graphs, the rate at which the probability approaches 1 does not depend on the particular graph being embedded. Results analogous to these are proved to be true for embeddings of graphs in a subset of Z^3 bounded by two parallel planes (a slab).

In order to investigate the knotting probability of embeddings of graphs in a rectangular prism (an infinitely long rectangular tube in Z^3), a pattern theorem for self-avoiding polygons in a prism is proved. From this it is possible to prove that for any given eulerian graph, the probability that an embedding of the graph in a prism is knotted goes to 1 as the number of edges in the embedding goes to infinity. Then, just as for Z^3, there is at least a subset of these graphs for which the rate that this probability approaches 1 does not depend on the particular graph.

Similar results are shown to hold in cases where restrictions are placed on the number of edges per branch in a graph embedding.

Key words. knots, graph embeddings, branched polymer, simple cubic lattice.

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1. Introduction. In 1988 Sumners and Whittington [1] investigated questions about knottedness of a closed curve of given length embedded in the three dimensional integer lattice, Z^3. They and, independently, Pippenger [2] showed that sufficiently long closed curves embedded in Z^3 are almost surely knotted. Soteros, Sumners and Whittington [3] extended the results of Sumners and Whittington in several directions. In particular, they showed that all but exponentially few sufficiently long closed curves embedded in Z^3 are highly composite knots, with any knot type appearing numerous times in the prime knot factorization. They also found that similar results hold for embeddings of graphs in Z^3.

These results are important to the study of models of polymers in dilute solution. Embeddings of a graph in Z^3 can be used to represent the possible conformations of a polymer with the structure of the given graph. Concerns about knottedness with regard to polymers are motivated by the fact that closed circular DNA has been observed to be knotted and that entanglements in proteins are believed to be relevant to their properties. There are at least two important questions that one would like to address using this model of polymers. How does knottedness depend on the particular structure of the polymer? How does knottedness depend on the geometrical constraints placed on the space in which the polymer is confined? In this paper, these two questions are addressed by studying

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the limiting behaviour, as the number of edges of the embedding goes to infinity, of the probability that an embedding of a graph in a subset of Z^3 is knotted. The subsets of Z^3 considered are Z^3 itself, slabs (subsets of Z^3 bounded by two parallel planes), and rectangular prisms (infinitely long rectangular tubes).

As a step towards answering the first question it is shown here, for each of the three lattice subsets, that there is a large class of graphs (including all planar graphs with no vertices of odd degree) for which the probability that an embedding of a graph in the given subset of Z^3 is knotted goes to one as the number of edges in the embedding goes to infinity and that the exponential rate at which the probability approaches one is independent of the specific graph. Thus, at least in terms of this limiting behaviour and this class of structures, knottedness is not very dependent on the particular structure of the polymer and all but exponentially few embeddings of the polymer are knotted. The approach to proving this result, however, depends on the particular subset of Z^3 considered. While the approach is quite similar for both Z^3 and slab geometries, in the case of the rectangular prism a new pattern theorem for self-avoiding polygons is required and proved. Furthermore, in the prism, the exponential growth rate of the number of embeddings of a graph is shown to be dependent on the particular structure of the graph while in Z^3 or in a slab it is not. Because of this, the class of graphs for which we address questions about knottedness in a prism is smaller than for Z^3 or the slab geometries.

The second question posed above is addressed here by studying the probability that an embedding of a simple closed curve, i.e., a self-avoiding polygon, confined to a particular lattice subset is knotted. This probability has been studied previously in [1,4] and the results from these works are reviewed here. It is shown that the probability is dependent on the lattice subset.

The knottedness of embeddings of graphs in Z^3 has been previously investigated in [3,5] and the results from these works are reviewed and generalized further here. The results presented regarding the knottedness of embeddings of graphs in slab and prism geometries are substantially new. In order to discuss the results in all three subsets, many of the established results for self-avoiding walks, self-avoiding polygons, and embeddings of graphs in the three subsets are reviewed.

The paper is organized as follows. In section 2, the terminology associated with using embeddings of graphs as models of branched polymers is reviewed and important results regarding growth constants for graph embeddings are presented. In section 3, questions related to knots in graphs embedded in Z^3 are addressed. In section 4, results regarding growth constants and knottedness for embeddings of graphs in a slab geometry are presented; graphs embedded in a slab geometry are shown to have properties parallel to those of graphs embedded in the whole space, Z^3. In section 5, the rectangular prism geometry is studied and in this case there are substantial differences from the two previous geometries. A pattern theorem for polygons in a prism, needed for the results presented in section 5, is presented in section 6.

2. Embeddings of Graphs in Z^3 as Models of Branched Polymers. In this paper the focus is on lattice models of branched polymers and in particular on models using the three dimensional integer lattice, i.e., the simple cubic lattice. The advantages of lattice models of polymers are that the excluded volume property (each monomer exists in a volume of space to the exclusion of any other monomer) is easily incorporated, that the "lattice polymer" has substantial conformational freedom despite the restrictions of the lattice, and perhaps most importantly, that rigorous mathematical analysis of lattice models is possible. It is expected that lattice models of polymers will exhibit qualitatively the same behaviour as "real" polymers. Furthermore, field theoretic arguments suggest that there exist universal quantites, i.e. critical exponents, which will be exactly the same for lattice models and for real polymers. In this paper, we will focus on lattice models of polymers whose branching structure is specified by an abstract graph. In order to introduce appropriate notation the standard lattice models for linear and ring polymers are reviewed first. Graph theory terminology is used to describe these models. In particular, the three dimensional integer lattice is defined to be the infinite graph with vertex set Z^3 and edge set $\{\{u,v\}|u,v \in Z^3, |u-v|=1\}$. Note that Z^3 will be used to represent either, depending on the context, the three dimensional integer lattice or its vertex set. Similarly for V a set of vertices in Z^3, V will be used to represent either the vertex set V or the subraph of Z^3 induced by this vertex set.

Self-avoiding walks are well known as good models of very long linear polymers in equilibrium in dilute solution. An n-step self-avoiding walk on the simple cubic lattice, Z^3, is an alternating sequence of $n+1$ distinct vertices and n directed edges, $u_0, (u_0,u_1), u_1, (u_1,u_2), u_2, ..., u_{n-1}, (u_{n-1}, u_n)$, u_n, such that the vertices $u_i \in Z^3$ for $i = 0, ..., n$, $u_0 = (0,0,0)$, and for each $i = 0, ..., n-1$ the directed edge (u_i, u_{i+1}) joins two nearest neighbour vertices in Z^3 (i.e. u_{i+1} and u_i differ only in one coordinate with the difference being ± 1). c_n is defined to be the number of n-step self-avoiding walks. As a model of a linear polymer composed of n monomers each n-step self-avoiding walk represents a possible polymer conformation and the self-avoidance ensures that there is an excluded volume around each monomer. The quantity $n^{-1}\log c_n$ thus represents the entropy per monomer of this polymer model and as $n \to \infty$ the limiting entropy per monomer has been proved to exist.

LEMMA 2.1 (HAMMERSLEY 1954 [6]). *The following limit exists:*

$$\kappa \equiv \lim_{n\to\infty} n^{-1} \log c_n. \tag{2.1}$$

κ is also known as the *connective constant* for Z^3. From Lemma 2.1 it is clear that

$$\mu \equiv \lim_{n\to\infty} c_n^{1/n} = e^{\kappa}, \tag{2.2}$$

where μ is known as the *growth constant* for self-avoiding walks in Z^3. Further results about c_n can be found in Madras and Slade [7].

Ignoring the orientation of the edges in a self-avoiding walk yields an undirected self-avoiding walk. Let w_n be the number of n-edge undirected self-avoiding walks (up to translation). Clearly,

$$w_n = \frac{c_n}{2} \tag{2.3}$$

and hence the growth constant for w_n will be μ.

Ring polymers in dilute solution have been successfully modelled using self-avoiding polygons. An n-edge *self-avoiding polygon* in Z^3 is an alternating sequence of n distinct vertices and n undirected edges, $u_0, \{u_0, u_1\}, u_1, \{u_1, u_2\}, u_2, ..., u_{n-1}, \{u_{n-1}, u_0\}, u_0$, such that for each $i = 0, ..., n-1$ the vertex $u_i \in Z^3$ and the edge $\{u_i, u_{i+1}\}$ joins two nearest neighbour vertices in Z^3. p_n is defined to be the number of n-vertex self-avoiding polygons (up to translation). Hammersley [8] proved that the growth constant for self-avoiding polygons in Z^3 is the same as that for self-avoiding walks.

LEMMA 2.2 (HAMMERSLEY 1961 [8]).

$$\lim_{n\to\infty} (2n)^{-1} \log p_{2n} = \kappa. \tag{2.4}$$

In order to obtain relationships between other lattice models and self-avoiding walks or polygons, it is also useful to study self-avoiding walks or polygons in wedges [9,10]. The following result is a consequence of the results for self-avoiding polygons in wedges in [10]. Given non-negative integers $\infty \geq \beta > \alpha > 0$, define the wedge $W(\alpha, \beta)$ to be the sublattice of Z^3 induced by the vertex set $\{(x, y, z) \in Z^3 | \alpha x \leq y \leq \beta x + \alpha + 1, x \geq 0, z \geq 0\}$. This definition of the wedge ensures that at least one self-avoiding polygon of arbitrary length contained in the (x, y)-plane can fit in the wedge. Let $p_n^{\alpha,\beta}$ be the number of n-edge self-avoiding polygons confined to $W(\alpha, \beta)$ and containing an edge between $(0, 0, 0)$ and $(0, 1, 0)$; similarly, let $c_n^{\alpha,\beta}$ be the number of n-step self-avoiding walks confined to $W(\alpha, \beta)$ and having its first step from $(0, 0, 0)$ to $(0, 1, 0)$. The wedge arguments in [10] lead to the following:

LEMMA 2.3 (SOTEROS 1992 [10]). *Given non-negative integers α and β such that $\infty \geq \beta > \alpha > 0$,*

$$\lim_{n\to\infty} (2n)^{-1} \log p_{2n}^{\alpha,\beta} = \lim_{n\to\infty} n^{-1} \log c_n^{\alpha,\beta} = \kappa. \tag{2.5}$$

Hence confinement of a self-avoiding polygon or walk to a wedge such as $W(\alpha, \beta)$ does not affect its growth constant. A very general wedge result has been obtained recently by Soteros *et al* [11]. From their results Lemma 2.3 is extended to the case that α and β are any real numbers.

The undirected self-avoiding walk and polygon models are included in a wider class of polymer models in which the structure of a polymer is given by an abstract graph τ and polymer conformations are represented by embeddings of τ in Z^3. In this wider class of models, the graph τ which represents the topology of a polymer is assumed to have no vertices of degree two (except in the case of a ring polymer); the *degree* of a vertex of a graph is defined to be the number of edges incident on the vertex and a *loop* (an edge from a vertex to itself) is assumed to contribute twice to the degree of a vertex. An edge of τ is used to represent a *branch* of the polymer. In the special case of a ring polymer τ is taken to be the *circle graph* which is defined to consist of one vertex (a vertex of degree two) and one loop. The circle graph is thus said to have one branch. Vertices of τ having degree greater than one are referred to as *branch points*. Conformations of a polymer with topology τ are represented by embeddings of τ in Z^3. An *embedding of τ in Z^3* is defined to be any subgraph of Z^3 which is isomorphic to τ when vertices of degree two are suppressed; that is, an embedding of τ is any subgraph of Z^3 which is *homeomorphic* to τ. Define G_r to be the set which includes the circle graph and the set of all connected graphs having at least one edge and no vertices of degree two and whose branch points all have degree less than or equal to r. Soteros *et al* [3] proved that an embedding of τ in Z^3 exists for any $\tau \in G_6$. Given $\tau \in G_6$, define $g_n(\tau)$ to be the number of embeddings of τ in Z^3 (up to translation) consisting of n edges.

Thus an n-edge self-avoiding polygon is an embedding of the circle graph consisting of n edges and $g_n(\text{circle}) = p_n$. Figure 2.1 b) shows the circle graph along with a 10 edge embedding of the circle graph in Z^3. Define the *line graph* to be the graph consisting of two vertices and one edge which joins the two vertices together. An n-edge undirected self-avoiding walk is thus an n-edge embedding of the line graph and $g_n(\text{line}) = w_n$. Figure 2.1 a) shows the line graph and a 10 edge embedding of the line graph in Z^3. Define the *figure eight graph* to be the graph with one vertex and two loops. Figure 2.1 c) depicts a figure eight graph and a 20-edge embedding of it in Z^3.

Based on the following result, the *growth constant*, $\lim_{n\to\infty}(g_n(\tau))^{1/n}$, for the number of embeddings of a graph exists and is independent of the specific graph.

LEMMA 2.4 (SOTEROS, SUMNERS AND WHITTINGTON 1992 [3]). *Given a graph $\tau \in G_6$*

$$\lim_{n\to\infty} n^{-1} \log g_n(\tau) = \kappa \tag{2.6}$$

where κ is the connective constant for self-avoiding walks and where if τ admits no embeddings with an odd number of edges then the limit is taken only through even values of n .

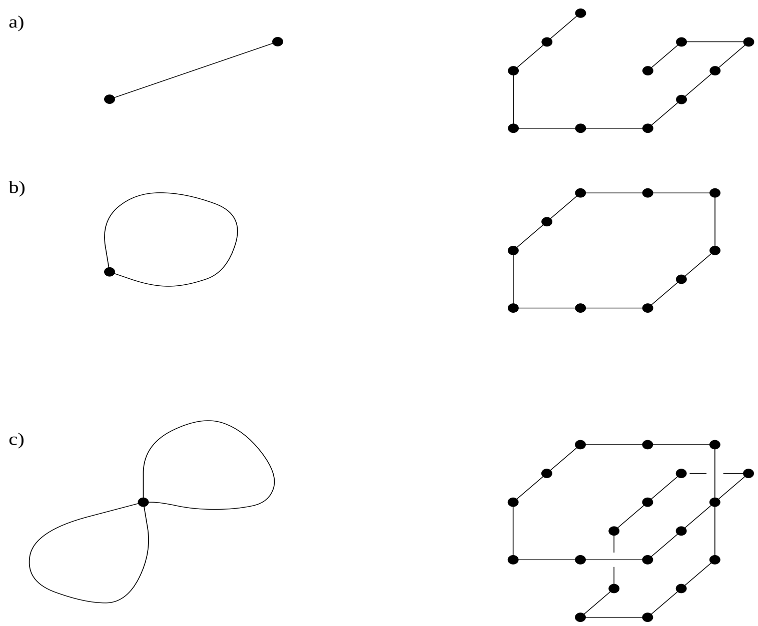

FIG. 2.1. *In a) the line graph and a 10-edge embedding of the line graph in Z^3 is depicted. In b) the circle graph and a 10-edge embedding of the circle graph in Z^3 is depicted. In c) the figure eight graph and a 20-edge embedding of the figure eight graph in Z^3 is depicted.*

Proof. The proof of this Lemma is reviewed here in order to introduce a basic approach to obtaining results concerning growth constants of graph embeddings. Let τ be any graph in G_6 and fix a labelling of the vertices and edges of τ. Let f be the number of edges in τ. We first note that given any embedding of τ, the vertices (except for those of degree two) and branches of the embedding can be labelled according to the labelling given for τ. In particular, label the vertices first and, when ambiguity arises in the labelling of vertices, label them according to the lexicographic ordering of their coordinates in Z^3. When ambiguity arises in the labelling of branches (i.e. two or more branches have the same labelled vertices at their ends), label them according to the lexicographic ordering of the coordinates of the vertex of each branch that is adjacent to its smallest end vertex.

An upper bound is obtained for $g_n(\tau)$ in terms of self-avoiding walks as follows. Consider any n-edge embedding of τ. Translate the embedding so that the first branch has its smallest (in terms of the labelling just described) end vertex at the origin. For each branch, orient the edges of the branch to go from its smaller to its larger end vertex. Thus each branch of the embedding can be viewed as a self-avoiding walk and therefore

$$g_n(\tau) \leq \sum_{\{m_i | \sum_{i=1}^{f} m_i = n\}} c_{m_1} c_{m_2} \cdots c_{m_f} \leq e^{\kappa n + o(n)} \tag{2.7}$$

where m_i represents the number of edges in branch i of τ.

A lower bound is obtained for $g_n(\tau)$ in terms of self-avoiding polygons as follows. Start with any embedding of τ in which the rightmost (maximum x-coordinate) plane of the embedding, $x = k$ say, contains the edge $\{(k, 0, 0), (k, 1, 0)\}$. It is always possible to find such an embedding with an even number of edges and, if there exists an embedding of τ with an odd number of edges, it is also possible to find such an embedding with an odd number of edges [3]. Let $m_e > 0$ be an even number for which such an m_e-edge embedding of τ exists and m_o be an odd number for which such an m_o-edge embedding of τ exists. For any $2n \geq m_e + 4$, let P be a $(2n - m_e)$-edge self-avoiding polygon confined to $W(0, \infty)$ and containing the edge $\{(0, 0, 0), (0, 1, 0)\}$. Translate P so that $(0, 0, 0)$ is translated to $(k + 1, 0, 0)$ and then *concatenate* P to the embedding of τ by adding the edges $\{(k, 1, 0), (k + 1, 1, 0)\}$ and $\{(k, 0, 0), (k + 1, 0, 0)\}$ and then deleting the edges $\{(k, 0, 0), (k, 1, 0)\}$ and $\{(k+1, 0, 0), (k+1, 1, 0)\}$. This results in the upper bound

$$p^{0,\infty}_{2n-m_e} \leq g_{2n}(\tau). \tag{2.8}$$

If τ has embeddings with an odd numbers of edges, a similar concatenation argument yields

$$p^{0,\infty}_{2n+1-m_o} \leq g_{2n+1}(\tau). \tag{2.9}$$

If τ does not admit any odd edge embeddings (for example if τ is the circle or the figure eight graph (see Figure 2.1 c)), taking logarithms, dividing by $2n$, letting $n \to \infty$, and using Lemma 2.3 in equations (2.7) (with n replaced by $2n$) and (2.8) gives the required result where the limit is taken only through even values. If τ does admit odd edge embeddings, equations (2.7), (2.8), and (2.9) lead to the required result where the limit is taken through all values of n. □

Polymer chemists are frequently interested in the case that the branches of a polymer all consist of the same number of monomers (i.e. the polymer chains making up the branched polymer structure are monodisperse). Thus it is useful to consider the case where the distribution of edges to the branches of a graph embedding is fixed. Given $\tau \in G_6$, let f be the number of edges of τ. Suppose $f \geq 2$. Given a fixed labelling of the vertices and edges of τ, we can define $g_n(\tau; (\phi_1, \phi_2, ..., \phi_f))$ to be the number of embeddings of τ in Z^3, distinct up to translation, composed of n edges with ϕ_i edges in its ith branch. The ϕ_i are positive integers such that $\sum_i \phi_i = n$ and the labelling of the branches of the embedding is determined, as described in the proof of Lemma 2.4, by the fixed labelling of τ. The ordered set of numbers $\phi \equiv (\phi_1, \phi_2, ..., \phi_f)$ will be referred to as the *edge distribution* of the embedding. In [10], the number of *uniform* or monodisperse embeddings of a graph was studied, $g_{nf}(\tau; (n, n, ..., n))$, and the following lemma resulted.

LEMMA 2.5 (SOTEROS 1992 [10]). *Given a bipartite graph $\tau \in G_6$*

$$\lim_{n\to\infty} (nf)^{-1} \log g_{nf}(\tau; (n, n, ..., n)) = \kappa. \tag{2.10}$$

Given a graph $\tau \in G_6$ which is not bipartite (i.e. has at least one cycle of odd length)

$$\lim_{n\to\infty} (2nf)^{-1} \log g_{2nf}(\tau; (2n, 2n, ..., 2n)) = \kappa. \tag{2.11}$$

Proof. The basic idea of the proof is to first get an upper bound on $g_{nf}(\tau; (n, n, ..., n))$ in terms of self-avoiding walks by noting that $g_{nf}(\tau; (n, n, ..., n)) \leq g_{nf}(\tau)$ and then using equation (2.7). A lower bound for $g_{nf}(\tau; (n, n, ..., n))$ is obtained by starting with an embedding of τ such that:

(i) Exactly one edge of each branch of τ lies in the rightmost plane, $x = k$, of the embedding. These rightmost edges lie in the line $z = 0$, $x = k$, $y \geq 0$.
(ii) The parity (even or odd) of the number of edges in a branch is the same for all branches.
(iii) Each edge in the line $z = 0$, $x = k$ is at least f edges apart from any other edge in the line.

Then, in order to create a new embedding of τ, for each $i = 1, ..., f$, a polygon in $W(i-1, i)$ is concatenated to the edge of the ith branch of τ contained in the rightmost plane $x = k$. This gives the lower bound

$$p^{0,1}_{n-m_1} p^{1,2}_{n-m_2} \cdots p^{f-1,f}_{n-m_f} \leq g_{nf}(\tau; (n, n, ..., n)) \tag{2.12}$$

where $(m_1, m_2, ..., m_f)$ is the edge distribution of the initial embedding of τ. Taking logarithms, dividing by nf, letting n go to infinity, and using Lemma 2.3 gives the required result. □

This type of argument can also be used to obtain results about other types of edge distributions. For example, consider the sequence of numbers $g_N(\tau; (\phi_1(n), ..., \phi_f(n)))$ for $n = 1, 2, 3, ...$, where $\phi_i(n)$ is a postive integer valued function of n and $N = \sum_{i=1}^{f} \phi_i(n)$. Let $\phi(n) \equiv (\phi_1(n), ..., \phi_f(n))$. In order for $g_N(\tau; \phi(n)) > 0$ when τ contains a cycle, constraints must be placed on the parity of the components of $\phi(n)$ to ensure that any cycle in an embedding of τ in Z^3 consists of an even number of edges. In particular, each embedding of a cycle must contain an even number of odd length branches. Define the *parity distribution* associated with an edge distribution $\phi(n)$ to be the f-tuple of parities whose ith component is the parity of $\phi_i(n)$. Suppose that $g_N(\tau; \phi(n)) > 0$ for $n \geq 1$ and, without loss of generality, that the sequence $\{\phi(n)\}_{n\geq 1}$ has the property that given an

$i \in \{1, 2, ..., f\}$ the parity of $\phi_i(n)$ is fixed for all $n \geq 1$, i.e., the sequence of $\phi(n)$'s has a fixed parity distribution. If the sequence does not have a fixed parity distribution, one considers separately each subsequence of $\{\phi(n)\}_{n\geq 1}$ that does have a fixed parity distribution; there can be at most 2^f such subsequences. Further suppose that given an $i \in \{1, 2, ..., f\}$ either $\phi_i(n)$ is a constant function or a strictly increasing function of n. If $\phi_i(n)$ is strictly increasing, we refer to the ith branch as *growing*; otherwise, the ith branch is referred to as *constant*. An upper bound for $g_N(\tau; \phi(n))$ is obtained in the same manner as in the proof of Lemma 2.4, namely, each embedding of τ is separated into f self-avoiding walks. To get a lower bound for $g_N(\tau; \phi(n))$ we again need to construct an appropriate embedding to which we can concatenate polygons in wedges. Since embeddings of τ exist with the parity and edge distributions given by $\{\phi(n)\}_{n\geq 1}$, it should be possible to find an embedding of τ having $\phi(1)$'s parity distribution, having $\phi_i(1)$ edges in each constant branch i, and having enough space between each branch of the embedding so that for each growing branch it is possible to concatenate a polygon to an edge of the branch and extend the branch so that it has a unique edge in the rightmost plane of the embedding. In this way one can construct an embedding of τ with properties (i) and (iii) as in the proof of Lemma 2.5 and with property (ii) revised as follows:

(ii*) The number of edges in branch i has the same parity as $\phi_i(1)$ and equals $\phi_i(1)$ if branch i is constant.

Establishing an appropriate lower bound then follows by concatenating polygons in wedges to the edges in the line $z = 0$, $x = k$ just as in the proof of Lemma 2.5. Thus, we obtain the following result.

LEMMA 2.6. *Given $\tau \in G_6$ with f edges, let $\{\phi(n)\}_{n\geq 1}$ be a sequence of edge distributions such that for $1 \leq i \leq f$, $\phi_i(n)$ is either a constant or strictly increasing function of n. If for each subsequence of $\{\phi(n)\}_{n\geq 1}$ with fixed parity distribution an embedding of τ with the properties (i), (ii*), and (iii) exists, then*

$$\lim_{n\to\infty} N^{-1} \log g_N(\tau; \phi(n)) = \kappa, \tag{2.13}$$

where $N = \sum_{i=1}^{f} \phi_i(n)$.

Thus the growth constant for embeddings of a graph does not depend on the fixed edge distribution sequence given for the graph.

3. Knots in Graphs in Z^3. In this section, results about knots in graph embeddings in Z^3 are discussed. Unless stated otherwise, the terminology used here will be the same as that defined in Soteros, Sumners and Whittington [3]. Any locally flat piecewise linear embedding of τ in 3-space is said to be a knot of τ. The set of equivalence classes of knots of τ (as defined in [3]) is denoted by $\mathcal{K}(\tau)$. For $K \in \mathcal{K}(\tau)$, the crossing number of K, $C(K)$, is the minimum number of crossings obtainable in any knot diagram for any knot $k \in K$ and we define

$$N_{\min}(\tau) = \min_{K \in \mathcal{K}(\tau)} C(K). \tag{3.1}$$

The knottedness of embeddings of a graph will be discussed in terms of embeddings in 3-space. Thus, in order to establish a point of reference, define $K \in \mathcal{K}(\tau)$ to be *unknotted* if there are members of K which realize $N_{\min}(\tau)$; in this case all members of K are said to be unknotted. Otherwise, $K \in \mathcal{K}(\tau)$ and all members of K are said to be *knotted.* An embedding of τ in Z^3 will be considered knotted if as an embedding in 3-space it is knotted.

Note that any embedding of the graph K_7 in 3-space contains a knotted cycle [12]. Although K_7 is not embeddable in Z^3, this example suggests the possibity that, based on the definition above, an unknotted embedding of a graph in Z^3 may contain a cycle which is a knotted self-avoiding polygon. It will be useful later to consider the set of graphs embeddable in Z^3 for which this is not possible. Thus, for $2 \leq r \leq 6$, let $\tilde{G}_r \subseteq G_r$ be the set of graphs such that for $\tau \in \tilde{G}_r$ any cycle in an unknotted embedding of τ in Z^3 is an unknotted embedding of a circle graph (i.e., an unknotted self-avoiding polygon). Note that $\tilde{G}_6$ contains the set of all planar graphs in G_6.

Given Lemmas 2.1-2.6, the main additional ingredient that is needed in order to prove results about knotted embeddings of a graph τ in Z^3 is an appropriate pattern theorem. A *pattern* will be defined to be any embedding of the line graph in Z^3. A *Kesten* pattern will be defined to be any pattern which appears at least three times in an embedding of the line graph. Let $g_n(\tau; \bar{P})$ be the number of n-edge embeddings of τ in Z^3 which do not contain the pattern P; let $g_n(\tau; P)$ be the number of n-edge embeddings of τ in Z^3 which contains the pattern P. Similarly, let $g_N(\tau; \phi(n), \bar{P})$ be the number of embeddings of τ in Z^3 composed of $N = \sum_{i=1}^{f} \phi_i(n)$ edges, with edge distribution $\phi(n) = (\phi_1(n), \phi_2(n), ..., \phi_f(n))$, and such that the pattern P does not appear in the embedding. A pattern theorem due to Kesten for self-avoiding walks yields the following pattern theorem for embeddings of the line graph.

LEMMA 3.1 (KESTEN 1963 [13]). *Let P be any Kesten pattern.*

$$\lim_{n \to \infty} n^{-1} \log g_n(\text{line}; \bar{P}) = \kappa(\bar{P}) < \kappa. \tag{3.2}$$

Combining this with Lemma 2.1 gives that

$$\lim_{n \to \infty} \frac{g_n(\text{line}; P)}{g_n(\text{line})} = \lim_{n \to \infty} 1 - e^{(\kappa(\bar{P}) - \kappa)n} = 1. \tag{3.3}$$

Hence, for n sufficiently large, all but exponentially few embeddings of the line graph contain the pattern P and

$$\lim_{n \to \infty} n^{-1} \log g_n(\text{line}; P) = \kappa. \tag{3.4}$$

Based on equation (2.7), one can obtain an upper bound for $g_n(\tau)$ in terms of $g_n(\text{line})$ by using the fact that $c_n = 2g_n(\text{line})$. The same reasoning allows one to obtain an upper bound for $g_n(\tau; \bar{P})$ in terms of $g_n(\text{line}; \bar{P})$ and for $g_N(\tau; \phi(n), \bar{P})$ in terms of $g_n(\text{line}; \bar{P})$ and gives the following two results.

LEMMA 3.2 (SOTEROS, SUMNERS AND WHITTINGTON 1992 [3]). *Let P be any Kesten pattern and τ any graph in G_6.*

$$\limsup_{n\to\infty} n^{-1} \log g_n(\tau; \bar{P}) \leq \kappa(\bar{P}) < \kappa. \tag{3.5}$$

That is, for sufficiently large n, the pattern P appears at least once in all but exponentially few embeddings of τ.

LEMMA 3.3. *Let P be any Kesten pattern and τ any graph in G_6. Given any edge distribution sequence $\{\phi(n)\}_{n\geq 1}$ for which equation (2.13) holds with $N = \sum_{i=1}^{f} \phi_i(n)$,*

$$\limsup_{n\to\infty} N^{-1} \log g_N(\tau; \phi(n), \bar{P}) \leq \kappa(\bar{P}) < \kappa. \tag{3.6}$$

That is, for sufficiently large n, the pattern P appears at least once in all but exponentially few embeddings of τ when the edge distribution is fixed.

A version of Lemma 3.3 for uniform embeddings of τ was given in [5].

In order to discuss knots in embeddings of τ in Z^3, the focus is on the pattern T^q which is formed by concatenating a sequence of q tight trefoils, T, where $q = \lceil 1 + \frac{N_{\min}(\tau)}{3} \rceil$. Figure 3.1 depicts a *tight trefoil*, T; if T appears in a self-avoiding polygon the polygon must be knotted. If T^q appears in a cycle in an embedding of τ in Z^3, then the crossing number of the embedding is $\geq 3q \geq N_{\min}(\tau)$ [3] and hence the embedding is knotted.

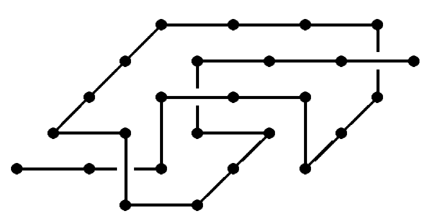

FIG. 3.1. *A tight trefoil pattern T in Z^3.*

Define $g_n^o(\tau)$ to be the number of unknotted n-edge embeddings of τ. Clearly if τ has no cycles then $g_n^o(\tau) = g_n(\tau)$. Sumners and Whittington [1] used a concatenation argument to show that for $p_n^o \equiv g_n^o(\text{circle})$

$$p_m^o p_n^o \leq p_{m+n}^o \tag{3.7}$$

and then they used Kesten's pattern theorem to prove the following result for unknotted self-avoiding polygons.

LEMMA 3.4 (SUMNERS AND WHITTINGTON 1988 [1]).

$$\lim_{n\to\infty}(2n)^{-1}\log p^o_{2n} \equiv \kappa_o < \kappa \tag{3.8}$$

and hence the probability that an n-edge self-avoiding polygon is knotted, $\frac{p_n - p^o_n}{p_n}$*, goes to unity as*

$$1 - e^{-\alpha n + o(n)} \tag{3.9}$$

when $n \to \infty$*, with* $\alpha \equiv \kappa - \kappa_o$*.*

The following theorem about the knottedness of graph embeddings in Z^3 is a consequence of Lemmas 3.2 and 3.4. Only graphs in which each branch of the graph is contained in a cycle need be considered; that is, graphs which have no cut edges. (A *cut edge* is any edge which when removed disconnects the graph.) An important subset of the graphs with no cut edges is the set of eulerian graphs; a graph is said to be *eulerian* if there exists a closed walk on the graph which uses each edge of the graph exactly once. Note that τ is eulerian if and only if every vertex of τ has even degree. The θ-graph (the graph with two vertices of degree 3 and three edges, each going from one vertex of the graph to the other) is an example of a graph with no cut edges that is not eulerian. The circle graph and the figure eight graph are eulerian.

THEOREM 3.1. *Suppose* $\tau \in G_6$ *has no cut edges,*

$$\kappa_o \le \liminf_{n} n^{-1}\log g^o_n(\tau) \le \limsup_{n\to\infty} n^{-1}\log g^o_n(\tau) \le \kappa(\bar{T}^q) < \kappa \tag{3.10}$$

(where as in Lemma 2.4 the limit is taken only through values of n for which $g^o_n(\tau) > 0$*) and hence the probability that an n-edge embedding of* τ *is knotted goes to unity at least as fast as*

$$1 - e^{-\beta n + o(n)} \tag{3.11}$$

and no faster than

$$1 - e^{-\alpha n + o(n)} \tag{3.12}$$

when $n \to \infty$*, with* $\beta = \kappa - \kappa(\bar{T}^q)$ *and* α *as defined in equation (3.9).*

If τ *is eulerian and* $\tau \in \tilde{G}_6$*,*

$$\lim_{n\to\infty}(2n)^{-1}\log g^o_{2n}(\tau) = \kappa_o \tag{3.13}$$

and hence the probability that an n-edge embedding of τ *is knotted goes to unity as*

$$1 - e^{-\alpha n + o(n)} \tag{3.14}$$

when $n \to \infty$*.*

Proof. For any $\tau \in G_6$, starting with an unknotted embedding of τ and then concatenating an unknotted embedding of a polygon yields a new unknotted embedding of τ. Thus following an argument similar to the one that leads to equations (2.8) and (2.9), there exists m such that

$$p_{n-m}^{o,0,\infty} \leq g_n^o(\tau) \tag{3.15}$$

where $p_n^{o,0,\infty}$ is the number of n-edge unknotted self-avoiding polygons in the wedge $W(0,\infty)$. Here we note that, given Lemma 3.4, Lemma 2.3 can also be proved for unknotted polygons in wedges with κ replaced by κ_o. Thus taking logarithms, dividing by n, and letting n go to infinity in equation (3.15) gives

$$\kappa_o \leq \liminf_n n^{-1} \log g_n^o(\tau) \tag{3.16}$$

where if τ does not admit any odd edge embeddings then the limit is taken only through even values of n.

In the case $\tau \in G_6$ has no cut edges, an upper bound on $g_n^o(\tau)$ can be obtained as in equation (2.7) except now no branch of τ can contain the pattern T^q. Thus

$$\begin{aligned} g_n^o(\tau) \leq &\quad 2^f \sum_{\{m_i \mid \sum_{i=1}^f m_i = n\}} g_{m_1}(\text{line}, \bar{T^q}) g_{m_2}(\text{line}, \bar{T^q}) \cdots g_{m_f}(\text{line}, \bar{T^q}) \\ (3.17) \leq &\quad e^{\kappa(\bar{T^q})n + o(n)}. \end{aligned}$$

Equation (3.17) and equation (3.16) lead to equation (3.10). (Equation (3.17) was first presented in [3].) The limiting behaviour of the probability that an n-edge embedding of τ is knotted is determined by equation (3.10) since it implies that for sufficiently large n

$$1 - e^{-\alpha n + o(n)} \geq \frac{g_n(\tau) - g_n^o(\tau)}{g_n(\tau)} \geq 1 - e^{-\beta n + o(n)} \tag{3.18}$$

with α and β as defined in the statement of the theorem.

If τ is eulerian then there exists a closed path which uses every edge of τ exactly once. Fix such a closed path. This path can be used to decompose an embedding of τ into at most f rooted (or possibly multiply rooted) self-avoiding polygons. Let f_p be the number of polygons that τ decomposes into. For each vertex of degree $2j$ of τ, j roots are needed. Thus $2n_4 + 3n_6$ roots must be distributed to the f_p polygons, where n_i is the number of vertices of degree i in τ. An upper bound on the number of ways to root and label the f_p polygons is given by

$$R_\tau(n) = 2^{f_p} \binom{f_p + 2n_4 + 3n_6 - 1}{2n_4 + 3n_6} n^{(2n_4+3n_6)f_p} \tag{3.19}$$

where n is the total number of edges in an embedding of τ. Recall that if $\tau \in \tilde{G}_6$, every cycle in an unknotted embedding of τ is unknotted. Thus for eulerian $\tau \in \tilde{G}_6$ the following upper bound for $g^o_{2n}(\tau)$ results

$$(3.20)\ g^o_{2n}(\tau) \leq R_\tau(2n) \sum_{\{m_i | \sum_{i=1}^{f_p} m_i = n\}} p^o_{2m_1} p^o_{2m_2} \cdots p^o_{2m_{f_p}} \leq e^{2n\kappa_o + o(n)}$$

where we have used equation (3.7) and Lemma 3.4 for the rightmost inequality. This combined with equation (3.16) gives equation (3.13). □

For any $\tau \in G_6$ let $\{\phi(n)\}_{n\geq 1}$ be an edge distribution sequence for which equation (2.13) holds. We define a *fast growing* branch of τ to be a branch i for which

$$1 \geq \lim_{n\to\infty} \frac{\phi_i(n)}{N} > 0. \tag{3.21}$$

Using this definition we obtain the following result.

THEOREM 3.2. *Given $\tau \in G_6$ with f edges and at least one cycle, if $\{\phi(n)\}_{n\geq 1}$ is an edge distribution sequence such that Lemma 2.6 holds, such that there exists an unknotted embedding of τ with edge distribution $\phi(1)$, and such that at least one branch of a cycle of τ is fast growing, then*

$$\begin{aligned} \kappa_o \leq & \liminf_{n\to\infty} N^{-1} \log g^o_N(\tau;\phi(n)) \\ \leq & \limsup_{n\to\infty} N^{-1} \log g^o_N(\tau;\phi(n)) \leq \kappa(\bar{T}^q) < \kappa. \end{aligned} \tag{3.22}$$

Furthermore, if all the fast growing branches of $\tau \in \tilde{G}_6$ are contained in an eulerian subgraph (not necessarily connected) of τ

$$\lim_{n\to\infty} N^{-1} \log g^o_N(\tau;\phi(n)) = \kappa_o. \tag{3.23}$$

Proof. Let τ be any fixed graph in G_6 and let $\{\phi(n)\}_{n\geq 1}$ be an edge distribution sequence for which Lemma 2.6 holds. Based on the argument that leads to equation (2.12), concatenating unknotted polygons in wedges to an unknotted embedding of τ with properties (i), (ii*), and (iii) results in the lower bound

$$p^{o,0,1}_{\phi_1(n)-m_1} p^{o,1,2}_{\phi_2(n)-m_2} \cdots p^{o,f-1,f}_{\phi_f(n)-m_f} \leq g^o_N(\tau;\phi(n)) \tag{3.24}$$

where $(m_1, m_2, ..., m_f)$ is the edge distribution of the initial unknotted embedding of τ. Taking logarithms, dividing by N, and letting n go to infinity then gives

$$\kappa_o \leq \liminf_{n\to\infty} N^{-1} \log g^o_N(\tau;\phi(n)). \tag{3.25}$$

Let i be a fast growing branch contained in a cycle of τ. To obtain the upper bound, we separate an n-edge embedding of τ into f embeddings of the line graph (as in equation (3.17)) except that the ith branch cannot contain the pattern T^q. Thus

$$\begin{aligned} g_N^o(\tau;\phi(n)) &\leq 2^f w_{\phi_1(n)}\cdots w_{\phi_{i-1}(n)} w_{\phi_{i+1}(n)}\cdots w_{\phi_f(n)} g_{\phi_i(n)}(\text{line},\bar{T^q}) \\ &\leq e^{\kappa(N-\phi_i(n))+\kappa(\bar{T^q})\phi_i(n)+o(N)}. \end{aligned} \tag{3.26}$$

Taking logarithms, dividing by N, and letting n go to infinity in this equation gives

$$\limsup_{n\to\infty} N^{-1}\log g_N^o(\tau;\phi(n)) < \kappa. \tag{3.27}$$

Further suppose that all fast growing branches of $\tau \in \tilde{G}_6$ are contained in an eulerian subgraph η of τ. Let f_p be the number of polygons that η separates into and let $R_\eta(n)$ be as defined in equation (3.19). Assume that the remaining branches of τ (i.e. those not part of η) are labelled from 1,2,...,f'. Starting with an N-edge unknotted embedding of τ with edge distribution $\phi(n)$, none of the polygons that η separates into can be knotted hence,

$$\begin{aligned} g_N^o(\tau;\phi(n)) &\leq R_\eta(N) 2^{f'} w_{\phi_1(n)}\cdots w_{\phi_{f'}(n)} p^o_{m_1}\cdots p^o_{m_{f_p}} \\ &\leq e^{\kappa_o N + o(N)} \end{aligned} \tag{3.28}$$

where m_i is the number of edges of the embedding in η's ith polygon and the fact that $\lim_{n\to\infty}\frac{\sum_{i=1}^{f'}\phi_i(n)}{N} = 0$ has been used to obtain the rightmost inequality. Equations (3.25) and (3.28) lead to equation (3.23). □

Note that this theorem was proved for the uniform case (i.e., $\phi(n) = (n,n,...,n)$) in [5]; a related theorem was proved in [3] for embeddings in which the fraction of edges in a designated cycle was fixed rather than the whole edge distribution being fixed. One can also use a more general version of Kesten's pattern theorem to prove that in the cases covered by Theorems 3.1 and 3.2 almost all the considered embeddings of a graph τ are highly composite knots [3,5].

In the next sections the extent to which these results hold for embeddings of graphs in subsets of Z^3 are explored.

4. Knots in Graphs in an L-Slab. An L-slab is the sublattice of Z^3 induced by the vertex set $\{(x,y,z) \in Z^3 | 0 \leq z \leq L\}$. The properties of self-avoiding walks and polygons in an L-slab have been reviewed in two recent papers by Tesi *et al* [4,14]. In order to address questions about knots in graphs in an L-slab, the same ingredients as those introduced in the last two sections are needed, namely, a result equating the growth constant for self-avoiding walks and self-avoiding polygons (as in Lemma 2.2), a result for the growth constant of self-avoiding polygons in wedges (as in Lemma 2.3), and a pattern theorem for self-avoiding walks (as in Lemma 3.1). In fact the arguments which led to the results just listed can be modified in a straightforward fashion to deal with self-avoiding polygons and walks in an L-slab, $L \geq 1$.

Define $p_n(L)$ to be the number (up to translation) of n-edge self-avoiding polygons confined to an L-slab and let $c_n(L)$ to be the number of n-step self-avoiding walks confined to an L-slab. From the work of Hammersley and Whittington (1985) [9] and Madras and Slade (1993) [7] we have that

LEMMA 4.1.

$$\lim_{n\to\infty} n^{-1}\log c_n(L) = \lim_{n\to\infty}(2n)^{-1}\log p_{2n}(L) = \kappa(L) < \kappa \tag{4.1}$$

where $\kappa(L)$ is strictly increasing in L and $\lim_{L\to\infty}\kappa(L) = \kappa$.

Given non-negative integers $\infty \geq \beta > \alpha > 0$, define $W(\alpha,\beta,L)$ to be the sublattice of an L-slab induced by the vertex set $\{(x,y,z) \in Z^3 | \alpha x \leq y \leq \beta x + \alpha + 1, 0 \leq x, 0 \leq z \leq L\}$. For $L \geq 0$, let $p_n^{\alpha,\beta}(L)$ be the number of n-edge self-avoiding polygons confined to $W(\alpha,\beta,L)$ and containing an edge between $(0,0,0)$ and $(0,1,0)$; similarly, let $c_n^{\alpha,\beta}(L)$ be the number of n-step self-avoiding walks confined to $W(\alpha,\beta,L)$ and having its first step from $(0,0,0)$ to $(0,1,0)$. The wedge arguments in [10,11] are easily modified to give:

LEMMA 4.2.

$$\lim_{n\to\infty}(2n)^{-1}\log p_{2n}^{\alpha,\beta}(L) = \lim_{n\to\infty} n^{-1}\log c_n^{\alpha,\beta}(L) = \kappa(L). \tag{4.2}$$

Tesi *et al* [4,14] have proved an appropriate pattern theorem for self-avoiding walks in an L-slab. Let $\mathcal{C}_{m_1,m_2}(L)$ be the set of self-avoiding walks completely contained in $D_{m_1,m_2}(L) = \{(x,y,z) \in Z^3 | 0 \leq x \leq m_1, 0 \leq y \leq m_2, 0 \leq z \leq L\}$ with one endpoint at the origin and the other at $(m_1,m_2,0)$. For any $m_1 > 0$ and $m_2 > 0$, a $K_{m_1,m_2}(L)$ pattern is defined to be an self-avoiding walk which appears in some element of $\mathcal{C}_{m_1,m_2}(L)$. The following pattern theorem holds.

LEMMA 4.3 (TESI *et al* [4,14]). *For any $m_1 > 0$ and $m_2 > 0$ and any $K_{m_1,m_2}(L)$ pattern P,*

$$\lim_{n\to\infty} n^{-1}\log c_n(L,\bar{P}) \equiv \kappa(L,\bar{P}) < \kappa(L) \tag{4.3}$$

where $c_n(L,\bar{P})$ is the number of n-step walks in an L-slab which do not contain the pattern P.

Arguments such as those given in [3] can be used to show that, for $L \geq 2$ and any graph $\tau \in G_6$, there exists an embedding of τ in an L-slab. Similarly, for $L = 1$ and any graph $\tau \in G_5$, there exists an embedding of τ in a 1-slab. Finally, in Soteros (1992) [10] it was shown that for $L = 0$ and any planar graph $\tau \in G_4$, there exists an embedding of τ in the 0-slab, i.e., the square lattice Z^2. The arguments that led to Lemma 2.4 have been modified for an L-slab in [15] for the case $L > 0$ and in [10] for the case $L = 0$ and used to prove the following.

LEMMA 4.4. *For $L > 1$ and any fixed graph $\tau \in G_6$*

$$\lim_{n\to\infty} n^{-1} \log g_n(\tau, L) = \kappa(L); \tag{4.4}$$

for $L = 1$ and any fixed graph $\tau \in G_5$

$$\lim_{n\to\infty} n^{-1} \log g_n(\tau, 1) = \kappa(1); \tag{4.5}$$

and for $L = 0$ and any planar graph $\tau \in G_4$

$$\lim_{n\to\infty} n^{-1} \log g_n(\tau, 0) = \kappa(0). \tag{4.6}$$

In all three cases the limits are taken only through values of n for which $g_n(\tau, L) > 0$.

The result, corresponding to Lemma 2.5, that uniform embeddings in an L-slab have the same growth constant as self-avoiding walks in an L-slab,

$$\lim_{n\to\infty} (nf)^{-1} \log g_n(\tau, L; (n, n, ..., n)) = \kappa(L), \tag{4.7}$$

was proved for $L = 0$ in [10] and for $L > 0$ in Whittington and Soteros [15]. Similar arguments can also be used to show that, for $L \geq 1$,

$$\lim_{n\to\infty} N^{-1} \log g_N(\tau, L; \phi(n)) = \kappa(L), \tag{4.8}$$

where $g_N(\tau, L; \phi(n))$ is the number of embeddings of τ in an L-slab with edge distribution $\phi(n)$ and where the restrictions put on $\{\phi(n)\}_{n\geq 1}$ are similar to to those listed in Lemma 2.6.

Using arguments analogous to those which prove Lemma 3.2, the following pattern theorem holds for embeddings of graphs in an L-slab.

LEMMA 4.5. *Given any $m_1 > 0$ and $m_2 > 0$ and any pattern P which is an undirected version of a $K_{m_1,m_2}(L)$ pattern, let $g_n(\tau, L; \bar{P})$ be the number of n-edge embeddings of τ in an L-slab (up to translation) which do not contain the pattern P. For $L > 1$ and τ any graph in G_6,*

$$\limsup_{n\to\infty} n^{-1} \log g_n(\tau, L; \bar{P}) \leq \kappa(L; \bar{P}) < \kappa(L); \tag{4.9}$$

for $L = 1$ and τ any graph in G_5,

$$\limsup_{n\to\infty} n^{-1} \log g_n(\tau, L; \bar{P}) \leq \kappa(L; \bar{P}) < \kappa(1). \tag{4.10}$$

For each $L \geq 1$ it is possible to construct a tight trefoil pattern $T(L)$ so that if $T(L)^q$ appears in a cycle of an embedding, the embedding will surely be knotted. The tight trefoil pattern T introduced in Figure 3.1 is in fact suitable for all $L \geq 1$. Based on Lemma 4.3 with P an appropriate tight trefoil, the following result for unknotted polygons in an L-slab has been proved.

LEMMA 4.6 (TESI *et al* 1994 [4]). *Let $p_n^o(L)$ be the number (up to translation) of n-edge unknotted self-avoiding polygons in an L-slab. Then the limit in the following inequality exists and satisfies*

$$\lim_{n\to\infty}(2n)^{-1}\log p_{2n}^o(L)=\kappa_o(L)<\kappa(L) \tag{4.11}$$

for all $L\geq 1$, $\kappa_o(L)$ is a concave function of L,

$$\lim_{L\to\infty}\kappa_o(L)=\kappa_o, \tag{4.12}$$

and

$$\lim_{L\to\infty}\kappa(L)-\kappa_o(L)=\alpha \tag{4.13}$$

where α is defined as in equation (3.9).

The numerical evidence presented in [4,14] indicates that $\alpha(L)\equiv\kappa(L)-\kappa_o(L)$ is a decreasing function of L and hence the probability of a polygon being knotted increases as the height L of the slab decreases.

Using Lemma 4.6 and arguing as in the proof of Theorem 3.1, the following theorem for knots in graphs in an L-slab results.

THEOREM 4.1. *For $L>1$ ($L=1$), suppose $\tau\in G_6$ (G_5) has no cut edges,*

$$\begin{aligned}\kappa_o(L)\leq\liminf_{n\to\infty}n^{-1}\log g_n^o(\tau,L) &\leq \limsup_{n\to\infty}n^{-1}\log g_n^o(\tau,L)\\ &\leq \kappa(\bar{T}^q,L)<\kappa(L)\end{aligned} \tag{4.14}$$

(where the limit is taken only through values of n for which $g_n^o(\tau,L)>0$) and hence the probability that an n-edge embedding of τ is knotted goes to unity at least as fast as

$$1-e^{-\beta(L)n+o(n)} \tag{4.15}$$

and no faster than

$$1-e^{-\alpha(L)n+o(n)} \tag{4.16}$$

when $n\to\infty$, with $\beta(L)=\kappa(L)-\kappa(\bar{T}^q,L)$ and $\alpha(L)=\kappa(L)-\kappa_o(L)$.

If $\tau\in\tilde{G}_6$ ($\tilde{G}_5$) is eulerian

$$\lim_{n\to\infty}(2n)^{-1}\log g_{2n}^o(\tau)=\kappa_o(L) \tag{4.17}$$

and hence the probability that an n-edge embedding of τ is knotted goes to unity as

$$1-e^{-\alpha(L)n+o(n)} \tag{4.18}$$

when $n\to\infty$.

A result analogous to Theorem 3.2 also holds for embeddings of τ with a fixed edge distribution sequence.

5. Knots in Graphs in an (L, M)-Prism. An (L, M)-rectangular prism (or tube), is defined to be the sublattice of Z^3 induced by the vertex set $\{(x, y, z) \in Z^3 | 0 \leq y \leq L, 0 \leq z \leq M\}$. Let $c_n(L, M)$ be the number of self-avoiding walks confined to an (L, M)-prism, let $p_n(L, M)$ be the number (up to translation) of n-edge self-avoiding polygons confined to an (L, M)-prism, and given a graph $\tau \in G_6$, let $g_n(\tau, L, M)$ be the number (up to translation) of n-edge embeddings of τ in an (L, M)-prism.

The procedure followed in the last two sections to obtain results about knots in graphs no longer works for embeddings of graphs in an (L, M)-prism. In fact the procedure fails at the first step because there is no result, such as the result in Lemma 4.1 for walks and polygons in an L-slab, which equates the growth constants for self-avoiding walks and polygons in a prism. Instead as the following two results indicate the number of self-avoiding polygons in an (L, M)-prism is exponentially smaller than the number of self-avoiding walks in an (L, M)-prism.

LEMMA 5.1 (SOTEROS AND WHITTINGTON 1989 [16]). *The following limit exits*

$$\lim_{n \to \infty} n^{-1} \log c_n(L, M) \equiv \kappa(L, M). \tag{5.1}$$

LEMMA 5.2 (SOTEROS AND WHITTINGTON 1989 [16]). *The limit in the following inequality exists and satisfies*

$$\lim_{n \to \infty} (2n)^{-1} \log p_{2n}(L, M) \equiv \kappa_p(L, M) < \kappa(L, M). \tag{5.2}$$

A pattern theorem for self-avoiding walks in an (L, M)-prism was also proved in [16]. Let $\mathcal{C}_b(L, M)$ be the set of self-avoiding walks completely contained in $D_b(L, M) = \{(x, y, z) \in Z^3 | 0 \leq x \leq b, 0 \leq y \leq L, 0 \leq z \leq M\}$ with one endpoint at the origin and the other at $(b, 0, 0)$. For any $b > 0$, a K_b pattern is defined to be any self-avoiding walk which can occur in some element of $\mathcal{C}_b(L, M)$.

LEMMA 5.3 (SOTEROS AND WHITTINGTON 1989 [16]). *For any $b >$ 0, let P be a K_b pattern, then*

$$\lim_{n \to \infty} n^{-1} \log c_n(L, M; \bar{P}) \equiv \kappa(L, M; \bar{P}) < \kappa(L, M). \tag{5.3}$$

With regards to embeddings of graphs in an (L, M)-prism, the following results indicates that if a graph has a cut edge then its growth constant is the same as that for self-avoiding walks, if a graph is eulerian then its growth constant is the same as that for self-avoiding polygons, otherwise it remains even to be proved that the growth constant exists.

LEMMA 5.4. *Given a graph $\tau \in G_6$ such that $g_n(\tau, L, M) > 0$ for some n, if τ has a cut edge*

$$\lim_{n \to \infty} n^{-1} \log g_n(\tau, L, M) = \kappa(L, M); \tag{5.4}$$

if τ is eulerian

$$\lim_{n\to\infty}(2n)^{-1}\log g_{2n}(\tau,L,M)=\kappa_p(L,M); \tag{5.5}$$

and if τ is not eulerian and has no cut edges

$$\begin{aligned}\kappa_p(L,M)\le\liminf_{n\to\infty}n^{-1}\log g_n(\tau,L,M)\le\quad&\limsup_{n\to\infty}n^{-1}\log g_n(\tau,L,M)\\ &<\kappa(L,M).\end{aligned} \tag{5.6}$$

Proof. In the case that τ has a cut edge an upper bound is obtained, just as in the proof of Lemma 2.4, by separating an embedding of τ into self-avoiding walks (each confined to an (L,M)-prism) to give

$$\begin{aligned}g_n(\tau,L,M)\quad&\le\sum_{\{m_i|\sum_{i=1}^{f}m_i=n\}}c_{m_1}(L,M)c_{m_2}(L,M)\cdots c_{m_f}(L,M)\\ &\le e^{\kappa(L,M)n+o(n)}.\end{aligned} \tag{5.7}$$

For the lower bound an argument similar to that used in [10, Theorem 3] is used. Fix a cut edge of τ. Obtain two rooted graphs, τ_L and τ_R, from τ by deleting the cut edge. Find an embedding of τ_L (τ_R) in an (L,M)-prism such that its root, the vertex which was connected to the designated cut edge of τ, is in the rightmost (leftmost) plane of the embedding. The two embeddings of τ_L and τ_R can now be concatenated together by concatenating the first vertex of an n-step *unfolded* walk (or bridge) to τ_L's root and then concatenating the walk's last vertex to τ_R's root (the concatenation of the walk to the roots is done using two short walks each with lengths less than $2(L+1)(M+1)$). This gives the lower bound

$$c_n^{\dagger}(L,M)\le g_{n+m}(\tau,L,M) \tag{5.8}$$

where m is the number of edges of the resulting embedding that were not initially part of the unfolded walk and $c_n^{\dagger}(L,M)$ is the number of n-step unfolded self-avoiding walks in an (L,M)-prism. It has been proved [17] (see also [7, section 8.2]) that

$$\lim_{n\to\infty}n^{-1}\log c_n^{\dagger}(L,M)=\kappa(L,M). \tag{5.9}$$

Hence taking logarithms, dividing by n, and letting $n\to\infty$ in equations (5.7) and (5.8) gives equation (5.4).

In the case that τ is eulerian, an argument similar to that used to obtain equation (3.13) is used. That is, an upper bound is obtained by separating τ into self-avoiding polygons and a lower bound is obtained by concatenating a polygon to an embedding of τ. Taking logarithms, dividing by n, and letting $n\to\infty$ in the resulting inequalities leads to equation (5.5).

For τ with no cut edges and not eulerian, for example τ a θ graph, a lower bound can be obtained by concatenating a polygon to an embedding of τ. This leads to the left-hand side of equation (5.6). Since every branch of τ is contained in a cycle, no branch of τ can contain either of the *filling patterns* depicted in [16, Figure 4] (these patterns cannot appear in any self-avoiding polygon). Thus equation (5.7) becomes

$$\begin{aligned} g_n(\tau, L, M) &\leq {\sum}' c_{m_1}(L, M; \bar{P_F}) c_{m_2}(L, M; \bar{P_F}) \cdots c_{m_f}(L, M; \bar{P_F}) \\ &\leq e^{\kappa(L,M;\bar{P_f})n + o(n)} \end{aligned} \tag{5.10}$$

where P_F is the appropriate filling pattern and the primed sum is over the set $\{m_i | \sum_{i=1}^{f} m_i = n\}$. Equation (5.10) and Lemma 5.3 imply equation (5.6). □

To obtain results for embeddings of graphs with a fixed edge distribution sequence, a pattern theorem for self-avoiding polygons in an (L, M)-prism is needed. Due to Lemma 5.2, a pattern theorem for self-avoiding walks in a prism does not imply a pattern theorem for self-avoiding polygons. Instead, a separate pattern theorem for self-avoiding polygons in an (L, M)-prism is needed. The required pattern theorem is introduced here and a proof is given in the next section.

Define $\mathcal{P}(L, M)$ to be the set of self-avoiding polygons in an (L, M)-prism. Let $\mathcal{P}_b(L, M) \subseteq \mathcal{P}(L, M)$ be the set of self-avoiding polygons confined to the subgraph of the prism given by the vertex set $V_b = \{(x, y, z) \in Z^3 | 0 \leq x \leq b, 0 \leq y \leq L, 0 \leq z \leq M\}$. Given any $b > 0$, a $\tilde{K}_b$ pattern is defined to be a configuration (including occupied and unoccupied edges) of any element of $\mathcal{P}_b(L, M)$ in V_b with the edges in the $x = 0$ and $x = b$ planes excluded. Given a $\tilde{K}_b$ pattern P, define $p_n(L, M; \bar{P})$ to be the number (up to translation) of n-edge polygons confined to an (L, M)-prism in which the pattern P does not occur. The following lemma is a consequence of the pattern theorem that is proved in the next section.

LEMMA 5.5. *For any integer $b \geq 2$ and any $\tilde{K}_b$ pattern P,*

$$\lim_{n \to \infty} n^{-1} \log p_n(L, M; \bar{P}) \equiv \kappa_p(L, M; \bar{P}) < \kappa_p(L, M). \tag{5.11}$$

The prism pattern theorems, Lemma 5.4 and Lemma 5.5, can be used to investigate the growth constant for embeddings of a graph with a fixed edge distribution sequence. Instead of exploring all possible types of graph embeddings, the focus is on several illustrative cases to show that the growth constant for graph embeddings in an (L, M)-prism can be highly dependent on the structure of the graph and the restrictions put on the edge distribution sequence. First some special graphs are defined. The *4-watermelon graph* is defined to be the graph with two vertices, v_1 and v_2, and four edges, each of the form $\{v_1, v_2\}$. A *dumbell graph* is the graph with two vertices of degree 3 and three edges, one edge from one vertex of the graph to the other and two loops, one from each vertex to itself. A *3-star* is a graph with one vertex of degree 3, 3 vertices of degree 1, and three edges, one from the vertex of degree 3 to each vertex of degree 1. The following theorem indicates that if the fast growing branches of τ form a chain with essentially free ends then the embeddings of τ have the same growth constant as self-avoiding walks; however, if instead there is a fast growing branch in a cycle or three fast growing branches form a 3-star the embeddings have less freedom or entropy than self-avoiding walks and the growth constant is reduced. Furthermore, if the fast growing branches of τ are contained in at most two loops of τ then the embeddings of τ have the same growth constant as self-avoiding polygons; however, if instead the fast growing branches are contained in at least three branches of a 4-watermelon graph the embeddings have less freedom or entropy and the growth constant is reduced.

LEMMA 5.6. *Given $L \geq 1$, $M \geq 1$, suppose that $\tau \in G_6$ is such that $g_n(\tau, L, M) > 0$ for some n and that $\{\phi(n)\}_{n\geq 1}$ is an edge distribution sequence for τ such that $g_N(\tau, L, M; \phi(n)) > 0$ for all $n \geq 1$ and for each i, $\phi_i(n)$ is either a constant or strictly increasing function of n.*

First suppose τ has a cut edge. Also suppose $\{\phi(n)\}_{n\geq 1}$ is such that all the fast growing branches of τ are cut edges and that when they are removed from τ, τ decomposes into components each of which was connected to at most two fast growing branches of τ. In this case

$$\lim_{n\to\infty} N^{-1} \log g_N(\tau, L, M; \phi(n)) = \kappa(L, M). \tag{5.12}$$

On the other hand, if $\{\phi(n)\}_{n\geq 1}$ is such that either there is a fast growing branch that is contained within a cycle or there are three or more fast growing branches connected to one branch point, then

$$\limsup_{n\to\infty} N^{-1} \log g_N(\tau, L, M; \phi(n)) < \kappa(L, M). \tag{5.13}$$

Now suppose τ has at least one cycle and $\{\phi(n)\}_{n\geq 1}$ is such that all fast growing branches are contained within an eulerian subgraph (not necessarily connected) of τ. Then in general

$$\limsup_{n\to\infty} N^{-1} \log g_N(\tau, L, M; \phi(n)) \leq \kappa_p(L, M). \tag{5.14}$$

Furthermore, if $\{\phi(n)\}_{n\geq 1}$ is such that all fast growing branches are contained in either of two loops of τ, then

$$\lim_{n\to\infty} N^{-1} \log g_N(\tau, L, M; \phi(n)) = \kappa_p(L, M). \tag{5.15}$$

However, if τ has a subgraph which is homeomorphic to the 4-watermelon graph and if $\{\phi(n)\}_{n\geq 1}$ is such that at least three of the watermelon branches each contain a fast growing branch of τ, then

$$\limsup_{n\to\infty} N^{-1} \log g_N(\tau, L, M; \phi(n)) < \kappa_p(L, M). \tag{5.16}$$

Proof. Let τ be any graph in G_6 such that $g_n(\tau, L, M) > 0$ for some n and that $\{\phi(n)\}_{n\geq 1}$ is an edge distribution sequence for τ such that $g_N(\tau, L, M; \phi(n)) > 0$ for all $n \geq 1$.

First suppose τ has a cut edge. Since $g_N(\tau, L, M; \phi(n)) \leq g_N(\tau, L, M)$, equation (5.4) in Lemma 5.4 gives the upper bound

$$g_N(\tau, L, M; \phi(n)) \leq e^{\kappa(L,M)N+o(N)}. \tag{5.17}$$

Next suppose $\{\phi(n)\}_{n\geq 1}$ is such that all the fast growing branches of τ are cut edges and that when they are removed from τ, τ decomposes into components each of which was connected to at most two fast growing branches of τ. In this case a lower bound can be obtained for $g_N(\tau, L, M; \phi(n))$ in terms of $\kappa(L, M)$ as follows. Suppose τ has f' growing branches. Remove each fast growing branch from τ, this results in a disconnected graph with $f' + 1$ components, $\tau_1, ..., \tau_{f'+1}$, where by relabelling as appropriate we can assume that the ith fast growing branch of τ connects component τ_i to component τ_{i+1} in τ. Then arguing as in the proof of Lemma 5.4, by concatenating together elements of an alternating sequence of component embeddings and unfolded walks the following lower bound is obtained

$$c^{\dagger}_{\phi_1(n)-m_1} \cdots c^{\dagger}_{\phi_{f'}(n)-m_{f'}} \leq g_N(\tau, L, M; \phi(n)) \tag{5.18}$$

where $m_1, ..., m_{f'}$ are independent of n. Since $\lim_{n\to\infty} \frac{\sum_{i=1}^{f'} \phi_i(n)}{N} = 1$, this lower bound and equation (5.17) leads to equation (5.12).

Now suppose $\{\phi(n)\}_{n\geq 1}$ is such that either there is a fast growing branch of τ that is contained within a cycle or there are three or more fast growing branches connected to one branch point. As noted in the proof of Lemma 5.4, any branch of τ which is contained in a cycle cannot contain the filling pattern P_F. Thus if the ith branch of τ is a fast growing branch that is contained within a cycle

$$\begin{aligned} g_N(\tau, L, M; \phi(n)) &\leq c_{\phi_i(n)}(L, M; \bar{P_F}) \prod_{j=1, j\neq i}^{f} c_{\phi_j(n)}(L, M) \\ &\leq e^{(N-\phi_i(n))\kappa(L,M)+\phi_i(n)\kappa(L,M;\bar{P_F})+o(N)}. \end{aligned} \tag{5.19}$$

Taking logarithms, dividing by N, and letting $n \to \infty$ in this equation gives equation (5.13). Similarly, if three or more branches of τ are joined at a single branch point then at least one of these branches cannot contain the filling pattern P_F (if all three contained P_F then at least two of the branches will intersect each other at a vertex other than the common branch point). In this case, let i, $i + 1$ and $i + 2$ be the labels of the three fast growing branches

$$g_N(\tau, L, M; \phi(n)) \leq \left[\sum_{j=0}^{2} c_{\phi_{i+j}(n)}(L, M; \bar{P_F})\right] \prod_{m=1, m\neq i+j} c_{\phi_m(n)}(L, M)$$

$$\leq e^{(N-\phi_k(n))\kappa(L,M)+\phi_k(n)\kappa(L,M;\bar{P_F})+o(N)} \tag{5.20}$$

where $k \in \{i, i+1, i+2\}$ and $\lim_{n\to\infty} \frac{\phi_k(n)}{N} = \min_{0\leq j\leq 2}\{\lim_{n\to\infty} \frac{\phi_{i+j}(n)}{N}\}$. Taking logarithms, dividing by N, and letting $n \to \infty$ in this equation again gives equation (5.13).

If the only fast growing branches of τ are in an eulerian subgraph (not necessarily connected) η of τ, then by separating the eulerian subraph into f_p self-avoiding polygons and the remaining branches of τ into f' self-avoiding walks the following upper bound is obtained,

$$\begin{aligned} g_N(\tau, L, M; \phi(n)) &\leq R_\eta(N)\left[\prod_{i=1}^{f'} c_{\phi_i(n)}(L, M)\right]\prod_{j=1}^{f'} p_{m_j}(L, M) \\ &\leq e^{\kappa_p(L,M)N+o(N)} \end{aligned} \tag{5.21}$$

where $R_\eta(N)$ is as defined in equation (3.19), m_i is the number of edges in η's ith self-avoiding polygon, and the fact that $\lim_{n\to\infty} \frac{\phi_i(n)}{N} = 0$ for $i = 1, ..., f'$ has been used to obtain the rightmost inequality. This leads to equation (5.14).

If τ is a figure eight graph, then a lower bound can be obtained for $g_n(\tau, L, M; \phi(n))$ in terms of $\kappa_p(L, M)$ by taking any two polygons with appropriate numbers of edges and then concatenating them (using O(LM) additonal edges) together to create an embedding of a figure eight graph. The resulting lower bound combined with equation (5.14) leads to equation (5.15). Furthermore, if, for example, $\{\phi(n)\}_{n\geq 1}$ is such that τ has at most two fast growing branches each of which forms a loop of τ (an example is the case that τ is a dumbbell graph in which its cut edge is not fast growing), then the argument just described for a figure eight graph works in a similar way to give equation (5.15).

If τ is a 4-watermelon graph, an upper bound for $g_n(\tau, L, M; \phi(n))$ can be obtained by separating τ into two doubly rooted self-avoiding polygons. There are three ways to pair off the branches of τ to form polygons. Given an embedding of τ there is always at least one way to pair off the branches so that one of the two resulting polygons does not contain the filling pattern $P_{\hat{F}}$ depicted in Figure 5.1 (the pattern is defined so that the branch points of the watermelon cannot be within the pattern and so that it cannot appear in more than two branches of the 4-watermelon graph). Given an embedding of τ, relabel the four branches so that branch 1 and 2 are used to form a polygon which does not contain pattern $P_{\hat{F}}$ and let this be the last in the sequence of polygons obtained from τ. Thus,

$$\begin{aligned} g_N(\tau, L, M; \phi(n)) &\leq N^4 p_{\phi_3(n)+\phi_4(n)}(L, M) p_{\phi_1(n)+\phi_2(n)}(L, M; \bar{P_{\hat{F}}}) \\ &\leq e^{(N-\phi_1(n)-\phi_2(n))\kappa_p(L,M)+(\phi_1(n)+\phi_2(n))\kappa_p(L,M;\bar{P_{\hat{F}}})+o(N)}. \end{aligned} \tag{5.22}$$

If at least three of the branches are fast growing then at least one of the branches 1, 2 will be fast growing. Taking logarithms, dividing by N, letting

$n \to \infty$ in the above equation gives equation (5.16) for the case that τ is a 4-watermelon graph. This same argument works if τ has a subgraph which is homeomorphic to a 4-watermelon graph and $\{\phi(n)\}_{n\geq 1}$ is such that each of three of the branches of the watermelon contain fast growing branches of τ. There are also other types of graphs and edge distribution sequences for which equation (5.16) will hold. □

Note that equation (5.13) was shown for $\phi(n) = (n, n, ..., n)$ (i.e. uniform embeddings) in [15].

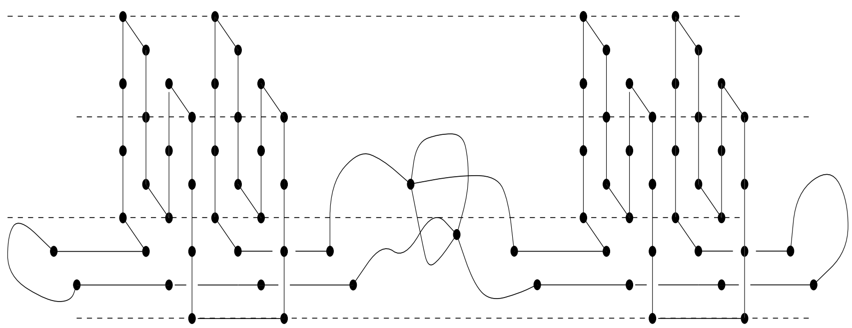

FIG. 5.1. *The bold pattern (either on the left or the right of the prism) is a filling pattern $\hat{P}_F$ which cannot appear in more than two branches of a 4-watermelon graph in a (3,3)-prism. A similar filling pattern exists for an (L, M)-prism.*

Next the probability that a graph embedding is knotted is investigated. Define $p_n^o(L, M)$ to be the number (up to translation) of unknotted self-avoiding polygons in an (L, M)-prism. Similarly, define $g_n^o(\tau, L, M)$ to be the number (up to translation) of unknotted embeddings of τ in an (L, M)-prism. A tight trefoil $\tilde{K}_b$ pattern is now needed. Consider T in Figure 3.1, suppose the left most vertex in T is the origin. T can be made into a $\tilde{K}_5$ pattern by adding in 5 connected edges starting at $(0, 0, -1)$ and ending at $(5, 0, -1)$ (or starting at $(0, -2, 0)$ and ending at $(0, -2, 5)$) and such a pattern can fit in an (L, M)-prism for $L \geq 3$, $M \geq 2$ (or $L \geq 4, M \geq 1$). Using the pattern theorem for self-avoiding polygons in a prism (Lemma 5.5) and a concatenation argument, the following result can be proved for any L and M for which a tight trefoil pattern in an (L, M)-prism exists.

LEMMA 5.7. *For L and M such that the (L, M)-prism contains a tight trefoil $\tilde{K}_b$ pattern for some $b > 0$,*

$$\lim_{n\to\infty} n^{-1} \log p_n^o(L, M) \equiv \kappa_o(L, M) < \kappa_p(L, M) \tag{5.23}$$

and hence the probability that a self-avoiding polygon in an (L, M)-prism is knotted goes to unity as

$$1 - e^{-\alpha(L,M)n+o(n)} \tag{5.24}$$

when $n \to \infty$, with $\alpha(L,M) = \kappa_p(L,M) - \kappa_o(L,M)$.

It is now possible to obtain results about knots in graphs in an (L,M)-prism using Lemma 5.7 and focussing on the cases in which the embeddings of a graph have growth constant equal to $\kappa_p(L,M)$.

THEOREM 5.1. *Let L and M be as in Lemma 5.7 and T be an appropriate tight trefoil $\tilde{K}_b$ pattern for some $b > 0$. Given eulerian $\tau \in G_6$ such that $g_n(\tau, L, M) > 0$ for some $n > 0$,*

$$\begin{aligned}\kappa_o(L,M) &\le \liminf_{n\to\infty} n^{-1} \log g_n^o(\tau,L,M) \\ &\le \limsup_{n\to\infty} n^{-1} \log g_n^o(\tau,L,M) \le \kappa_p(L,M;\bar{T}^q) < \kappa_p(L,M). \qquad (5.25)\end{aligned}$$

Further, given any $\tau \in G_6$ and an edge distribution sequence such that equation (5.15) is true and there exists an unknotted embedding of τ with edge distribution $\phi(1)$,

$$\begin{aligned}\kappa_o(L,M) &\le \liminf_{n\to\infty} N^{-1} \log g_N^o(\tau,L,M;\phi(n)) \\ &\le \limsup_{n\to\infty} N^{-1} \log g_N^o(\tau,L,M;\phi(n)) \\ &\le \kappa_p(L,M;\bar{T}^q) < \kappa_p(L,M). \qquad (5.26)\end{aligned}$$

In both these cases the probability that an appropriate n-edge embedding of τ in an (L,M)-prism is knotted goes to unity at least as fast as

$$1 - e^{-\beta(L,M)N + o(N)} \qquad (5.27)$$

and no faster than

$$1 - e^{-\alpha(L,M)N + o(N)} \qquad (5.28)$$

when $n \to \infty$, with $\beta(L,M) \equiv \kappa_p(L,M) - \kappa_p(L,M;\bar{T}^q)$ and $\alpha(L,M)$ as in Lemma 5.7.

For $\tau \in \tilde{G}_6$, these results can be strengthened to:

$$\lim_{n\to\infty} n^{-1} \log g_n^o(\tau,L,M) = \kappa_o(L,M) \qquad (5.29)$$

for eulerian graphs and

$$\lim_{n\to\infty} N^{-1} \log g_N^o(\tau,L,M;\phi(n)) = \kappa_o(L,M) \qquad (5.30)$$

for any τ and edge distribution sequence such that equation (5.15) is true. In both these cases the probability that an appropriate n-edge embedding of τ is knotted goes to unity as

$$1 - e^{-\alpha(L,M)N + o(N)} \qquad (5.31)$$

when $n \to \infty$.

Proof. Obtain bounds for $g_n^o(\tau,L,M)$ and $g_N^o(\tau,L,M;\phi(n))$ as in the proofs of equations (5.5) and (5.15), except instead of obtaining bounds in terms of arbitrary self-avoiding polygons either self-avoiding polygons which do not contain T^q or unknotted self-avoiding polygons (depending on whether $\tau \in G_6 - \tilde{G}_6$ or $\tau \in \tilde{G}_6$) are used. ∎

6. A Pattern Theorem for Self-Avoiding Polygons in a (L, M)-Prism. In this section a transfer matrix approach, the same as that used by Alm and Janson in their study of self-avoiding walks in one-dimensional lattices [18], is used to prove a pattern theorem for self-avoiding polygons in a rectangular prism.

An (L, M)-prism is equivalent to $Z \times H(L, M)$, where $H(L, M)$ is the finite subgraph of Z^2 induced by the vertex set $\{(y, z) \in Z^2 | 0 \leq y \leq L, 0 \leq z \leq M\}$, and hence, in the terminology of [18], an (L, M)-prism is a one-dimensional lattice. An (L, M)-prism can also be thought of as an alternating sequence of *hinges* and *sections* where for any $i \in Z$ the ith hinge, $H_i(L, M)$, is defined to be the subgraph of the prism induced by the vertex set $\{(i, y, z) \in Z^3 | 0 \leq y \leq L, 0 \leq z \leq M\}$ and the ith section, $S_i(L, M)$, is defined to be the set of edges which join $H_{i-1}(L, M)$ to $H_i(L, M)$ in the prism.

A self-avoiding polygon in an (L, M)-prism is said to span m sections of the prism if the edges of the self-avoiding polygon are contained in $H_{i-1}(L, M) \cup S_i(L, M) \cup H_i(L, M) \cup ... \cup S_{i+m-1}(L, M) \cup H_{i+m-1}(L, M)$ for some $i \in Z$. Clearly, given an n-edge self-avoiding polygon in an (L, M)-prism there exists some $m \in \{1, ..., \frac{n-2}{2}\}$ such that the polygon spans m sections of the prism; define m to be the *span* of the given self-avoiding polygon.

Without loss of generality, assume that the first hinge and section of any self-avoiding polygon in an (L, M)-prism are respectively $H_0(L, M)$ and $S_1(L, M)$ and define the *last* section and hinge to be $S_m(L, M)$ and $H_m(L, M)$, respectively, where m is the span of the polygon. Furthermore, for any polygon in an (L, M)-prism the edges of the polygon can be directed and ordered in the following way: consider the vertices joined by an edge of the polygon to the polygon's bottom vertex (the first vertex of the polygon in a lexicographic ordering of the coordinates of the polygon's vertices), of these choose the smallest (lexicographically) vertex and direct an edge from the bottom vertex to this vertex. This edge is considered the first in the ordering of the edges. The ordering and orientation of the remaining edges continues in a cyclic fashion around the polygon. Given a self-avoiding polygon in an (L, M)-prism with span m, define a *pattern* with span k of the polygon to be the polygon's *configuration* in a sublattice of the form $S_i(L, M) \cup H_i(L, M) \cup ... \cup H_{i+k-2}(L, M) \cup S_{i+k-1}(L, M)$ for $1 \leq i \leq m - k + 1$. The polygon's configuration in such a sublattice of the prism consists of the sublattice, the set of directed edges of the polygon in the sublattice, and if there are e edges of the polygon in the sublattice then they are ordered from 1 to e according to their ordering in the polygon. We say the pattern of span k corresponding to a polygon's configuration in $S_i(L, M) \cup H_i(L, M) \cup ... \cup H_{i+k-2}(L, M) \cup S_{i+k-1}(L, M)$ *occurs* at the ith section of the polygon. Figure 6.1 depicts a self-avoiding polygon in a $(0, 4)$-prism and its associated patterns with span 2. Given $k \geq 2$, define $\Pi(k)$ to be the set of distinct patterns with span k that occur in at least one self-avoiding polygon in an (L, M)-prism.

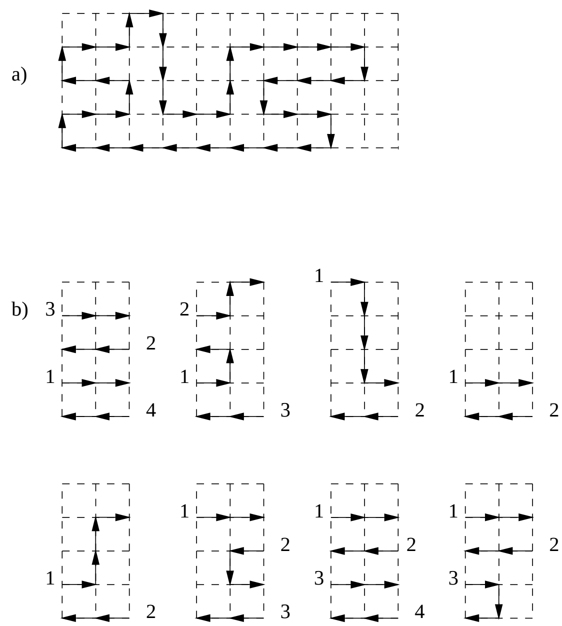

FIG. 6.1. *(a) A self-avoiding polygon in a* $(0,4)$*-prism along with (b) its eight associated patterns with span 2. The numbering on the sides of each pattern indicates the order in which the separate walks making up the pattern should be traversed. Thus the pattern occuring at section 1 of the polygon is different from the pattern occuring at section 7.*

Consider $\hat{\mathcal{P}}(L, M)$, the set of self-avoiding polygons in an (L, M)-prism with the following properties: the only edge in $H_0(L, M)$ is the edge between $(0, 0, 0)$ and $(0, 0, 1)$; the only edges in $S_1(L, M)$ are the edge between $(1, 0, 0)$ and $(0, 0, 0)$ and the edge between $(0, 0, 1)$ and $(1, 0, 1)$; the only edges in $S_m(L, M)$ are the edge between $(m, 0, 0)$ and $(m-1, 0, 0)$ and the edge between $(m-1, 0, 1)$ and $(m, 0, 1)$, for m the span of the polygon; the only edge in $H_m(L, M)$ is the edge between $(m, 0, 0)$ and $(m, 0, 1)$; and if the edges of the polygon are oriented in a cyclic fashion starting from $(0, 0, 0)$ to $(0, 0, 1)$, then the orientation of the edge in $H_m(L, M)$ is from $(m, 0, 1)$ to $(m, 0, 0)$. Let $\hat{p}_n(L, M)$ be the number of such self-avoiding polygons with n-edges.

The following result indicates that the growth constant for $\hat{p}_n(L, M)$ is the same as the growth constant for $p_n(L, M)$.

LEMMA 6.1.

$$\lim_{n\to\infty} n^{-1} \log \hat{p}_n(L, M) = \kappa_p(L, M). \tag{6.1}$$

Also, for any integer $k \geq 1$ *and any pattern* $\pi \in \Pi(k)$, π *can occur in an* *element of* $\hat{\mathcal{P}}(L, M)$.

Proof. Clearly

$$\hat{p}_n(L, M) \leq p_n(L, M). \tag{6.2}$$

To get a lower bound for $\hat{p}_n(L, M)$, start with any n-edge polygon in an (L, M)-prism. Orient and order the edges of the polygon in a cyclic fashion as described previously. It is always possible to concatenate an oriented polygon (with on the order of $(2L + 2M)$ edges) to the first edge and another oriented polygon (with on the order of $(2L + 2M)$ edges) to the last edge in the rightmost plane, so that the resulting polygon is an element of $\hat{\mathcal{P}}(L, M)$. Thus

$$p_n(L, M) \leq \hat{p}_{n+O(2L+2M)}(L, M) \tag{6.3}$$

where the function $O(2L+2M)$ does not depend on n. Taking logarithms, dividing by n, and then letting n go to infinity in equations (6.3) and (6.2) results in equation (6.1).

Also, given a pattern $\pi \in \Pi(k)$ there exists a self-avoiding polygon in an (L, M)-prism such that π occurs in the self-avoiding polygon. Fix such a self-avoiding polygon and now, as in the argument leading to the lower bound for $\hat{p}_n(L, M)$, concatenate polygons to the first and last hinge of the initial polygon to create an element of $\hat{\mathcal{P}}(L, M)$. Thus an element of $\hat{\mathcal{P}}(L, M)$ has been created in which the pattern π occurs. □

For any integer $k \geq 1$ and given a pattern $\pi \in \Pi(k)$, define $p_n(N, M; \bar{\pi})$ to be the number (up to translation) of n-edge polygons in an (L, M)-prism that do not have π as a pattern. Similarly, define $\hat{p}_n(N, M; \bar{\pi})$ to be the number of n-edge polygons of $\hat{\mathcal{P}}(L, M)$ that do not have π as a pattern. The following is a pattern theorem for self-avoiding polygons in an (L, M)-prism.

THEOREM 6.1. *For any integer* $k \geq 2$ *and any pattern* $\pi \in \Pi(k)$,

$$\begin{aligned}\lim_{n\to\infty} n^{-1}\log p_n(L, M; \bar{\pi}) = \lim_{n\to\infty} n^{-1}\log \hat{p}_n(L, M; \bar{\pi}) &\equiv \kappa_p(L, M; \bar{\pi}) \\ &< \kappa_p(L, M).\end{aligned} \tag{6.4}$$

Proof. Note first that if the second limit in the above equation exists then the arguments of Lemma 6.1 imply that

$$\lim_{n\to\infty} n^{-1}\log p_n(L, M; \bar{\pi}) = \lim_{n\to\infty} n^{-1}\log \hat{p}_n(L, M; \bar{\pi}). \tag{6.5}$$

In particular, given the pattern π, one can always convert a polygon in an (L, M)-prism into an element of $\hat{P}(L, M)$ by a concatenation process which ensures that if π does not occur in the original polygon then it does not occur in the final polygon. Thus in the remainder of the proof the focus will be on the set of polygons in $\hat{P}(L, M)$.

Given $k \geq 2$, consider the set of all possible patterns with span k, $\Pi(k)$. Each such pattern can be considered as a polygon configuration of

$S_1(L,M)\cup H_1(L,M)\cup\ldots\cup H_{k-1}(L,M)\cup S_k(L,M)$. Since these patterns are contained in a finite subgraph of the lattice there is clearly a finite number of such patterns. Order them from 1 to $|\Pi(k)|$. For the ith pattern, define e_i to be the number of polygon edges contained in $S_1(L,M)\cup H_1(L,M)$. We can construct a transfer matrix $G(x)=(g_{i,j}(x))$ in the following way:

$$g_{i,j}(x)=\begin{cases} x^{e_i} & \begin{array}{c}\text{if the configuration of pattern } i \text{ on}\\ S_2(L,M)\cup H_2(L,M)\cup\ldots\cup H_{k-1}(L,M)\cup S_k(L,M)\\ \text{equals the configuration of pattern } j \text{ on}\\ S_1(L,M)\cup H_1(L,M)\cup\ldots\cup H_{k-2}(L,M)\cup S_{k-1}(L,M)\end{array}\\ & \\ 0 & \text{otherwise.}\end{cases}$$

(6.6)

Define the pattern $\phi\in\Pi(k)$ to be the pattern with the following configuration: the first polygon edge goes from (0,0,1) to (1,0,1), the second edge goes from (1,0,1) to (2,0,1),..., the kth edge goes from ($k-1$,0,1) to (k,0,1), the $k+1$st edge goes from (k,0,0) to ($k-1$,0,0), the $k+2$nd edge goes from ($k-1$,0,0) to ($k-2$,0,0), ..., the ($2k$)th edge goes from (1,0,0) to (0,0,0). Let ϕ also represent the index of ϕ in the labelling of all patterns in $\Pi(k)$.

Consider a sequence of $r\geq 2$ patterns in $\Pi(k)$ of the form ϕ, π_{i_2}, π_{i_3}, ..., $\pi_{i_{r-1}}$, ϕ such that $g_{\phi,i_2}(x)\neq 0$, $g_{i_{r-1},\phi}(x)\neq 0$, and $g_{i_j,i_{j+1}(x)}\neq 0$ for $2\leq j\leq r-2$. Then this sequence defines a pattern with span $r+k-1$ in which pattern ϕ occurs at the 1st and rth section and pattern π_{i_j} occurs at the jth section, for $j=2,\ldots,r-1$. The number of edges in this pattern is $2e_\phi+\sum_{j=2}^{r-1}e_{i_j}+2(k-1)$ where $e_\phi=2$ and the weight associated with this pattern in $(G(x)^{r-1})_{\phi,\phi}$ is $x^{e_\phi+\sum_{j=2}^{r-1}e_{i_j}}$. (The notation $(A)_{i,j}$ refers to the i,jth element of matrix A.)

Any pattern with span $r+k-1$ in which ϕ occurs at the 1st and rth section can be decomposed into a sequence of r patterns from $\Pi(k)$ as above. Note that for $r=2,\ldots,k$, the only pattern with span $r+k-1$ in which ϕ occurs at the 1st and rth section is the pattern which has ϕ occuring at each section. Also note that given $r\geq k$, a pattern with span $r+k-1$ and $2e_\phi+\sum_{j=2}^{r-1}e_{i_j}+2(k-1)$ edges corresponds to a self-avoiding polygon in $\hat{\mathcal{P}}(L,M)$ with span $r-k+1$ and $2e_\phi+\sum_{j=2}^{r-1}e_{i_j}-2(k-2)$ edges. Such a polygon is constructed from the pattern by deleting the $2(k-1)$ polygon edges of ϕ in $S_1(L,M)\cup H_1(L,M)\cup\ldots\cup S_{k-1}(L,M)\cup H_{k-1}(L,M)$, deleting the $2(k-1)$ polygon edges of ϕ in $H_r(L,M)\cup S_{r+1}(L,M)\cup H_{r+1}(L,M)\cup\ldots\cup S_{r+k-1}(L,M)$, and then adding edges from $(k-1,0,0)$ to $(k-1,0,1)$ and from $(r,0,1)$ to $(r,0,0)$. Translating the polygon so that the vertex $(k,0,0)$ is translated to $(0,0,0)$ results in a self-avoiding polygon in $\hat{\mathcal{P}}(L,M)$ with the properties as listed above. Figure 6.2 shows an example.

Thus the generating function $F(x)=\sum_{n=2}\hat{p}_{2n}(L,M)x^{2n}$ satisfies the

FIG. 6.2. *A pattern (on the left) starting and ending with $\phi \in \Pi(4)$ in a $(0,4)$-prism along with its associated self-avoiding polygon (on the right) in $\hat{\mathcal{P}}(0,4)$.*

following:

$$x^{2(k-3)}F(x) = (G(x)^{k-1})_{\phi,\phi}+(G(x)^k)_{\phi,\phi}+\ldots = (G(x)^{k-1}(I-G(x))^{-1})_{\phi,\phi} \tag{6.7}$$

where each non-zero term on the right hand side has a factor of x^{2k-2} (x^{2k-2} is the smallest power of x associated with a sequence of k correctly connected patterns with span k). Note that

$$(G(x)^{k-1}(I-G(x))^{-1})_{\phi,\phi} = \frac{\det(G(x)^{k-1})\det((I-G(x))(G(x)^{k-1})^{-1};\phi,\phi)}{\det(I-G(x))}. \tag{6.8}$$

Given any $x > 0$, it can be shown that for any pair of patterns i, j there exists an integer m such that $(G(x)^m)_{i,j} > 0$. (To see this, start with a polygon in $\hat{\mathcal{P}}(L,M)$ in which pattern i occurs and concatenate it to a polygon in $\hat{\mathcal{P}}(L,M)$ in which pattern j occurs. This yields a polygon in $\hat{\mathcal{P}}(L,M)$ in which pattern i occurs at some section and pattern j occurs at a later section. From this obtain a sequence of m correctly connected patterns starting with pattern i and ending in pattern j.) Also, $(G(x))_{\phi,\phi} = x^2 > 0$ for $x > 0$. Thus for $x > 0$, $G(x)$ is an irreducible and aperiodic matrix and Frobenius theory [19] implies that the spectral radius, $\rho(x)$, of $G(x)$ is a simple root of $\det(\lambda I - G(x))$, that $G(x)$ has a strictly positive eigenvector associated with $\rho(x)$, and that $\rho(x)$ is the only eigenvalue of modulus $\rho(x)$. $\rho(0) = 0$ and $\rho(x)$ is an unbounded, increasing, continuous function on $[0,\infty)$, hence there exists a unique $x_o > 0$ such that $\rho(x_o) = 1$. From equation (6.8), $F(x)$ has poles only when $\frac{1}{\det(I-G(x))}$ has poles, that is, when 1 is an eigenvalue of $G(x)$. Thus based on the results and arguments of [18, Lemma 9 and Theorem 3] $F(x)$ is analytic for $|x| < x_o$ and has one simple pole when $|x| = x_o$, namely, $x = x_o$. In particular, as $x \to x_o$

$$\begin{aligned}(x_o - x)F(x) &= (x_o - x)x^{6-2k}(G(x)^{k-1}(I-G(x))^{-1})_{\phi,\phi} \\ &\to x_o^{6-2k}(\zeta^T G'(x_o)\eta)^{-1}(\eta)_\phi(\zeta^T)_\phi > 0\end{aligned} \tag{6.9}$$

where η and ζ^T are strictly positive eigenvectors of $G(x_o)$ associated with $\rho(x_o) = 1$ and normalized so that $\zeta^T\eta = 1$. Thus, there exists $\alpha > 0$ such that

$$\hat{p}_n(L,M) = \alpha x_o^{-n} + o(x_o^{-n}) \qquad \text{as } n \to \infty \tag{6.10}$$

and taking $\kappa_p(L,M) = -\log x_o$ we obtain

$$\lim_{n\to\infty} n^{-1}\log \hat{p}_n(L,M) = \kappa_p(L,M). \tag{6.11}$$

Let $\pi \in \Pi(k)$ be a specific pattern, $\pi \neq \phi$. Let π represent the label of pattern π in $\Pi(k)$. Consider the generating function $\bar{F}(x) = \sum_{n=2} \hat{p}_{2n}(N,M;\bar{\pi})x^{2n}$. Then clearly

$$x^{2(k-3)}\bar{F}(x) = (\bar{G}(x)^{k-1})_{\phi,\phi}+(\bar{G}(x)^{k})_{\phi,\phi}+\ldots = (\bar{G}(x)^{k-1}(I-\bar{G}(x))^{-1})_{\phi,\phi} \tag{6.12}$$

where $\bar{G}(x)$ is obtained from $G(x)$ by deleting its πth row and column. The argument goes through just as before so that there exists $\bar{x}_o > 0$ and $\bar{\alpha} > 0$ such that

$$\hat{p}_n(N,M;\bar{\pi}) = \bar{\alpha}\bar{x}_o^{-n} + o(\bar{x}_o^{-n}) \qquad \text{as } n \to \infty \tag{6.13}$$

and the spectral radius, $\bar{\rho}(\bar{x}_o)$, of $\bar{G}(\bar{x}_o)$ equals 1. Now consider the matrix $G_\pi(x)$ obtained from $G(x)$ by replacing the πth row and column by a row and column of zeroes. Then the spectral radius, $\rho_\pi(x)$, of $G_\pi(x)$ equals $\bar{\rho}(x)$. Furthermore, $G_\pi(x) \leq G(x)$ and at least one element of $G_\pi(x)$ is strictly less than the corresponding element of $G(x)$. Frobenius theory [19] then implies that $\rho_\pi(x) < \rho(x)$ and hence for $x = x_o$, $\rho_\pi(x_o) < \rho(x_o) = 1$ and therefore $\bar{x}_o > x_o$. Thus,

$$\lim_{n\to\infty} n^{-1}\log \hat{p}_n(N,M;\bar{\pi}) = -\log \bar{x}_o < \kappa_p(L,M). \tag{6.14}$$

If $\pi = \phi$, redefine ϕ so that the y-coordinate of each polygon vertex is N instead of 0 and then a similar argument to that given above will yield equation (6.14). □

We note that it is possible to generalize this result to deal with other one dimensional lattices or to deal with patterns on the scale of hinges or sections (see [18] for such generalizations in the case of self-avoiding walks). In a subsequent work [20], questions related to the average number of times a particular pattern occurs in a self-avoiding polygon in a prism will be addressed.

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