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The Number of Smallest Knots on the Cubic Lattice

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It has been shown that the smallest knots on the cubic lattice are all trefoils of length 24. In this paper, we show that the number of such unrooted knots on the cubic lattice is 3496.

KEY WORDS: Knots; knotted polygons; cubic lattice; self-avoiding walks.

1. THE MINIMAL PROJECTION OF $P(24)$

The study of polygons on the cubic lattice has led to fairly large amount of literature. See Hammersley[2] and Kesten[3] for the early work on this object. For a complete reference, see Madras and Slade.[4] Knotting in polygons on the cubic lattice is an interesting mathematical problem in this area.[5,7] In Diao,[1] it is proved that 24 is the minimal number of steps needed for a polygon on the cubic lattice to be knotted. In this paper, we enumerate all possible knotted polygons on the cubic lattice with 24 steps.

Throughout this paper, a polygon always means a polygon on the cubic lattice and $P(n)$ means a polygon of n steps. The projection of $P(24)$ onto a coordinate plane is a weighted graph on the square lattice with the weight of each edge being the number of steps projected onto it. A step is called an x step if it is parallel to the x axis, similarly for y and z steps. Let a, b, and c be the number of x, y, and z steps in $P(24)$, then we have $a+b+c=24$, hence the sum of the two smaller ones of a, b, and c will be at most 16. This number is called the minimal projection number and is denoted by m. The corresponding projection of $P(24)$ onto a coordinate plane has total weight $=m \leqslant 16$. This projection is called the minimal projection of $P(24)$ and is denoted by $G(m)$. Notice that m must be even and the sum of weights of edges sharing a common vertex (called the

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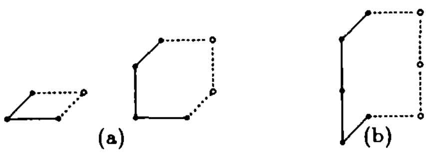

Fig. 1. The square move and the rotation.

degree of that vertex) is also even. We will assume that the xy plane is the minimal projection plane for convenience.

A polygon is reducible if it is topologically equivalent to a shorter polygon. Two polygons are l-equivalent if they are topologically equivalent and have the same length. Since 24 is the minimal number of steps needed for a polygon to be knotted, any knotted $P(24)$ is nonreducible. We will be looking at the minimal projections of $P(24)$ and eliminate most of them. The number of cases we will need to study is large but manageable. It is actually quite small compare with the total number of $P(24)$, which should be around 10^{11}–10^{12}.[6]

A continuous sequence of steps of $P(24)$ is called a path. A 1-path is a path such that its projection onto the xy plane contains only single edges. Let L be a 1-path of $P(24)$ such that its projection is half of a unit square and that the vertex on the unit square not covered by L is not occupied by $G(m)$ either. If L is replaced by a 1-path L' that has the same length and endpoints as that of L such that the projection of L' goes to the other half of the unit square, then the new polygon so obtained is l-equivalent to the previous one. Such a move is called a square move, as shown in Fig. 1a. Also, without changing the length and knot type of $P(24)$, any path L of $P(24)$ whose projection is an edge on $G(m)$ with one end open [call it a $B(1)$] can be replaced by a path L' that has the same length and endpoints as that of L such that its projection is a different $B(1)$ provided that the open end vertex of this new $B(1)$ is not occupied by $G(m)$. Such a move is called a rotation, as shown in Fig. 1b.

Since a knotted $P(24)$ is nonreducible, its $G(m)$ cannot have the situations in Fig. 2, since they all give a reducible $P(24)$. A marked number

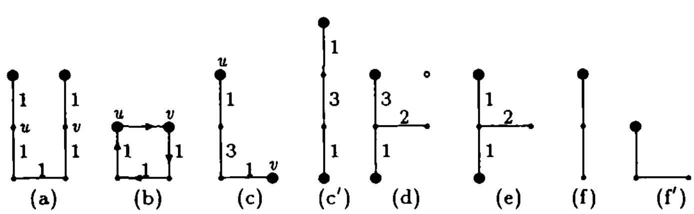

Fig. 2. Impossible projections for a knotted $P(24)$.

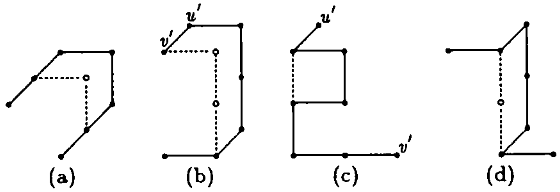

Fig. 3. Examples of reducible paths.

indicates the weight of the corresponding edge, and a vertex connected to the rest of $G(m)$ is marked with a bigger dot.

Figure 3 shows typical examples of Figs. 2a–2d and how they can be reduced. Figures 2e and 2f are either reducible or require too many edges to be nonreducible. One can draw a few pictures to see this or refer to ref. 1.

Lemma 1. If $P(24)$ is knotted, then $G(m)$ cannot be a tree. Furthermore, there exists a loop of $G(m)$ which bounds every other loop of $G(m)$ (if there is any).

Lemma 1 is proved in ref. 1 for $P(22)$. The proof for $P(24)$ is essentially the same with very little modification, so we refer for it to ref. 1. Let $\Delta(p)$ be the loop in $G(m)$ defined in Lemma 1, where p is its length. If $p \geqslant 14$, $G(m)$ is obviously reducible. There are 25 different shapes for $\Delta(12)$ (up to a rigid move), which are listed in Fig. 4.

The only one in Fig. 4 that can give a knot projection is the one marked with a single asterisk (see Fig. 7c). Every other shape can be

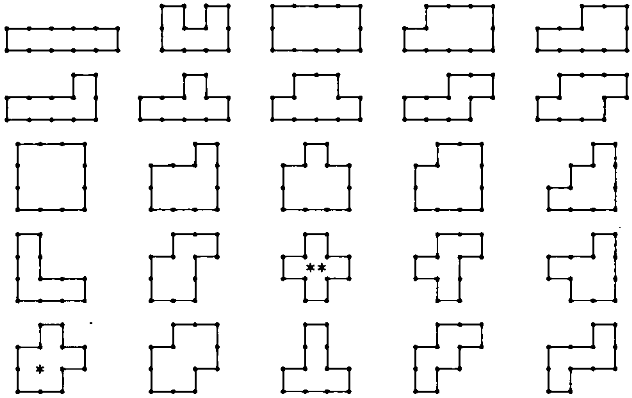

Fig. 4. All possible $\Delta(12)$'s.

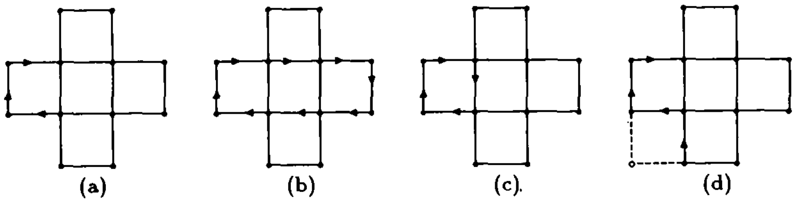

Fig. 5. Cases from Fig. 4(**).

eliminated, since the corresponding $P(24)$ is reducible. This can be seen by using Fig. 2 and the facts that there are at most four edges available to fill in the graph and a vertex must have an even degree. The only one not so obvious is the one marked with two asterisks, when the four edges form a square in the middle, as shown in Fig. 5a. For the four 1-paths similar to the one shown in Fig. 5a with arrows, one of the situations shown in Figs. 5b–5d must happen. Figure 5b is eliminated since it gives two polygons. Figure 5c contains a reducible pattern (Fig. 2b), so is eliminated. The indicated square move in Fig. 5d yields a $G(m)$ like Fig. 7c. That means if there is a knotted $P(24)$ with projection as in Fig. 5d, then it can be obtained from a knotted $P(24)$ with the projection of Fig. 7c by a square move. But we will see later that no such square move can be made on any knot with projection of Fig. 7c (see Fig. 8c).

Figure 6 gives all possible shapes of $\Delta(10)$ and $\Delta(8)$.

Figures 6a and 6d–6f can be eliminated easily since there are always reducible path no matter how the other edges (at most 6, since $p = 10$ in these cases) are filled in. It is shown in ref. 1 that Fig. 6b requires at least 26 steps for the corresponding polygon to be knotted. So Fig. 6b is

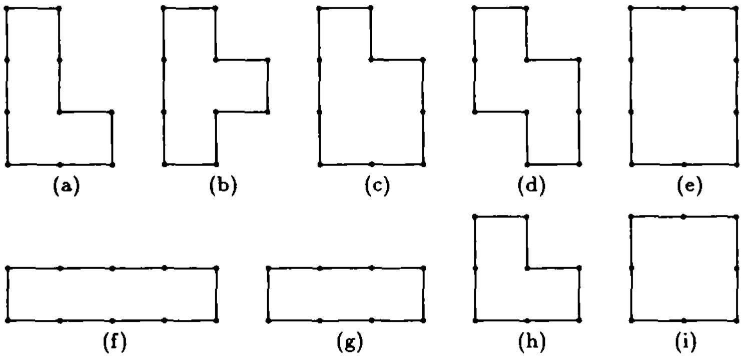

Fig. 6. All possible shapes of $\Delta(8)$ and $\Delta(10)$.

eliminated. Figure 6g is discussed and eliminated in ref. 1 for $m \leqslant 14$. We leave it to the reader to verify that it can also be eliminated for $m = 16$. Figures 6c, 6h, and 6i are candidates for knot projections.

$\Delta(6)$ is a rectangle of width 1 and length 2. It is a candidate for knot projection. $\Delta(4)$ is a unit square and the other edges (if there are any) can only be attached to its corners as $B(1)$'s. A single $B(1)$ at a corner can create a bigger loop by a square move (may need a rotation first), which corresponds to $p = 6$. But as we will see later, any knotted $P(24)$ with the projection of Fig. 7a has no such square move. So there are either two $B(1)$'s attached or no $B(1)$'s attached at each vertex of $\Delta(4)$. Again, to avoid a square move, the paths in these $B(1)$'s have to follow strict directions, which results in either too many edges or two components. So $\Delta(4)$ is not a candidate. To summarize, there are five possible shapes left for Δ. What is left is to decide how the other edges can be attached to these shapes to yield a knot projection. We state the result in the following lemma, but leave the details to the reader to verify.

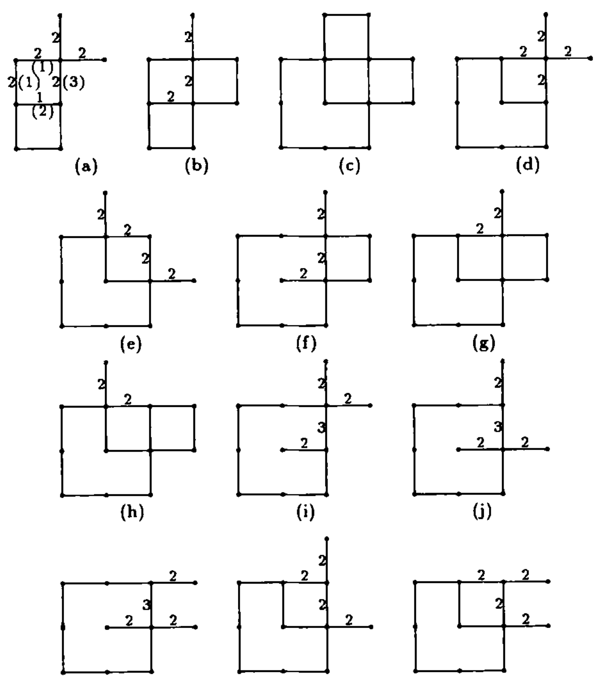

Fig. 7. Minimal projections of knotted $P(24)$.

Lemma 2. If $P(24)$ is knotted, then $G(m)$ can be transformed to one of the graphs given in Fig. 7 by a rigid motion (i.e., any combination of reflection, rotation, and translation).

Remark. The numbers in Fig. 7 indicate the weights of the corresponding edges and the unmarked edges are all single edges.

2. THE ENUMERATION

Two polygons on the cubic lattice are regarded as the same if one can be translated to another by letting $x_1 = x + a$, $y_1 = y + b$, and $z_1 = z + c$ for certain integers a, b, and c. Otherwise they are said to be different. Such polygons are called unrooted polygons. Under this definition, the same (unrooted) polygons have the same minimal projection.

In Figs. 7a and 7b, $m = 14$, hence there are three possibilities for the projection plane, since its other projections are graphs of total weight exceeding 14. Once the plane is fixed, there are eight different graphs that can be transformed to each of Figs. 7a and 7b by a rigid motion, since they are not symmetric about any axis. Thus, any $P(24)$ with its minimal projection as Fig. 7a or Fig. 7b corresponds to $3 \cdot 8 = 24$ different ones. If this $P(24)$ is a trefoil, then its mirror image about the projection plane is different from itself, since a translation does not change the chirality. Yet this reflection does not change its projection. Therefore, such a trefoil $P(24)$ corresponds to 48 different ones.

In Figs. 7c–7m the total weight is $m = 16$. The projection of the corresponding $P(24)$ to any coordinate plane will also be 16. So we assume that the projection plane is the xy plane. Each trefoil $P(24)$ with a projection of Fig. 7c, 7d, or 7e corresponds to eight different ones (notice their symmetry property), yet each trefoil $P(24)$ with a projection in one of Figs. 7f–7m corresponds to 16 different ones.

Figure 8 gives 13 trefoil $P(24)$'s whose minimal projection graphs correspond to the ones given in Fig. 7, respectively. The direction of projection is the vertical direction. Their mirror images about the projection plane have been included in the possibilities discussed above.

The dashed lines in the pictures hint at different ways to draw such a $P(24)$ without changing its projection and its knot type. For example, Fig. 9 shows three different $P(24)$ all with the projection of Fig. 7a. One can get another three like the one marked with a dashed line. Since these two parts do not interfere with each other, they combine into $3 \cdot 3 = 9$ different ones. The other ones are all counted in a similar manner. The final count: nine ways each for Figs. 7a and 7b, 63 for Fig. 7c, 31 for Fig. 7d, 5

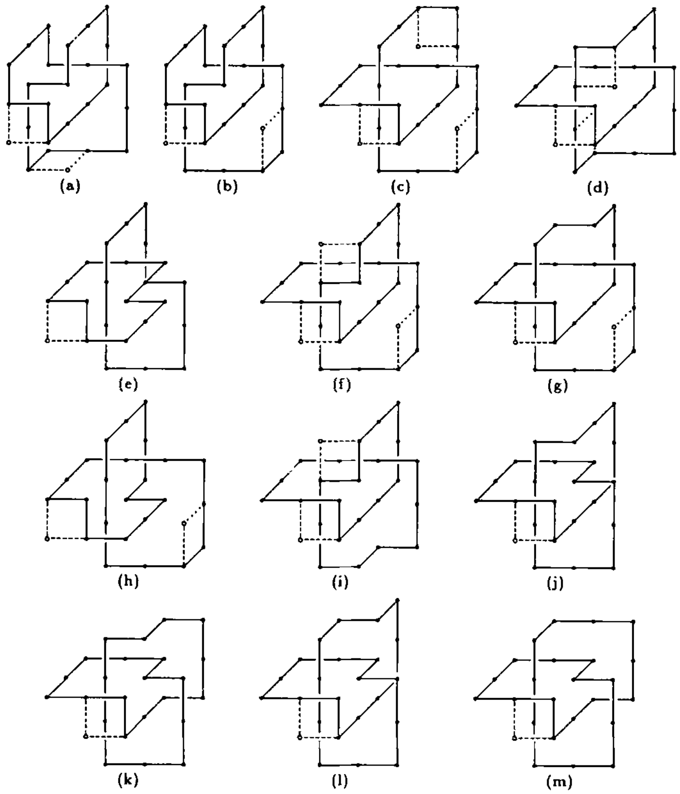

Fig. 8. The realization of knot projections.

for Fig. 7e, 39 for Fig. 7f, 21 for Fig. 7g, 18 for Fig. 7h, 13 for Fig. 7i, and 6 for each of Figs. 7j–7m. The total number of knotted $P(24)$'s is

$$48 \cdot (9+9) + 8 \cdot (63+31+5) + 16 \cdot (39+21+18+13+6+6+6+6) = 3496$$

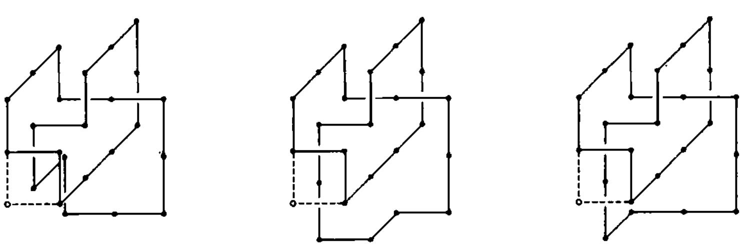

Fig. 9. Different knotted $P(24)$ with the same projection, that of Fig. 7a.

Since the polygons are unrooted, it follows that the number of rooted polygons of 24 steps that are knotted is $24 \cdot 3496 = 83{,}904$. We conclude this paper by stating the above as the following theorem.

Theorem. On the cubic lattice, there are 3496 unrooted polygons of 24 steps that are knotted and 83,904 rooted polygons of 24 steps that are knotted. Furthermore, they are all trefoils.

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