

Almost unknotted embeddings of graphs and surfaces

S G Whittington, University of Toronto, Toronto M5S3H6, Canada ¹

Abstract : We consider the number of embeddings of almost unknotted Θ_k -graphs, $3 \leq k \leq 6$, in the simple cubic lattice Z^3 . We show that to exponential order this number is the same as the number of unknotted Θ_k -graphs. This implies that almost unknotted Θ_k -graphs are exponentially rare in the set of embeddings of Θ_k -graphs. We construct almost unknotted surfaces in Z^4 by spinning and show that to exponential order the numbers of almost unknotted spun Θ_k are equal to the numbers of unknotted spun Θ_k , $4 \leq k \leq 6$. The case of $k = 3$ is open.

1 Introduction

In the early 1960s Frisch and Wasserman [1] and independently Delbrück [2] conjectured that sufficiently long ring polymers would be knotted with high probability. This became known as the Frisch-Wasserman-Delbrück conjecture and was settled for a lattice model [3, 4] and for two continuum models [5, 6] in a set of papers published about twenty five years later. For the lattice case, suppose that p_n is the number of polygons (embeddings of simple closed curves in the simple cubic lattice, Z^3) with n edges, where polygons are counted up to translation. For instance, $p_4 = 3$, $p_6 = 22$ and $p_8 = 207$. It is known [7] that the limit

$$\lim_{n \rightarrow \infty} n^{-1} \log p_n \equiv \kappa \quad (1)$$

exists and it is easy to establish that $\log 3 \leq \kappa \leq \log 5$. If p_n^0 is the number of unknotted polygons with n edges then it is known [3, 4] that the limit

$$\lim_{n \rightarrow \infty} n^{-1} \log p_n^0 \equiv \kappa_0 \quad (2)$$

and that

$$\kappa_0 < \kappa. \quad (3)$$

This establishes the Frisch-Wasserman-Delbrück conjecture for the lattice polygon model. There are some extensions in the literature to knotted embeddings of graphs [8, 9] and to linking of lattice polygons [10].

A theta graph (actually a Θ_3 -graph) is a multiply connected graph with two vertices of degree 3 and three edges, resembling the Greek letter θ . We shall sometimes call any graph homeomorphic to this graph a theta graph. We can extend this to a Θ_k -graph which is a multiply connected graph with two vertices of degree k and k edges. A rather complicated embedding in R^3 of a Θ_4 -graph is shown in Figure 1. Embeddings of theta graphs in R^3 can be knotted (eg if any cycle is knotted) or unknotted (ambient isotopic to a planar embedding). Kinoshita [11] gave an example of an embedding of a theta graph which is not ambient isotopic to the planar embedding but has no knotted cycle. It becomes unknotted if any edge is deleted. Such embeddings are called *almost unknotted embeddings*. Examples for Θ_k , $k > 3$ have been given by Suzuki [12] and an important theorem about the existence of almost unknotted embeddings was established by Kawauchi [13]. Figure 1 shows an almost unknotted embedding of Θ_4 .

¹E-mail: swhittin@chem.utoronto.ca

2 Almost unknotted embeddings of theta graphs

If we think of embedding Θ_k , $3 \leq k \leq 6$, in Z^3 we can choose to stratify the embeddings by the total number of edges (n) in the embedding. An embedding of Θ_k has k sequences of edges with the first and last edge in each sequence incident on a vertex of degree k . If there is the same number of edges in each sequence of edges we say that the embedding is *uniform* [9]. If we restrict ourselves to uniform embeddings then the total number of edges, n , must be divisible by k . We shall consider only uniform embeddings. The results for non-uniform embeddings are very similar [14, 15].

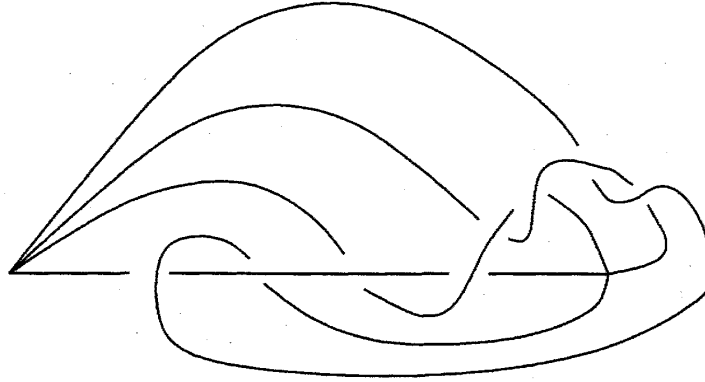


Figure 1: An almost unknotted Θ_4 graph.

Let $\theta_k(n)$ be the number of uniform embeddings of Θ_k in Z^3 with a total of n edges. Recall that $\theta_k(n) = 0$ unless k divides n . Let $\theta_k^0(n)$ be the number of unknotted uniform embeddings of Θ_k and let $\theta_k^*(n)$ be the number of almost unknotted uniform embeddings of Θ_k with n edges. It is known [9] that

$$\lim_{n \rightarrow \infty} n^{-1} \log \theta_k(n) = \kappa \quad (4)$$

and that

$$\lim_{n \rightarrow \infty} n^{-1} \log \theta_k^0(n) = \kappa_0 \quad (5)$$

From (3) this implies that unknotted uniform embeddings are exponentially rare.

This raises the interesting question as to whether almost unknotted embeddings are rare with respect to unknotted embeddings. It has been proved [14, 15] that

$$\lim_{n \rightarrow \infty} n^{-1} \log \theta_k^*(n) = \kappa_0 \quad (6)$$

for $3 \leq k \leq 6$ so almost unknotted embeddings and unknotted embeddings are equinumerous to exponential order.

The proof uses explicit lower and upper bounds on $\theta_k^*(n)$. The lower bound uses a result about polygons confined to wedges and to explain the idea we consider the square lattice Z^2 . Consider the vertices of Z^2 with integer coordinates (x, y) such that

1. $x \geq 0$,
2. $y \geq 0$ and
3. $y \leq 1 + \alpha x$, $\alpha > 0$.

These constraints define a *wedge*, $W(\alpha)$. If we write $p_n(W)$ for the number of polygons containing the edge $(0, 0) - (0, 1)$, confined to $W = W(\alpha)$ then Hammersley and Whittington [16] proved that

$$\lim_{n \rightarrow \infty} n^{-1} \log p_n(W) = \kappa_2 \quad (7)$$

independent of α for $\alpha > 0$, where κ_2 is the connective constant of the square lattice. This result also works for Z^3 and has been extended to more general wedges [10, 16]. In three dimensions essentially the same argument works to show that $\lim_{n \rightarrow \infty} n^{-1} \log p_n^0(W) = \kappa_0$, where $p_n^0(W)$ is the number of unknotted n -edge polygons in a suitably defined wedge W .

To construct a lower bound we construct an almost unknotted embedding of Θ_k which fits in a box (the shaded region in Figure 2) and has one edge from each of the k branches in the right most plane of the box. We then construct k disjoint wedges (see Figure 2) incident on this box and put unknotted polygons in each wedge. With the original embedding of Θ_k fixed we allow the numbers of edges of each of the unknotted polygons to grow. These objects are almost unknotted embeddings of Θ_k and can be constructed to have n/k edges in each of the k branches [15]. This yields the lower bound

$$\liminf_{n \rightarrow \infty} n^{-1} \log \theta_k^*(n) \geq \kappa_0. \quad (8)$$

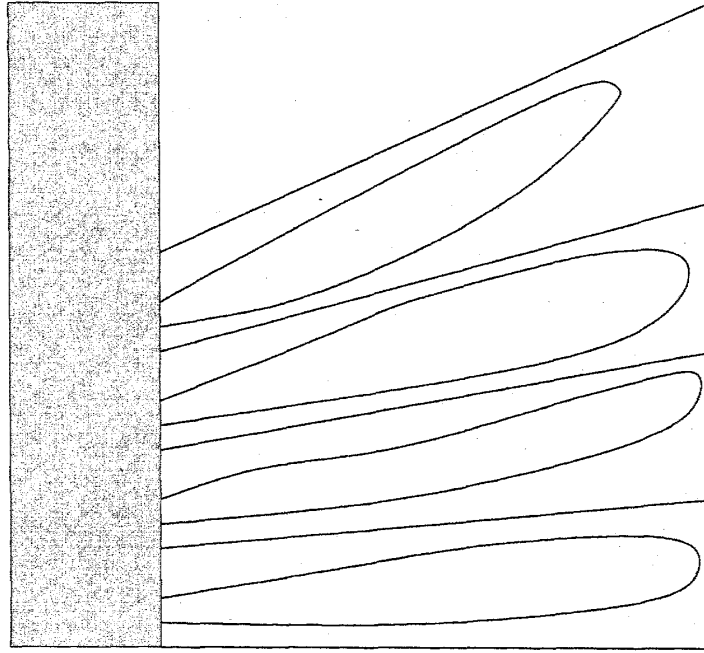


Figure 2: A set of disjoint wedges.

To construct upper bounds we first look at the cases where k is even (ie $k = 2$ and 4). In these cases the graph is Eulerian. Consider a cubic box of side $L = 2n$. Embed $k/2$ circles as unknotted polygons each with $2n/k$ edges in all possible ways in the box. The number of ways to do this is $[p_{2n/k}^0]^{k/2} e^{o(n)}$ where the $e^{o(n)}$ term accounts for the number of ways to translate the polygons within the box. This gives an upper bound on the number of almost unknotted embeddings so

$$\limsup_{n \rightarrow \infty} n^{-1} \log \theta_k(n) \leq \lim_{n \rightarrow \infty} n^{-1} \log [p_{2n/k}^0]^{k/2} = \kappa_0. \quad (9)$$

This, together with (8), gives the required result for $k = 2$ and 4 . For k odd this approach does not work but a proof can be constructed [14, 15] based on the Loomis-Whitney inequality [17].

3 Spun theta graphs and almost unknotted surfaces

One can ask if something similar happens in higher dimensions. If an unknotted Θ_3 is spun up a dimension to give a surface in R^4 then the surface is a 2-sphere with a disc sewn along its equator. The spinning operation is as follows. One of the vertices of degree 3 is removed to give three vertices each of degree 1. These vertices sit in a plane and the remainder of the graph is in the half-space bounded by this plane. This object is then spun about this plane to give a surface in R^4 . If the original Θ_3 was knotted then the surface in R^4 is knotted, *ie* it is not ambient isotopic to the standard 2-sphere with a disc sewn along its equator. If the original Θ_3 is almost unknotted then the resulting surface is also almost unknotted. This is clear because none of the 2-spheres will be knotted but, since π_1 is invariant under spinning, the resulting surface is knotted. Of course, the situation is essentially the same for spun Θ_4 (see Figure 3), Θ_5 and Θ_6 . For instance a Θ_4 gives two 2-spheres with coincident equators.

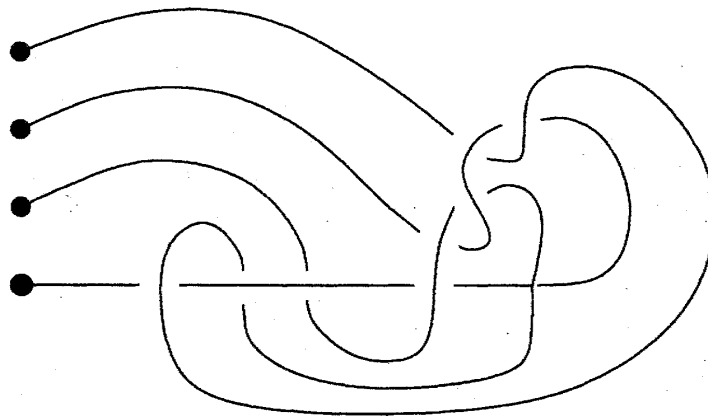


Figure 3: A spun Θ_4 can be obtained by spinning a Θ_4 graph. If the Θ_4 graph is almost unknotted so is the resulting spun Θ_4 .

An analogous spinning operation can be carried out for the lattice case, ensuring that the resulting surface is embeddable in Z^4 [15].

We write $S_k(n)$ for the number of embeddings of spun Θ_k in Z^4 with n plaquettes and $S_k^0(n)$ and $S_k^*(n)$ for the numbers of embeddings of spun Θ_k in Z^4 which are unknotted or almost unknotted. The same kinds of argument as those described in Section 2 work in higher dimension [15] to prove that

$$\lim_{n \rightarrow \infty} n^{-1} \log S_k^*(n) = \lim_{n \rightarrow \infty} n^{-1} \log S_k^0(n) \leq \lim_{n \rightarrow \infty} n^{-1} \log S_k(n) \quad (10)$$

for $4 \leq k \leq 6$. The case $k = 3$ is still open [15]. Note the non-strict inequality in higher dimension. This is because we lack a pattern theorem for dimensions higher than 3.

Spinning to give hypersurfaces in Z^p , $p > 4$, works in an analogous way [15].

Acknowledgment

This research was supported by NSERC of Canada.

References

- [1] H. Frisch and E. Wasserman, *J. Am. Chem. Soc.* **83** (1961), 3789.
- [2] M. Delbrück, *Proc. Symp. Appl. Math.* **14** (1962), 55.
- [3] D.W. Sumners and S.G. Whittington, *J. Phys. A: Math. Gen.* **21** (1988), 1689.
- [4] N. Pippenger, *Discrete Appl. Math.* **25** (1989), 273.
- [5] Y. Diao, D. Pippenger and D.W. Sumners, *J. Knot Theory and its Ramifications* **3** (1994), 419.
- [6] Y. Diao, *J. Knot Theory and its Ramifications* **4** (1995), 189.
- [7] J.M. Hammersley, *Proc. Camb. Phil. Soc.* **57** (1961), 516.
- [8] C. E. Soteros, D.W. Sumners and S.G. Whittington, *Math. Proc. Camb. Phil. Soc.* **111** (1992), 75.
- [9] C.E. Soteros, *J. Phys. A: Math. Gen.* **25** (1992), 3153.
- [10] C. E. Soteros, D.W. Sumners and S.G. Whittington, *J. Knot Theory and its Ramifications* **8** (1999), 49.
- [11] S. Kinoshita, *Pacific J. Math.* **42** (1972), 89.
- [12] S. Suzuki, *Kobe J. Math.* **1** (1984), 19.
- [13] A. Kawauchi, *Osaka J. Math.* **26** (1989), 743.
- [14] N. Madras, *J. Phys. Conf. Series* **42** (2006), 213.
- [15] N. Madras, D.W. Sumners and S.G. Whittington, *J. Knot Theory and its Ramifications* (in press).
- [16] J.M. Hammersely and S.G. Whittington, *J. Phys. A: Math. Gen.* **18** (1985), 101.
- [17] L.H. Loomis and H. Whitney, *Bull. Amer. Math. Soc.* **55** (1949), 961.