TOPOLOGY OF SPATIAL GRAPHS

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Abstract

In this article, we explain some introductory facts of spatial graphs and then introduce a concept of the unknotting number of a spatial graph generalizing the usual unknotting number of a knot. We explain that there are infinitely many prime spatial graphs which are almost identical to a given graph. We apply this result to a prion-tangle, a topological model of prion proteins to obtain a linking property of a prion-tangle.

Keywords: Spatial graph, Warping degree, Unknotting number, Topological model of prion proteins

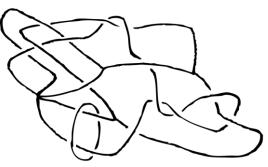


Figure 1: A spatial graph

1. Introduction

We consider a finite graph Γ without any vertices of degrees 0 and 1. A *spatial graph* of Γ is defined to be a topological embedding image G of Γ into Euclidean 3-space R^3 such that there is an orientation-preserving homeomorphism h: $R^3 \to R^3$ sending G to a polygonal graph in R^3 (see Fig.1). Spatial graphs are one of the main research objects in knot theory [1]. We consider a spatial graph G by ignoring the degree 2 vertices for our convenience, so that we have an edge with just one vertex (see Fig.2). For an edge α of a spatial graph G, let $G \setminus \alpha$ denote the spatial sub-graph obtained from G by deleting α with the vertices missed which is called the α -reduction. When α is an edge with only one degree 3 vertex, we have a degree one vertex in $G \setminus \alpha$. In this

case, we may understand the edge reduction $G \setminus \alpha$ as the graph obtained by deleting the arc with the degree one vertex. If Γ is a loop, then G is called a *knot*, and it is *trivial* if it is the boundary of a disk in R^3 (see Fig.3). When Γ is the disjoint union of finitely many loops, G is called a *link*, and it is trivial if it is the boundary of mutually disjoint disks in R³ (see Fig.4). A knot is considered as a link with one component. Since the 3-sphere S³ is topologically the one point compactification of R^3 adjoining the infinite point $\{\infty\}$, we can also consider spatial graphs as graphs in S³ without making a confusion. In Section 2, we explain a diagram of a spatial graph. In Section 3, the notion of the equivalence on spatial graphs is explained to describe a central problem, the equivalence decision problem. The equivalence of spatial graphs is also stated there in terms of the generalized Reidemeister moves. A role of a constituent link of a spatial graph is also observed there. In Section 4, we explain how the notion of the unknotting number of a knot is generalized to the notions of the unknotting number and the Γ -unknotting number of a spatial graph. In Section 5, we show the existence theorem of prime spatial graphs which are almost identical to every given spatial graph. In Section 6, we apply the existence theorem to a prion-tangle which is a topological model of prion proteins based on the Prusiner theory^[2] to show a linking property of the prion-tangles.

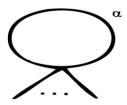


Figure 2: An edge α with just one vertex





A trivial knot

A non-trivial knot (Trefoil knot)

Figure 3





A trivial link

A non-trivial link (Hopf link)

Figure 4

2. Spatial graph diagrams

For a vector ${\bf a}$ orthogonal to a plane P in ${\bf R}^3$, let $p_{\bf a} \colon {\bf R}^3 \to P$ be the orthogonal projection to P. Assume that every point ${\bf x} \in p_{\bf a}(G)$ has one of the following neighborhoods in $p_{\bf a}(G)$ (see Fig. 5):

- (1) $p_a^{-1}(x) \cap G = \{x^*\}$ with x^* a non-vertex point of G.
- (2) $p_{a}^{-1}(x) \cap G = \{x_{+}^*, x_{-}^*\}$ with x_{+}^* and x_{-}^* non-vertex points of G.
- (3) $p_a^{-1}(x) \cap G = \{x^*\}$ with x^* a vertex of G of degree ≥ 3 .

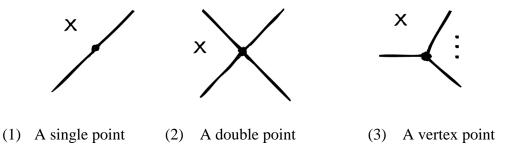


Figure 5: A projection image point x of a spatial graph

In (2), we take x_+^* and x_-^* so that they satisfy the inner product inequality $a \cdot x_+^* > a \cdot x_-^*$. Then x_+^* is called an *upper crossing point* and x_-^* is called a *lower crossing point*. We put the following definition:

DEFINITION 2.1.

A diagram $D=D_G$ of a spatial graph G is the image $p_a(G)$ in a plane $P \subseteq R^3$ for an orthogonal vector \mathbf{a} to P together with the upper-lower crossing point information on every double point so that a small open neighborhood of every lower crossing point is removed (see Fig. 1).

3. Equivalence of spatial graphs

Two spatial graphs G and G' are *equivalent* if there is an orientation-preserving homeomorphism h: $R^3 \to R^3$ sending G onto G'. A fundamental topological problem on spatial graphs is:

PROBLEM 3.1 (Equivalence Decision Problem).

By an effective method, decide whether or not two given spatial graphs of a graph Γ are equivalent.

A special problem relating to the molecular chemistry is:

PROBLEM 3.2(Chirality Problem).

Determine whether or not a given spatial graph is equivalent to the mirror image.

Even for knots and links, these problems are unsolved, although lots of effective methods on

topological invariants are known. The following theorem is a fundamental result in knot theory and sometimes useful in arguments on the equivalence decision problem.

THEOREM 3.3 [1], [3], [4], [5], [6].

Two spatial graphs G and G' are equivalent if and only if any diagram D of G is deformed into any diagram D' of G' by a finite sequence of the generalized Reidemeister moves I-V (see Fig. 6).

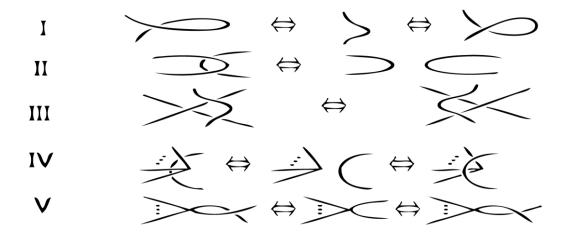


Figure 6: The Reidemeister moves I-III and the generalized Reidemeister moves I-V

A *consituent link* of a spatial graph G is a link contained in G. The following proposition is direct from the definition of an equivalence of spatial graphs:

PROPOSITION 3.4.

If two spatial graphs G^* and G are equivalent, then there is a graph-isomorphism $q: G^* \to G$ such that every constituent link L^* of G^* is equivalent to the corresponding constituent link $L=q(L^*)$ of $G=q(G^*)$.

A spatial graph of the graph Γ shown in Fig. 7(1) is called a θ -curve. A θ -curve is *trivial* if it is equivalent to the θ -curve in a plane as in Fig. 7(1). We see that the θ -curve in Fig. 7(2) is non-trivial, because the trivial θ -curve has only three trivial constituent knots shown in Fig. 8(1) and the θ -curve in Fig. 7(2) has a non-trivial constituent knot (Trefoil knot) shown in Fig. 8(2).

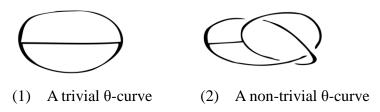


Figure 7





(1) The constituent knots of a trivial θ -curve (2) A non-trivial constituent knot

Figure 8

As we see in this example, knot theory is useful in determining non-equivalence for some spatial graphs. A difficult point of Problems 3.1 and 3.2 comes from the fact that the converse of Proposition 3.4 does not hold for any spatial graph G with at least one vertex with degree ≥ 3 , which will be explained in Section 5. Here is one famous example of a non-trivial θ -curve with only the trivial constituent knots.

EXAMPLE 3.5 (Kinoshita's θ -curve).

The θ -curve K shown in Fig. 9 is called *Kinoshita's* θ -curve^[7] which has only the trivial constituent knots shown in Fig. 10. The non-triviality of K can be proved by a traditional knot theoretical method such as Alexander ideals^[1]. A different geometric proof is given by considering the double branched covering of S³ branched along a constituent trivial knot, because the ambient manifold is again the 3-sphere S³ and the remaining arc lifts to a non-trivial knot whereas, for a trivial θ -curve, the remaining arc must lift to a trivial knot.

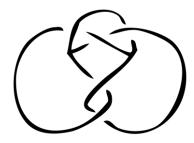


Figure 9: Kinoshita's θ -curve



Figure 10: The constituent knots of Kinoshita's θ -curve

4. The unknotting number of a spatial graph

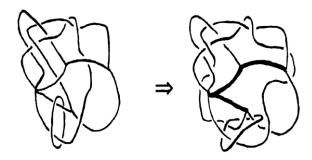


Figure 11: Deforming a diagram into a based diagram

The unknotting number of a knot or link is a well-known topological invariant^[1]. We explain here how this notion is generalized to the unknotting number and the Γ -unknotting number of a spatial graph by introducing the concepts of an unknotted spatial graph and a Γ -unknotted spatial graph. A connected spatial graph G is obtained from a maximal tree T (a smallest tree graph containing all the vertices of degrees ≥ 3 of G) by adding the remaining edges which we call T-edges. By definition, $T = \phi$ if G is a knot, and T is one vertex if G has just one vertex of degree ≥ 3 . Let D be a diagram of G, and D_{α} the sub-diagram of D corresponding to a T-edge α of G. The diagram D is a based diagram (on a based tree T) and denoted by (D;T) if there are no crossing points of D belonging to T. For a spatial graph G with connected components G_i (i=1,2,...,r), a based diagram (D,T) of G is a union of based diagrams (D_i,T_i) of G_i (i=1,2,...,r) such that D is a diagram of G and there are no crossing points of D belonging to T=T₁UT₂U...UT_r. We can deform every diagram of a spatial graph G into a based diagram by a finite sequence of the generalized Reidemeister moves (see Fig. 11). Let (D;T) be a based diagram of a connected spatial graph G. A T-edge diagram D_{α} is monotone if there is an orientation on the edge α such that a point going along the oriented T-edge diagram D_{α} from a vertex if $T\neq \phi$ or from a non-vertex point if $T=\varphi$ meets first the upper crossing point at every crossing point (see Fig. 12). A based diagram (D;T) of a connected graph G is monotone if the T-edge diagram D_{α} is monotone for every T-edge α and there is an ordered sequence on the T-edges such that the T-edge diagram D_{α} is upper than the T-edge diagram $D_{\alpha'}$ for every ordered pair $\alpha < \alpha'$ (see Fig. 13). In general, a based diagram (D;T) of a graph G with connected components G_i (i=1,2,...,r) is monotone if (D;T) is a union of monotone diagrams (D_i,T_i) of G_i (i=1,2,...,r) such that the diagram D_i is upper than the diagram D_i for every i<j after, if necessary, changing the indices of G_i (i=1,2,...,r). The warping degree d(D;T) of a based diagram (D;T) is the least number of crossing changes on the T-edge diagrams of (D;T) needed to obtain a monotone diagram. For example, the diagram in Fig. 14 is a monotone diagram obtained from a based diagram of the spatial graph of Fig. 1 by crossing changes. The *complexity* of the based diagram (D;T) is the pair cd(D;T)=(c(D;T), d(D;T)) together with the dictionary order where c(D;T) denotes the crossing number of (D;T). We put the following definitions^{[6],[8]}.

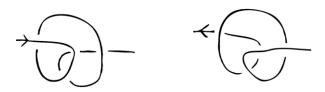


Figure 12: Monotone T-edge diagram



Figure 13

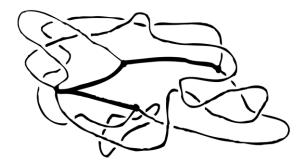


Figure 14: A monotone diagram

DEFINITION 4.1.

The *complexity* $\gamma(G)=(c_{\gamma}(G),d_{\gamma}(G))$ of a spatial graph G is the minimum in the dictionary order of the complexities cd(D;T) for all based diagrams (D;T) of G.

The complexity $\gamma(G)$ is a topological invariant of G. We call the topological invariants $c_{\gamma}(G)$ and $d_{\gamma}(G)$ the γ -crossing number and the γ -warping degree of G, respectively. The complexity $\gamma(G)$ goes down until G becomes a graph in a plane by the crossing change or the splice at a suitable crossing point on G. As similar notions, we have the crossing number c(G) which is the minimum of the crossing numbers c(D) of all diagrams D of G and the warping degree c(G) which is the minimum of the warping degrees c(D) of all based diagrams c(D) of G. The warping degrees of knots and links have been more or less discussed c(D), c(D),

DEFINITION 4.2.

A spatial graph G is *unknotted* if d(G)=0, γ -unknotted if $d_{\gamma}(G)=0$, and Γ -unknotted if G is a γ -unknotted spatial graph of a graph Γ such that $c_{\gamma}(G)$ is minimal for all spatial graphs of Γ .

A link L is unknotted if and only if L is a trivial link, and a spatial graph G of a plane graph Γ is Γ -unknotted if and only if G is equivalent to a graph in a plane. For example, in Fig. 15, a Γ -unknotted spatial graph K_6 of the 6-complete graph Γ_6 and a Γ -unknotted spatial graph K_7 of the 7-complete graph Γ_7 are shown. In these notions, the following Conway-Gordon theorem must keep in mind.

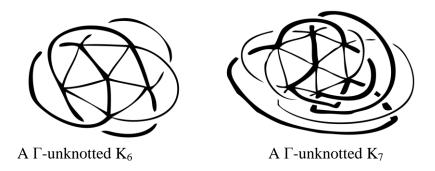


Figure 15

THEOREM 4.3 (Conway-Gordon^[12]).

Every spatial 6-complete graph K_6 contains a non-trivial constituent link and every spatial 7-complete graph K_7 contains a non-trivial constituent knot.

For example, K_6 and K_7 in Fig. 15 have a Hopf link constituent link and a Trefoil constituent knot, respectively. Nevertheless, we have the following properties of an unknotted spatial graph:

THEOREM 4.4^[8].

- (1) For every graph Γ , there are only finitely many unknotted spatial graphs G of Γ up to equivalences.
- (2) An unknotted connected spatial graph G is deformed into a maximal tree of G by a sequence of the α -reductions on trivial edges α shown in Fig. 16.
- (3) An unknotted connected spatial graph G is equivalent to a trivial bouquet of circles after the edge contractions of a maximal tree (see Fig. 17).

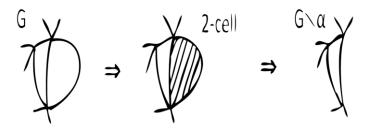


Figure 16: A trivial edge reduction

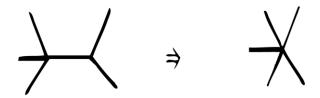


Figure 17: An edge contraction

The following notion^[8] is a natural generalization of the unknotting number of a knot or a link. A similar notion is further generalized to a spatial graph with at least two degree one vertices^[8].

DEFINITION 4.5.

The unknotting number u(G) (or the Γ -unknotting number $u_{\Gamma}(G)$, respectively) of a spatial graph G is the minimal number of crossing changes needed to obtain a diagram of an unknotted spatial graph (or a Γ -unknotted spatial graph, respectively) from a diagram of a spatial graph equivalent to G.

For example, Kinoshita's θ -curve G in Fig. 9 has $u(G) = u_{\Gamma}(G) = 1$, because the crossing change at any crossing point except one crossing point gives an unknotted θ -curve which is also a Γ -unknotted θ -curve (The crossing change at this exceptional crossing point gives a θ -curve equivalent to the mirror image of Fig. 7(2)). As another example, the spatial graph G of a plane graph Γ in Fig. 18 is unknotted, so that u(G)=0, but is not Γ -unknotted because a Hopf constituent link is contained. We have $u_{\Gamma}(G)=1$ by taking the crossing change at any crossing point. In general, we can see that *for any graph* Γ *and any positive integer* n, *there is a spatial graph* G *of* Γ *such that* $u(G)=u_{\Gamma}(G)=n^{[8]}$.

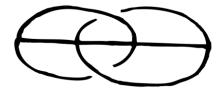


Figure 18: An unknotted, non-Γ-unknotted spatial graph

5. Existence of spatial graphs with the same constituent knots and links

In this section, we explain how the converse of Proposition 3.4 does not hold. For this purpose, we use the following notion where a similar useful notion is studied by Taniyama et al. ^[13].

DEFINITION 5.1.

A spatial graph G is *prime* if G is not equivalent to any spatial graph G' in the cases (0)-(2) (see Fig. 19):

- (0) There is a plane in R³ which does not meet G' and separates G' into two spatial sub-graphs.
- (1) There is a plane in R³ meeting G' in one point which separates G' into two spatial graphs (with at most one vertex of degree one).
- (2) There is a plane in R^3 meeting G' in two points x_1 , x_2 which separates G' into two spatial graphs G'_1 , G'_2 (with at most two vertices of degree one) such that the spatial graph $G'_i \cup [x_1, x_2]$ with $[x_1, x_2]$ the interval between the points x_1 , x_2 is not equivalent to a trivial knot for i=1,2.

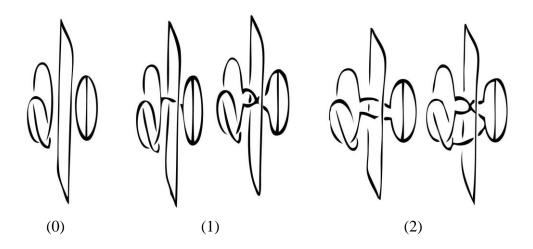


Figure 19: Non-prime spatial graphs

A spatial graph G^* is said to be *almost identical* to a spatial graph G if G^* is not equivalent to G and there is a graph-isomorphism $g: G^* \to G$ such that the α^* -reduction $G^* \setminus \alpha^*$ is equivalent to the α -reduction $G \setminus \alpha$ for every edge α^* of G^* and $\alpha = q(\alpha^*)$. We have the following theorem:

THEOREM 5.2 [14], [15].

For every spatial graph G, there are infinitely many (up to equivalences) prime spatial graphs G* which are almost identical to G. This family contains the following families:

- (1) A family of infinitely many prime spatial graphs G^* with $\max\{u(G)-2, 1\} \le u(G^*) \le \max\{u(G), 1\}$.
- (2) A family of infinitely many prime spatial graphs G^* with $\max\{u_{\Gamma}(G)-2, 1\} \leq u_{\Gamma}(G^*) \leq \max\{u_{\Gamma}(G), 1\}.$

The first half of this theorem is proved by the topological imitation theory^[14]. The latter half of this theorem is proved by observing that a technique on the crossing change in the topological imitation theory^[15] is applicable to the unknotting numbers u(G) and $u_{\Gamma}(G)$ of a spatial graph G by the same way as we have done for the unknotting number of knots and links. By a special feature of the topological imitation theory, the compact exteriors $E(G^*)$ of the spatial graphs G^* regarded as graphs in S^3 are hyperbolic 3-manifolds with non-torus components totally geodesic. Thus, the compact exteriors $E(G^*)$ are far from the compact exterior of an unknotted spatial graph which is seen to be a handlebody from Theorem 4.4. The following corollary, obtained directly

from Theorem 5.2 shows how the converse of Proposition 3.4 does not hold.

COROLLARY 5.3.

For every spatial graph G with at least one vertex of degree ≥ 3 , there are infinitely many (up to equivalences) prime spatial graphs G^* with a graph-isomorphism $q: G^* \rightarrow G$ such that every constituent link L^* of G^* is equivalent to the constituent link $L=q(L^*)$ of G. In this family, there are infinitely many prime spatial graphs G^* with max $\{u(G)-2, 1\} \leq u(G^*) \leq \max\{u(G), 1\}$ and infinitely many prime spatial graphs G^* with max $\{u_{\Gamma}(G)-2, 1\} \leq u_{\Gamma}(G^*) \leq \max\{u_{\Gamma}(G), 1\}$.

A spatial graph G of a plane graph Γ is said to be *minimally knotted* if G is almost identical to a graph in a plane (in R³). Theorem 5.2 was used to confirm the Simon-Wolcott conjecture^[16] that there is a minimally knotted spatial graph of every plane graph. Since a graph G in a plane (in R³) has $u(G)=u_{\Gamma}(G)=0$, we have the following corollary with additional properties:

COROLLARY 5.4.

For every plane graph Γ , there are infinitely many (up to equivalences) minimally knotted prime spatial graphs G^* of Γ with $u(G^*)=u_{\Gamma}(G^*)=1$.

6. An application to a topological model of prion proteins

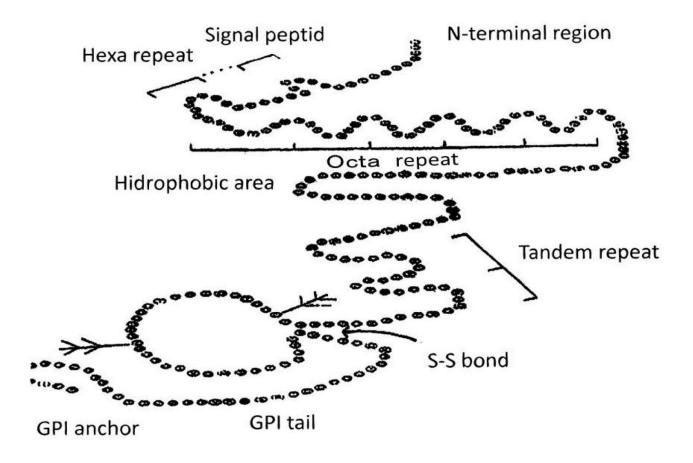


Figure 20: Prion Precursor Protein

An illustration of Prion precursor protein is in Fig. 20^[17] (where the responsibility of this English translation comes to the author). Some points of the Prusiner theory ^[2] on a prion protein are the following points (1)-(3):

- (1) By losing the N-terminal region, Prion precursor protein changes into Cellular PrP, denoted by PrP^{C} or Scrapie PrP, denoted by PrP^{SC} , and α -helices change into β -sheets.
- (2) The 1-dimensional structures on PrP^C and PrP^{SC} are the same and a main difference of PrP^C and PrP^{SC} may come from a difference of the conformations of PrP^C and PrP^{SC}.
- (3) There is one S-S bond.

Let

$$H^+ = \{ (x_1, x_2, x_3) \in R^3 \mid x_3 \ge 0 \}$$
 and $H^- = \{ (x_1, x_2, x_3) \in R^3 \mid x_3 \le 0 \}$

be the upper-half and lower-half 3-dimensional spaces, and

$$\partial H^+ = \partial H^- = \{ (x_1, x_2, x_3) \in \mathbb{R}^3 \mid x_3 = 0 \}$$

the boundary plane. We consider a topological model of prion proteins on PrP^c and PrP^{SC} to investigate a topological difference between PrP^c and PrP^{SC} as follows (see Fig.21):

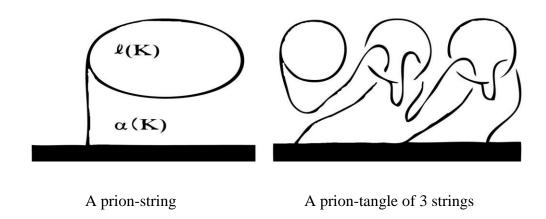


Figure 21

DEFINITION 6.1.

A *prion-string* K in the upper-half 3-space H^+ is a union of a trivial loop I(K) (called the *S-S loop*) in the interior of H^+ and an arc $\alpha(K)$ (called the *GPI-tail*) in H^+ joining a point (called the *S-S vertex*) in $\ell(K)$ with a point (called the *GPI-anchor*) in ∂H^+ . A *prion-tangle of* r *strings* is the union of mutually disjoint r prion-strings whose S-S loops form a trivial link

We note that the one point compactification $(R^3 \cup \{\infty\}, H^- \cup \{\infty\})$ is homeomorphic to a pair (S^3,B) with B a 3-ball in the 3-sphere S^3 . Given a prion-tangle T, we can construct a graph G(T) in S^3 by shrinking the 3-ball B to a point in S^3 , which may be considered as a spatial graph in R^3 in a unique sense up to equivalences (see Fig. 22). Two prion-tangles T and T' are *equivalent* if there is an orientation-preserving homeomorphism h: $H^+ \to H^+$ sending T to T'. By a shape of prion-tangles, we see the following lemma:

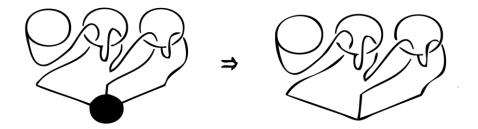


Figure 22: Constructing a spatial graph from the prion-tangle of 3-strings in Fig. 21

LEMMA 6.2.

Two prion-tangles T and T' are equivalent if and only if the spatial graphs G(T) and G(T') are equivalent.

In terms of diagrams of prion-tangles, we obtain the following corollary by combining Theorem 3.3 with Lemma 6.2:

COROLLARY 6.3.

Two prion-tangles T and T' are equivalent if and only if any diagram D of T is deformed into any diagram D' of T' by a finite sequence of the generalized Reidemeister moves I-V in the interior of H⁺ after a suitable position change of the GPI-anchors.

If G(T) is unknotted, Γ -unknotted or prime, then we say that the prion-tangle T is *unknotted*, Γ -unknotted or prime, respectively. A prion-tangle T^* is almost identical to a prion-tangle T if the spatial graph $G(T^*)$ is almost identical to the spatial graph G(T), which is equivalent to saying that T^* and T are not equivalent and there is a graph-isomorphism $q\colon T^*\to T$ such that for every S-S loop or GPI-tail α^* of T^* and $\alpha=q(\alpha^*)$, the α^* -reduction $T^*\setminus \alpha^*$ is equivalent to the α -reduction $T\setminus \alpha$. A prion-tangle T is *trivial* if T is equivalent to a prion-tangle with no crossing point. For a prion-tangle, we see that T is trivial if and only if T is unknotted if and only if T is T-unknotted. For example, the prion-tangle of 3 strings in Fig. 21 is trivial. A prime prion-tangle is non-trivial. Our topological model of prion proteins occurred by supposing that the GPI-tails of some prion-strings happened to cross each other or to pass through the S-S vertices of prion-strings. Some elementary properties of prion-tangles are investigated by Yoshida^[19] who also makes some calculations of the Yamada polynomial^[18] useful in identifying spatial graphs. For example, every prion-tangle T of one string is a trivial prion-tangle because T has a unique edge with the vertex of degree one whose contraction gives a trivial knot. As a consequence of Theorem 5.2, we can observe the following property on prion-tangles.

THEOREM 6.4.

For every prion-tangle T of $r(\ge 2)$ strings, there are infinitely many (up to equivalences) prime prion-tangles T^* almost identical to T. Further, this family contains infinitely many prime prion-tangles in the following two types:

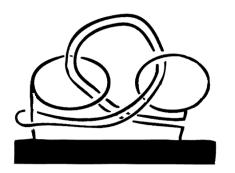
Type I: A prime prion-tangle T* constructed from T by one crossing-change on the GPI tails.

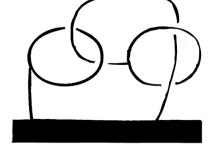
TypeII: A prime prion-tangle T* constructed from T by a GPI-tail passing through an S-S vertex once.

Some examples of types I and II are shown in Fig. 23 where the type II example is given by Yoshida^[19], who showed that this example gives a minimal crossing diagram among the non-trivial prion-tangle diagrams by showing that the prion-tangles with diagrams of crossing numbers ≤ 3 are trivial. By Theorem 6.2, we can observe the following *prime addition property of prion-tangles*:

COROLLARY6.5 (Prime Addition Property).

Let T and T' be any prion-tangles such that T and T' are separated by an upper-half plane in H^+ . Then the prion-tangle $T \cup T'$ is changed into a prime prion-tangle with T and T' as sub-tangles both by one crossing-change on the GPI tails and by a GPI-tail passing through an S-S vertex once.





An example of Type I

An example of Type II

Figure 23

7. Conclusion

The spatial graph induced from a prion-tangle is a spatial graph of a connected plane graph obtained from a finite number of loops by connecting a base point to a point of every loop with an edge and has a unique trivial constituent link. Since it is a relatively simple object in knot theory, a complete classification of prion-tangles may be expected. In our topological models of Cellular PrP's and Scrapie PrP's, we suppose that the Cellular PrP's are trivial prion-tangles and the Scrapie PrP's are non-trivial prion-tangles. Then the prime addition property of prion-tangles may support a conformal difference of Cellular PrP and Scrapie PrP, and also may explain a mysterious fact that the Scrapie PrP's are produced from the Scrapie PrP's and the Cellular PrP's, namely $sPrP^{SC} + tPrP^{C} \rightarrow (s+t) PrP^{SC}$.

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