K. KOBAYASHI KODAI MATH. J. **17** (1994), 511—517

ON THE SPATIAL GRAPH

By Kazuaki Kobayashi

In this article we will explain about spatial graph. Spatial graph is a spatial presentation of a graph in the 3-dimensional Euclidean space \mathbb{R}^3 or the 3-sphere S^3 . That is, for a graph G we take an embedding $f: G \to \mathbb{R}^3$, then the image $\tilde{G} := f(G)$ is called a spatial graph of G. So the spatial graph is a generalization of knot and link. For example the figure 0 (a), (b) are spatial graphs of a complete graph with 4 vertices.



Fig. 0.

Spatial graph theory has an application for molecular biology or stereochemistry to distinguish topological isomer. In this paper we will assume all homeomorphisms and embeddings piecewise linear or edgewise differentiable unless otherwise is stated. To distinguish spatial graphs there are nine equivalence relations among them;

- (1) ambient isotopic
- (3) cobordant
- (5) I-equivalent

- (2) homeomorphic as a pair
- (4) isotopic
- (6) graph homotopic
- (8) graph homologous

(7) weakly graph homotopic(9) Z₂ graph homologous.

Those definitions are as follows. Let $f, g : G \to \mathbb{R}^3$ be spatial presentations of G and I = [0, 1] a unit interval.

Then f and g are

- (1) <u>ambient isotopic</u> if there is a level preserving locally flat embedding $\Phi: G \times I \to \mathbf{R}^3 \times I$ between f and g that is, $\Phi(G,0) = f(G), \Phi(G,1) = g(G),$
- (2) homeomorphic as a pair if there is a homeomorphism $\Phi : (\mathbf{R}^3, f(G)) \to (\mathbf{R}^3, g(G)),$
- (3) <u>cobordant</u> if there is a locally flat embedding $\Phi: G \times I \to \mathbb{R}^3 \times I$ between f and g,
- (4) $\frac{\text{isotopic}}{\text{and } g_i}$ if there is a level preserving embedding $\Phi: G \times I \to \mathbb{R}^3 \times I$ between f
- (5) *I*-equivalent if there is an embedding $\Phi: G \times I \to \mathbf{R}^3 \times I$ between f and g,
- (6) graph homotopic if g is obtained from f by a series of self-crossing changes and

Received June 12, 1993.

KAZUAKI KOBAYASHI

ambient isotopies,

- (7) weakly graph homotopic if g is obtained from f by a series of crossing changes of adjacent edges and ambient isotopies,
- (8) graph homologous if there is a locally flat embedding $\Phi : (G \times I) \notin \bigcup S_i \to \mathbb{R}^3 \times I$ with $\Phi(G \times \{0\}) \subset \mathbb{R}^3 \times \{0\}$ and $\Phi(G \times \{1\}) \subset \mathbb{R}^3 \times \{1\}$ where S_i is a closed orientable surface and S_i is attached on $\operatorname{Int}(e \times I)$ for an edge $e \in E(G)$ by the connected sum and
- (9) \mathbb{Z}_2 graph homologous if in (8) S_i may be non-orientable.

THEOREM 1 ([T1]). The relations among the above equivalence relations are as follows;



Fig. 1.

And those are examples showing the differences for these equivalence relations (Figure 2).



512

By the above examples, in general a spatial graph \hat{G} contains a set of non-trivial knots and links. This means that to distinguish spatial graphs we can use all invariants for knots and links such as; fundamental group, Alexander polynomial, Conway polynomial, Jones polynomial, 2-variable Jones polynomial, Kauffman polynomial, linking number, unknotting number, genus of knot, signature of knot, torsion number, Milnor μ - and $\overline{\mu}$ -invariant etc. And these invariants are well known by knot theorists.

On the other hand there are several invariants directly defined for spatial graphs. Those are; fundamental group, Alexander polynomial, Kauffman polynomial, Yamada polynomial, Topological symmetry group, 1st kind Taniyama invariant, Taniyama-Wu group and 2nd kind Taniyama invariant. In this paper we'll explain Topological symmetry group and 1st and 2nd kind Taniyama invariants.

Topological symmetry group of a spatial graph G.

Let Aut(G) be the group of automorphisms of a graph G and $\tilde{G} = f(G)$ a spatial graph of G where $f: G \to \mathbb{R}^3$ is an embedding. And let

 $\operatorname{TSG}^+(\widetilde{G}) = \{ \tau \in \operatorname{Aut}(G) | \phi \circ f = f \circ \tau \text{ for an orientation preserving homeomorphism} \phi \text{ of } \mathbf{R}^3 \}$

 $TSG^{-}(\tilde{G}) = \{ \tau \in Aut(G) | * \circ \phi \circ f = f \circ \tau \text{ where } * \text{ is an orientation reversing involution of } \mathbb{R}^{3} \}$

And let $\operatorname{TSG}(\widetilde{G}) = \operatorname{TSG}^+(\widetilde{G}) \cup \operatorname{TSG}^-(\widetilde{G}).$

PROPOSITION 2. (1) If \tilde{G} is a plane graph, $\mathrm{TSG}^+(\tilde{G}) = \mathrm{TSG}^-(\tilde{G})$. (2) If G is a non-planar graph, $\mathrm{TSG}^+(\tilde{G}) \cap \mathrm{TSG}^-(\tilde{G}) = \emptyset$ for any spatial graph \tilde{G} of G.

So we consider as $TSG^+(\tilde{G}) = TSG^+(\tilde{G}) \times \{id.\}$ and $TSG^-(\tilde{G}) = TSG^-(\tilde{G}) \times \{*\}$. Then we may consider $TSG(\tilde{G})$ as a subgroup of $Aut(G) \times \mathbb{Z}_2$.

PROPOSITION 3. Let G be a graph. Then

- for any spatial graph G of G, TSG(G) = Aut(G) × Z₂ if and only if G is a forest,
 i.e. 1st Betti number β₁(G) = 0,
- (2) there is a spatial graph \tilde{G} of G such that $TSG(\tilde{G}) = Aut(G) \times \mathbb{Z}_2$ if and only if G is a planar graph,
- (3) there is a spatial graph \tilde{G} of G such that $TSG(\tilde{G}) = \{e\}$ if and only if G has not a vertex v with deg(v) = 1 or 2,
- (4) for any spatial graph \tilde{G} of G, $TSG(\tilde{G}) = \{e\}$ if and only if G contains a subgraph homeomorphic to K_5 or $K_{3,3}$ and $Aut(G) = \{e\}$.

This is a characterization of graphs by TSG.

Examples.



Fig. 3.

And there are some results for TSG of some spatial graphs.

Before stating the result, we'll define the standard spatial graph of a pseudo Hamilton graph and the composition of groups.

Standard spatial graph (presentation) of a pseudo Hamilton graph.

Let G be a pseudo Hamilton graph, that is, a graph with a path Δ containing all vertices of G. We call such a path Δ a Hamilton path. Let B_p be a book with p sheets and the binder Ξ (Figure 4).



Fig. 4.

Take an embedding $\phi: (G, \Delta) \to (B_p, \Xi)$ satisfying the following conditions;

(1) For any edge $e \in E(G) - E(\Delta)$, $\phi(e) \subset P_i$ for a sheet P_i .

(2) For any sheet P_i , there is at least one edge $e \in E(G) - E(\Delta)$ with $\phi(e) \subset P_i$.

Then we call ϕ (or $\phi(G)$) a book presentation of G with respect to a Hamilton path Δ (briefly B.P.H. Δ). When the number of sheets, p, is minimum, $\min\{p|\phi : (G, \Delta) \rightarrow (B_p, \Xi) \text{ a B.P.H. } \Delta\}$, We call $\phi(G)$ a standard spatial graph of G and denote it $\tilde{G}^{\star} = \phi(G)$.

Composition of groups.

514

Let X and Y be finite sets of order m and n respectively. And let A and B be permutation groups acting on X and Y respectively. Then the composition A[B] of A and B is defined and acting on $X \times Y$ as follows; For elements $a \in A, b_1, b_2, \dots, b_m \in$ B, $(a; b_1, b_2, \dots, b_m) \in A[B]$ and the action is defined by $(a; b_1, b_2, \dots, b_m)(x_i, y_j) =$ $(ax_i, b_iy_i).$

Topological symmetry group of some spatial graphs.

PROPOSITION 4. (1) (Mason) If \tilde{G} is a plane graph, $TSG(\tilde{G}) = Aut(G) \times \mathbb{Z}_2$.

- (2) (Yoshimatsu [Y]) For $G = K_5$ or $K_{3,3}$, $TSG(\tilde{G}^*) = Aut(G)$ where \tilde{G}^* is a standard spatial graph of G.
- (3) (Motohashi (see [K-T])) For any spatial graph $\widetilde{K_n}$ of K_n $(n \ge 6)$, $\mathrm{TSG}(\widetilde{K_n}) \subset$ Aut (K_n) by the projection pr : $\mathrm{TSG}(\widetilde{G}) \subset \mathrm{Aut}(G) \times \mathbb{Z}_2 \to \mathrm{Aut}(G)$.

PROPOSITION 5 (Toba [Toba]). (1) $\operatorname{TSG}(\widetilde{K_6}^{\star}) = S_2[S_3].$ (2) There is a spatial $\widetilde{K_6}$ such that $\operatorname{TSG}(\widetilde{K_6}) \subset \operatorname{TSG}(\widetilde{K_6}^{\star}).$

- (3) For any $\widetilde{K_6}$, $|\text{TSG}(\widetilde{K_6})| < |\text{TSG}(\widetilde{K_6}^*)|$.

1st kind Taniyama invariant.

This is an invariant for spatial graphs and defined by Taniyama ([T3]) which is a generalization of Arf invariant of knot.

DEFINITION 6. Let G be a finite graph, $\Gamma = \Gamma(G)$ the set of all cycles of G and $\mathbf{Z}_n = \mathbf{Z}/n\mathbf{Z}$ the additive group of order n. Let $\omega : \Gamma \to \mathbf{Z}_n$ be a map which we call a weight on Γ and $f: G \to \mathbf{R}^3$ a spatial presentation of G. Then we define $\alpha_{\omega}(f)$ by

$$lpha_\omega(f) := \sum_{\gamma \in \Gamma} \omega(\gamma) a_2(f(\gamma)) \pmod{\mathfrak{n}}$$

where $a_2(K)$ is the coefficient of z^2 in the Conway polynomial $\nabla_K(z)$ of a knot K.

DEFINITION.7. For an edge e of a graph G, we give an arbitrary orientation and Γ_e is a subset of Γ which consists of cycles containing the edge $e, \Gamma_e := \{\gamma \in \Gamma | \gamma \supset e\}$. We give an orientation to each $\gamma \in \Gamma_e$ by the orientation of e. Then we say that the weight $\omega: \Gamma \to \mathbf{Z}_n$ balanced on e if the homological sum $\sum_{\gamma \in \Gamma_e} \omega(\gamma) \gamma = 0$ in $H_1(G: \mathbf{Z}_n)$. This dose not depend on the orientation of e.

THEOREM 8 ([T3]). Let $\omega : \Gamma \to \mathbb{Z}_n$ be an weight which is balanced on each edge of G. Then α_{ω} is a graph homotopy invariant. That is, if two embeddings $f, g: G \to \mathbf{R}^3$ are graph homotopic, then $\alpha_{\omega}(f) \equiv \alpha_{\omega}(g) \pmod{n}$.

DEFINITION 9. Let e_1, e_2 be adjacent edges of G. We give an arbitrary orientation to e_1 and let $\Gamma_{e_1,e_2} = \{\gamma \in \Gamma | \gamma \supset e_1, e_2\}$ be a set of cycles of G containing e_1 and e_2 . We give an orientation to each $\gamma \in \Gamma_{e_1,e_2}$ by the orientation of e_1 . We say that an weight $\omega: \Gamma \to \mathbf{Z}_n$ is balanced on a pair of adjacent edges e_1, e_2 if $\sum_{\gamma \in \Gamma_{e_1, e_2}} \omega(\gamma) \gamma = 0$ in $H_1(G: \mathbf{Z}_n)$.

KAZUAKI KOBAYASHI

THEOREM 10 ([T3]). Let $\omega : \Gamma(G) \to \mathbb{Z}_n$ be an weight that is balanced on each pair of adjacent edges of G. Then α_{ω} is an weakly graph homotopy invariant. That is, if embeddings $f, g: G \to \mathbb{R}^3$ are weakly graph homotopic, then $\alpha_{\omega}(f) \equiv \alpha_{\omega}(g) \pmod{n}$.

We call α 1st kind Taniyama invariant.

Taniyama-Wu group and 2nd kind Taniyama invariant.

Let G be an arbitrary oriented finite graph and A(G) a free abelian group over **Z** generated all pair of disjoint edges $b_{ij} = (e_i, e_j)$ $(e_i \cap e_j = \emptyset)$ of G where $b_{ji} = b_{ij}$. For any pair of edges $e_i \in E(G)$ and vertex $v_j \in V(G)$ $(v_j \notin e_i)$, (e_i, v_j) , we define an element r(i, j) of A(G) as follows; if the oriented edges $e_{k1}, e_{k2}, \dots, e_{ku}$ go out from the vertex v_j , the oriented edges $e_{11}, e_{12}, \dots, e_{1v}$ come into the vertex v_j and the oriented edges $e_{m1}, e_{m2}, \dots, e_{mw}$ joint with the vertex v_j and the terminal vertex of e_i , then $r(i, j) := \sum_{p=1}^{u} (e_{kp}, e_i) - \sum_{q=1}^{v} (e_{1q}, e_i)$. And if v_j is a terminal vertex of e_i , then r(i, j) = 0.

Example. For the following Figure 5, $r(i, j) = (e_1, e_i) - (e_3, e_i) - (e_7, e_i) + (e_{10}, e_i)$



Fig. 5.

Let $\mathbf{R}(G)$ be a subgroup of A(G) generated by all r(i, j)'s.

DEFINITION 11. We call the qoutient group, L(G) := A(G)/R(G), Taniyama-Wu group.

For a diagram of an oriented spatial graph, we define the sign $\varepsilon(P)$ of a crossing point P as figure 6.



DEFINITON 12. Let G be an arbitrarily oriented finite graph and $f: G \to \mathbb{R}^3$ a spatial presentation. Take a pair, $b_{ij} = (e_i, e_j)$, of disjoint edges e_i, e_j $(e_i \cap e_j = \emptyset)$, and let $a_{ij} = \sum_{P \in f(e_i) \cap f(e_j)} \varepsilon(P)$. We define

$$l(f) := \sum_{i < j} a_{ij} b_{ij} \in A(G)$$

and take an equivalence class $\mathcal{L}(f) := [l(f)]$ in L(G).

516

THEOREM 13 ([T2]). Two spatial graph $f_1(G)$, $f_2(G)$ are graph homologous if and only if $\mathcal{L}(f_1) = \mathcal{L}(f_2)$.

We call $\mathcal{L}(f)$ 2nd kind Taniyama invariant.

References

- [K] K. Kobayashi, Standard spatial graph, Hokkaido Math.J. vol. XXI (1) (1992) 117-140.
- [K-T] K. Kobayashi and C. Toba, Topological symmetry group of spatial graph, Proc. TGRC-KOSEF 3 (1993) 153-171.
- [T] C. Toba, Topological symmetry group of spatial graph and its related topics, Master Theses (Tokyo Woman's Christian Univ.) (1993).
- [T1] K. Taniyama, Cobordism, homotopy and homology of graphs in R³, Topology 33(3) (1994) 509-523.
- [T2] K. Taniyama, Homology classification of spatial embeddings of a graph, (preprint).
- [T3] K. Taniyama, Link homotopy invariants of graphs in \mathbb{R}^3 , Revista Mat. Univ. Complut. Madrid. 7(1) (1994) 129–144.
- [W] W.T. Wu, A theory of imbedding, immersion and isotopy of polytopes in a Euclidean space, Science Press. Peking, (1965).
- [Y] Y. Yoshimatsu, Topological symmetry group of standard spatial graph of K₅, Master Theses (Tokyo Woman's Christian Univ.) (1992) (in Japanese).

DEPARTMENT OF MATHEMATICS TOKYO WOMAN'S CHRISTIAN UNIVERSITY 167 SUGINAMIKU, ZENPUKUZI 2-6-1 TOKYO, JAPAN