# On the three-fold irregular branched coverings of spatial four-valent graphs and its applications

Shin'ichi Kinoshita

*School of Science, Kwansei Gakuin University, Nishinomiya 662, Japan*

Let $L$ be a spatial four-valent graph. Then one of the effective tools for studying the topological position of $L$ in the 3-sphere is to consider the three-fold irregular branched coverings of $L$ [1]. In this paper we will show that this technique can also be applied to some hypothetical three-valent molecular graphs in topological stereochemistry.

## 1. Introduction

In this section we briefly explain the concept of three-fold irregular branched coverings of spatial four-valent graphs. A reader who is not familiar to knot theory may skip this section and go on to the next, in which we will state the same contents in non-technical terms and rules.

Let $L$ be a four-valent graph in a 3-sphere $S^3$ and $G(L) = \pi_1(S^3 - L, \mathrm{o})$, the fundamental group of the complementary domain of $L$ in $S^3$. We choose a Wirtinger presentation of $G(L)$, each of whose generators, say $x_i$, is a closed path beginning at o, going around edge $e_i$ of $L$ once and coming back to o, as shown in fig. 1.1. Now let $S_3$ be the symmetric group of degree 3 and $\{(12), (23), (13)\} = \{a, b, c\}$. A representation $\varphi$ (sometimes called a monodromy map) of $G(L)$ onto $S_3$ is a homomorphism of $G(L)$ onto $S_3$, and we restrict our study to the case where each $\varphi(x_i)$ is either $a, b$ or $c$ for every $i$. If we consider the images of $x_i$'s, instead of the $x_i$'s themselves, only two cases can occur (up to conjugation) at each crossing in a regular projection of $L$, as shown in fig. 1.2. Since $L$ is four-valent, at each vertex of $L$ only three cases can occur, as shown in fig. 1.3.

Now we consider the covering $M_\varphi(L)$ of $S^3 - L$, whose fundamental group is isomorphic to the inverse image of $\{1, (23)\}$, where 1 is the identity of $S_3$. Then we can construct the branched covering whose branch points are the spatial graph $L$. Take a small 2-sphere which encloses a vertex and intersects with $L$ at four points, then consider the lift of this 2-sphere in $M_\varphi(L)$. It is the disjoint union of a torus and a 2-sphere for the case fig. 1.3(1), and a 2-sphere for the cases fig. 1.3(2) and fig. 1.3(3). To make the branched covering a three-dimensional manifold, we have to exclude the case fig. 1.3(1), that is to say, we consider only the representation which

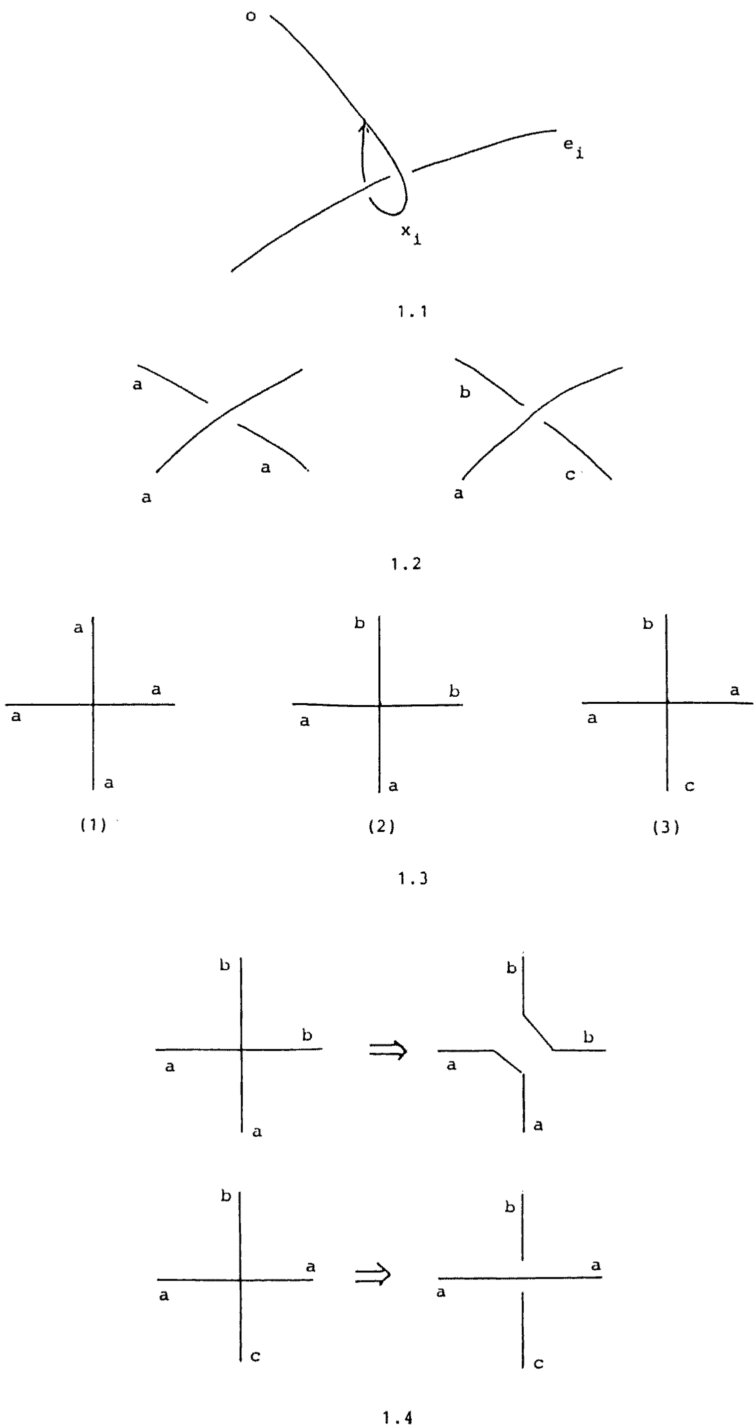



Fig. 1.

satisfies either case fig. 1.3(2) or case fig. 1.3(3) at each vertex. Then, the branched covering $M_\varphi(L)$ associated with a representation $\varphi$, if it exists, is an orientable three-dimensional manifold.

To identify $M(L)$, we may apply the operation, shown in fig. 1.4, which deforms the spatial graph $L$ to a link $L'$. Here we should note that link $L'$ depends on the choice of the regular projection of $L$, so that it is not uniquely determined. It can be seen, however, that $M_\varphi(L)$ is homeomorphic to $M_{\varphi'}(L')$, the three-fold irregular branched covering of $L'$, whose representation $\varphi'$ is inherited from $\varphi$. Hence, we can identify $M_\varphi(L)$ through $M_{\varphi'}(L')$, where the latter can be identified or at least investigated by applying the theory of three-dimensional manifolds. We will elucidate this procedure with examples in the following.

## 2. 3-colorability

In this section we use the term 3-colorability to explain what we did in the former section (see also ref. [2]). Suppose a spatial four-valent graph is given, and we consider its regular projection and its diagram. (A regular projection of a spatial graph $L$ is a projection of $L$ into a plane such that (i) only multiple points of the projection are double points, and there are only finite number of them, and (ii) no double point is the image of any vertex of $L$. A diagram is a regular projection with over/under information at each crossing.) A segment of a diagram is a path which is one of the following:

(1) a path from one undercrossing to the next undercrossing,
(2) a path from one vertex to the first undercrossing,
(3) a path from one vertex to the another vertex without undercrossing, and
(4) a circle which does not have any undercrossing.

Now we choose three colors, denoted by $a, b$ and $c$. We associate each segment with one of these three colors, subjecting the following rules (up to renaming the colors):

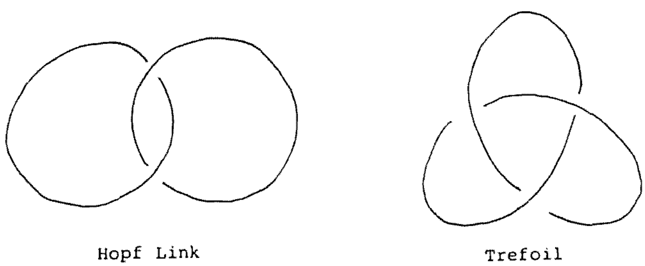
(1) at each crossing, either all three colors are present or just one color appears (see fig. 1.2),
(2) at each vertex, four segments are colored in the cyclic order of either $a, a, b, b$ or $a, b, a, c$ (see fig. 1.3), and
(3) at least two colors appear in the diagram.

(Though we are going to study 3-colorability of spatial four-valent graphs, there are cases, where only 2-colors may be present (see fig. 2.6). The latter cannot occur, if the spatial graph is a knot, a simple closed curve in a 3-sphere.)

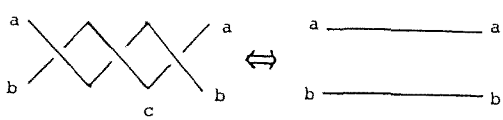
If a diagram of a spatial four-valent graph permits such a coloring, the spatial four-valent graph is called 3-colorable. The 3-colorability of a spatial four-valent graph is a topological invariant and it does not depend on the choice of its diagrams; i.e. either all of its diagrams are 3-colorable or none of them are 3-colorable. Some knots and links are 3-colorable (for instance, a trefoil knot), but there are knots and links which are not 3-colorable (for instance, a trivial knot and a Hopf link) (see fig. 2.1.)

Now suppose that a spatial four-valent graph $L$ is 3-colorable, and choose one of its diagrams with a coloring. Then, applying at each vertex the deformation shown in fig. 1.4, we can modify $L$ into a link $L'$, whose coloring is inherited from that of $L$. The link $L'$ may depend on the choice of the diagrams. However, if we permit the modification shown in fig. 2.2, two different links obtained from two different diagrams of a spatial four-valent graph turn out to be equivalent, i.e. one can modify one to the other under a finite number of these modifications (and moves permitted in topology, of course).

Here, we give an example for explaining the above discussion. A spatial $\theta_4$-curve consisting of two vertices and four edges, where each edge joins two vertices, is




2.1

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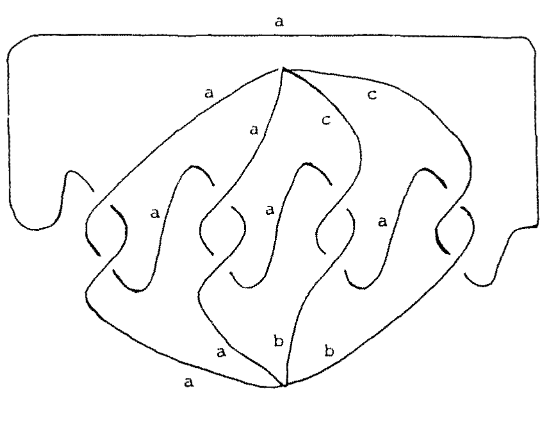
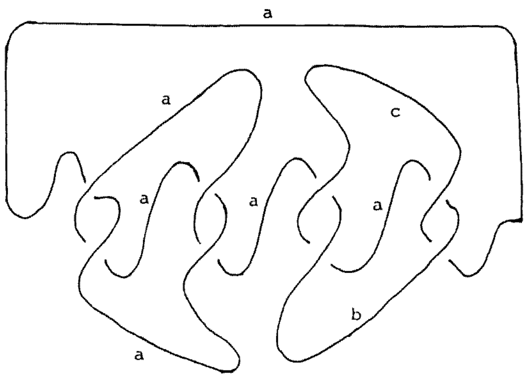



2.3

Fig. 2.

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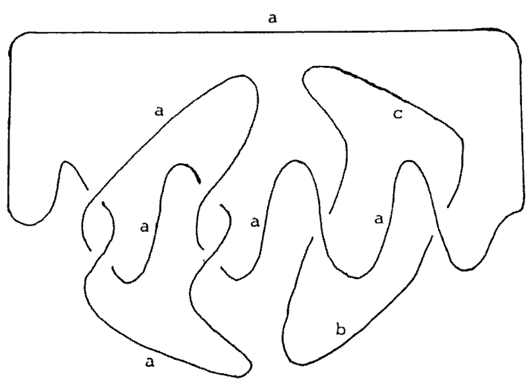
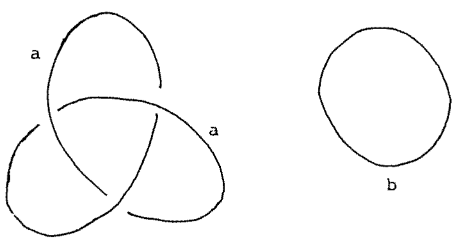



2.5




2.6

Fig. 2. Continued.

given in fig. 2.3 (see also ref. [3]). We, for instance, choose one coloring as indicated in fig. 2.3. (Actually there are four essentially different colorings up to renaming colors). Then, we apply at each vertex the deformation shown in fig. 1.4 (see fig. 2.4). After applying the modification shown in fig. 2.1 (see fig. 2.5) and moving the diagram, we have a diagram which is the disjoint union of a diagram of a trefoil knot $k_1$ and a trivial knot $k_2$ (see fig. 2.6). Note that $k_1$ and $k_2$ are differently colored.

To find a topological invariant of this coloring, we need some knowledge on knot theory. There is a polynomial invariant $\Delta_k(t)$ of a knot $k$, called the Alexander polynomial. For instance, $\Delta_{k_1}(t) = t^2 - t + 1$ for a trefoil knot $k_1$ and $\Delta_{k_2}(t) = 1$ for a trivial knot $k_2$. Then we consider $d = |\Delta_{k_1}(-1) \cdot \Delta_{k_2}(-1)| = 3 \cdot 1 = 3$, which turns out to be a topological invariant of this coloring of this $\theta_4$-curve.

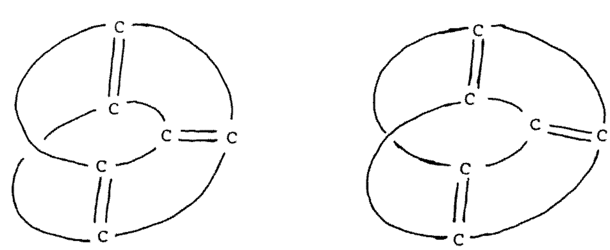
To a reader who read section 1, we explain the above discussion as follows: First note that to associate a coloring of 3-colors is equivalent to giving a representation of the group $G$ onto $S_3$. Then, the modification of diagrams given in fig. 2.1 does not change the three-fold irregular branched covering associated to the representation. Finally, when a diagram is modified to a disjoint union of a diagram of a knot $k_1$ and that of $k_2$, where $k_1$ and $k_2$ are differently colored, the three-fold irregular branched covering associated to a representation is homeomorphic to the sum of the two-fold branched covering of $k_1$ and that of $k_2$. Hence $d = |\Delta_{k_1}(-1) \cdot \Delta_{k_2}(-1)|$ is equal to the product of one-dimensional torsion numbers of the three-fold irregular branched covering associated to the given representation.

*Remark*

When a knot diagram is given, the Alexander polynomial $\Delta_k(t)$ can be calculated easily with a computer. Also, there is another direct method to compute $|\Delta_k(-1)|$.

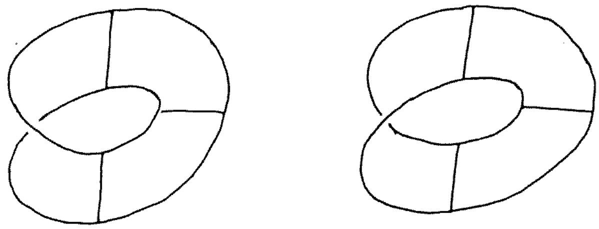
## 3. Applications

First let us consider two molecules synthesized by Walba [4], which are shown in fig. 3.1, where a single line stands for a chain of atoms combined by single covalent bonds, and double lines for a direct double covalent bond. It is has been proved by Simon [5] that these molecules are topologically chiral, i.e. they are not equivalent in topological stereochemistry. Now let us consider this situation in the setting of knot theory of spatial graphs. We may represent these two molecules in two ways. One way is to represent them as spatial three-valent graphs, as shown in fig. 3.2, and the other as spatial four-valent graphs, as shown in fig. 3.3. We note that

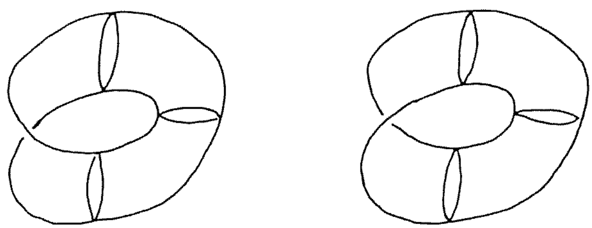



3.1

Fig. 3.



3.2



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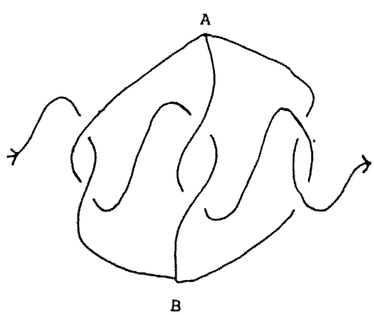


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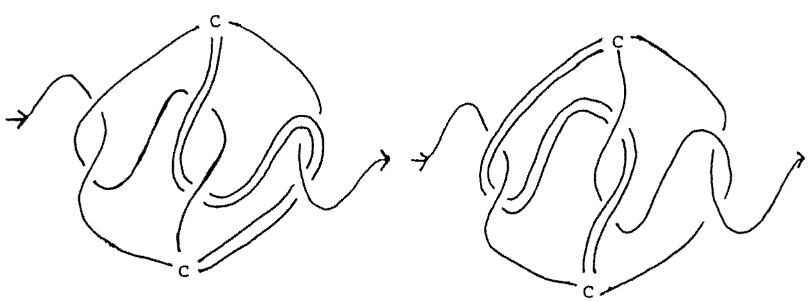
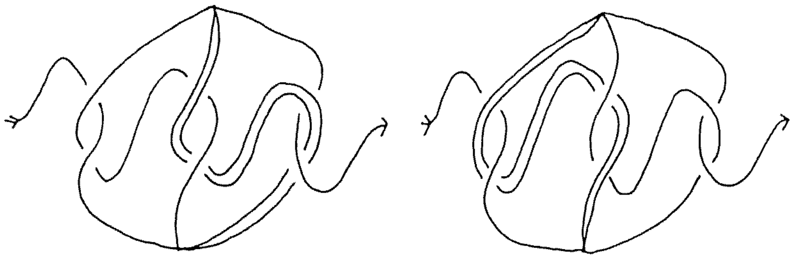


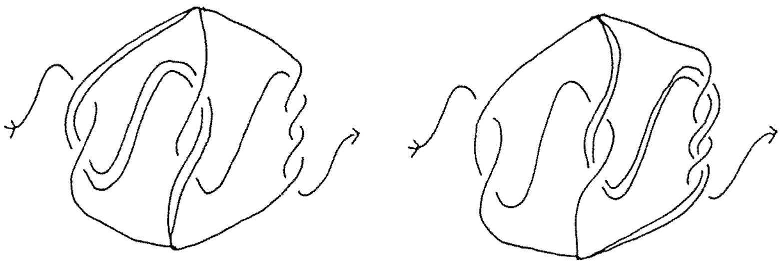

3.5

Fig. 3. Continued.



$L_1$ $L_2$

3.6



$L_3$ $L_4$

3.7

Fig. 3. Continued.

two spatial graphs in fig. 3.2. are topologically equivalent as spatial graphs, but two spatial graphs in fig. 3.3 are not topologically equivalent. (Simon's proof mentioned above can be applied to this case, too.) The above examples, though chemically very interesting, may be somewhat misleading, when we explain the transition from knot theory of molecules to that of spatial graphs. So, we introduce rather simple examples, which will clarify this transition. Suppose, for instance, a spatial $\theta_3$-curve is given as shown in fig. 3.4, where vertices $A$ and $B$ are joined by three edges. We replace $A$ and $B$ with carbon atoms, so that the spatial $\theta_3$-curve presents a molecular graph now. Then, one of the three edges should stand for a double covalent bond and we have hypothetical molecular graphs such as shown in fig. 3.5. We need not worry about the fact that the double covalent bonds are presented by curves. These are topological figures, so that double covalent bonds can be straighten up by moving other simple bonds. Then we can consider these molecular graphs as spatial four-valent graphs as shown in fig. 3.6. Are they topologically equivalent as spatial graphs? The answer is negative, which will be shown below. We will only sketch the outline of the proof. Since the spatial graphs $L_1$ and $L_2$ in fig. 3.6 are four-valent, we apply the technique explained in sections 1 and 2. First we count the numbers of representations of $G(L_1)$ and $G(L_2)$ onto $S_3$ (i.e. the numbers of essentially different 3-color colorings), respectively. Each of them is four. Next we count the numbers $d$ introduced in section 2. They are four 1's for $L_1$, and one 1 and three 7's for $L_2$. Hence, the spatial graphs $L_1$ and $L_2$ are not topologically equivalent, nor are the two molecular graphs in fig. 3.5. Actually, for $L_1$ all of four three-fold irregular branched coverings are 3-spheres and for $L_2$ only one of the three-fold irregular branched coverings is a 3-sphere, but the other three are identical 3-manifolds with one-dimensional torsion number 7. Now we give another simple example. Let $L_3$ and $L_4$ be two spatial $\theta_4$-curves as shown in fig. 3.7. Note that these spatial $\theta_4$-curves are constructed from the same $\theta_3$-curve. We apply the same technique to distinguish $L_3$ and $L_4$. When we count the numbers of possible representations of $G(L_3)$ and $G(L_4)$ onto $S_3$ (i.e. the numbers of essentially different 3-color colorings), respectively, it is four for $L_3$ and two for $L_4$. Hence, we already know that $L_3$ and $L_4$ are not topologically equivalent. The four $d$'s for $L_1$ are one 1 and three 11's and the two $d$'s for $L_2$ are 1 and 2. Four three-fold irregular branched coverings for $L_1$ are a 3-sphere and three identical 3-manifolds with one-dimensional torsion number 11. Two three-fold irregular branched coverings for $L_2$ are a 3-sphere and a projective 3-space.

## 4. Discussion

(1) Our method of using three-fold irregular branched coverings does not succeed in proving the chirality of spatial graphs in fig. 2.4.

(2) However, Simon's method [5] may encounter difficulty, if a spatial graph contains a non-trivial knot, whose two-fold branched covering we have to consider. Then, we may need to construct a link theory in a 3-manifold, which would be much more complicated than that in a 3-sphere.

(3) Though our method is also related to 3-manifold theory, in computation it actually does not go beyond 3-sphere.

(4) The number of representations in our method (i.e. the number of 3-color colorings) can be easily counted with a computer.

## References

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