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Dynnikov Three-Page Diagrams of Spatial 3-Valent Graphs

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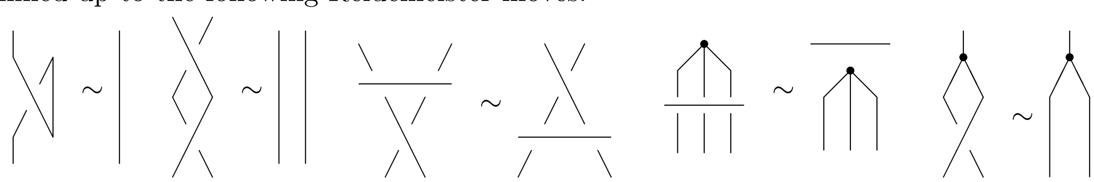
Recently, Dynnikov suggested a new way of encoding nonoriented links by three-page diagrams [1], and this permitted him to obtain an algebraic classification of the isotopy classes of nonoriented links (see [2]). We generalize this approach to 3-valent graphs. A finite graph is said to be 3-*valent* if exactly three edges meet at any vertex. We consider only 3-valent nonoriented graphs, which can be disconnected and have loops and multi-edges. By a *spatial graph* we mean an embedding of a graph in $\mathbb{R}^3$ under which the edges become finite polygonal lines. We study the spatial graphs up to an ambient isotopy, where an *ambient isotopy between two graphs* is a continuous family of homeomorphisms $\phi_t \colon \mathbb{R}^3 \to \mathbb{R}^3$, $t \in [0,1]$, such that $\phi_0 = \mathrm{id}$ and ϕ_1 sends one of these graphs to the other. Isotopy invariants of spatial graphs were studied in [3, 4]. For other equivalence relations (including concordance, homotopy, and homology), see [5].

The notion of spatial graph is motivated both theoretically and practically. First, the problem to classify the spatial graphs up to isotopy is a special case of the general topological problem of classifying the embeddings in Euclidean space. We simultaneously obtain a natural extension of the classical knot theory to more complex one-dimensional objects. Many invariants of ordinary links, including the Alexander polynomials and Vassiliev invariants, can be generalized to graphs [6, 7]. As well as the ordinary links, the spatial graphs can readily be represented by plane diagrams determined up to the following Reidemeister moves:



Second, spatial graphs are useful mathematical models for long protein molecules in organic chemistry and molecular biology. As is known, a twisted α-spiral is a stable primary structure of a DNA molecule consisting of several hundred atoms [8]. The stability is caused by hydrogen connections. Adding these connections to the molecule as virtual edges, we obtain a 3-valent graph in $\mathbb{R}^3$. One of the main problems in modern biology is to predict the real shape of a molecule in dependence on its atomic composition [9]. In particular, it is of interest to find out what spatial graphs can be obtained for a given molecule. Diverse chemical properties are determined precisely by the spatial structure of the molecule. For instance, it is of importance whether or not a molecule can take the shape reflection symmetric to the original shape [10]. The principal difficulty is that any biological system is open to any action of external forces. Some ferments can change the topological type of a molecule. However, this process can be controlled, which helps to synthesize certain compounds [11].

The discussion below follows [12]. Consider the semigroup Stg with the set of generators $\mathbb{A} = \{a_i, b_i, c_i, d_i, e_i, f_i, g_i, h_i; i \in \mathbb{Z}_3\}$ and the following 90 defining relations ($i = 1, 2, 3$; one of relations (4) can be omitted by using (3)):

(1) $a_i = a_{i+1}d_{i-1}$, $b_i = a_{i-1}c_{i+1}$, $c_i = b_{i-1}c_{i+1}$, $d_i = a_{i+1}c_{i-1}$,

(2) $e_i = d_i g_i = g_{i-1}b_{i+1} = a_{i+1}h_{i-1}$, $f_i = h_i b_i = d_{i+1}h_{i-1} = g_{i-1}c_{i+1}$,

(3) $d_1 d_2 d_3 = 1$,

(4) $b_i d_i = d_i b_i = 1$,

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(5) $(d_{i-1}c_{i-1})x = x(d_{i-1}c_{i-1})$, where $x \in \{c_i, e_i, b_{i-1}d_id_{i-1}\}$,

(6) $uv = vu$, where $u \in \{a_{i-1}b_{i-1}, e_{i-1}b_{i-1},\ b_{i+1}d_{i-1}d_{i+1}b_{i-1}\}$, $v \in \{a_i, b_i, c_i, e_i, b_{i-1}d_id_{i-1}\}$.

Theorem 1. *Any spatial graph can be encoded by an element of the semigroup Stg.*

Theorem 2. *Spatial graphs are isotopic if and only if the elements representing them coincide in Stg.*

Theorem 3. *An element of Stg encodes a spatial graph if and only if this element is central, i.e., commutes with any element of this semigroup.*

The proof of Theorem 3 is similar to that of Lemma 3 in [2]. Let P_1, P_2, P_3 be three half-planes in $\mathbb{R}^3$ whose boundaries coincide: $\partial P_1 = \partial P_2 = \partial P_3 = \alpha$ (see the right-hand part of the figure below). Set $\mathbb{Y} = P_1 \cup P_2 \cup P_3$. Let us choose an orientation on the axis α. By a *three-page diagram* (*a* 3*-diagram*) of a spatial graph Γ we mean an embedding of the graph Γ in $\mathbb{Y}$ such that

(a) all 3-valent vertices of Γ belong to α;

(b) (transversality with respect to α) the intersection $\Gamma \cap \alpha = A_1 \cup \cdots \cup A_m$ is finite;

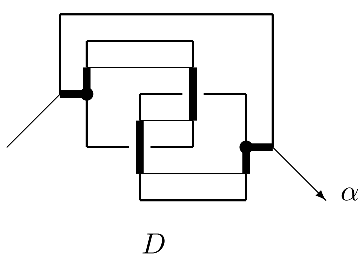
(c) two arcs abutting upon a vertex of degree two belong to different half-planes;

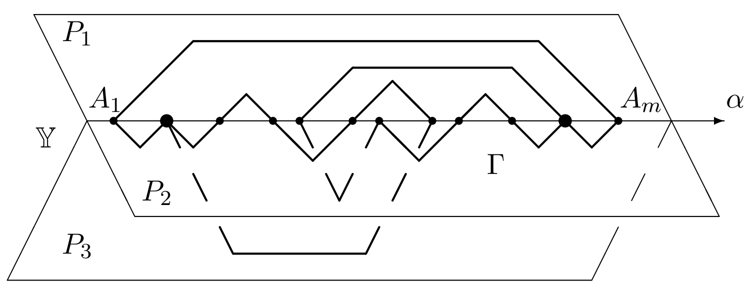
(d) two of three arcs abutting upon a 3-valent vertex belong to one half-plane and the third arc belongs to another;

(e) (monotonicity) the restriction of the orthogonal projection $\mathbb{R}^3 \to \alpha \approx \mathbb{R}$ to any *arch* (a connected component of the intersection $\Gamma \cap P_i$) is a monotone function for any $i = 1, 2, 3$.

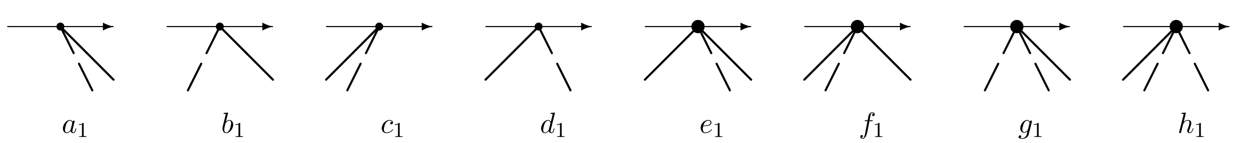
Proof of Theorem 1. A 3-diagram is said to be *special* if any arch in the half-plane P_2 is either of length 2, i.e., joins a vertex A_i with the vertex A_{i+2}, or of length 1, in which case it contains a 3-valent vertex. For a plane diagram of a graph we will construct a special three-page diagram determining the same spatial graph. Let us mark a small segment (an *intermediate bridge*) of the upper arc for any crossing of our plane diagram D and two small outgoing arcs (a *primary bridge*) for any 3-valent vertex.

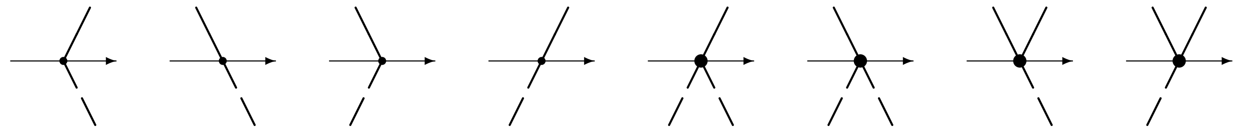
Let us choose an arbitrary non-self-intersecting orientable path in the plane of D such that the ends of the path are outside D and the path passes along each bridge exactly once and intersects the remaining part of the diagram transversally. Deform the plane of the diagram in such a way that the path becomes a segment of a straight line α. Next, we attach a half-plane P_2 along this line and push out any bridge to P_2 so that any intermediate bridge becomes a single trivial arch and any primary bridge becomes a pair of arches meeting at a 3-valent vertex:



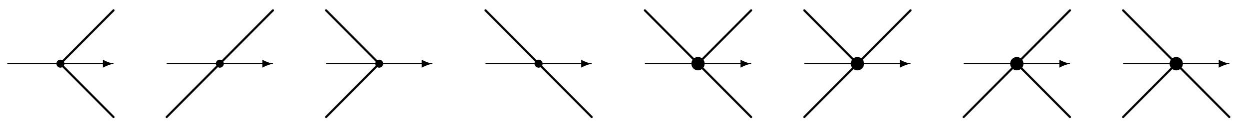


Clearly, the entire 3-diagram of a spatial graph can uniquely be recovered from a part of this diagram in a small neighborhood of the axis α. To this end, it suffices to join the oppositely directed units, starting from the innermost ones, in each of the half-planes. In the vicinity of α, a 3-diagram can consist of elements of the following 24 types:





a_2 b_2 c_2 d_2 e_2 f_2 g_2 h_2



a_3 b_3 c_3 d_3 e_3 f_3 g_3 h_3

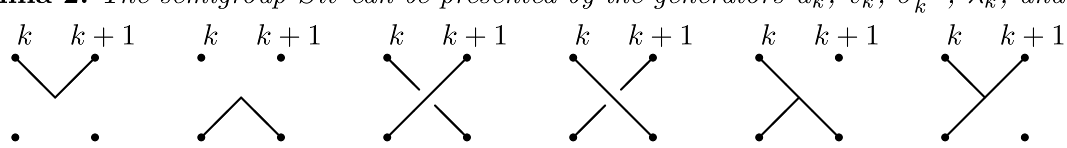
Let W be the set of all words in this alphabet $\mathbb{A}$ including the empty word $\varnothing$. For a given 3-diagram Γ, let us successively write out the above types of all vertices on the axis α. We obtain a word $w_\Gamma \in W$ (for the diagram in the figure, one has $w_\Gamma = a_3e_1b_3d_3a_2b_3b_1c_2b_3d_3h_3c_3$). Note that in this way one can obtain only the so-called *balanced* words rather than all words in W. A simple geometric criterion for a word to be balanced is as follows: all units outgoing from points on the axis must be joined with one another. This condition can readily be represented algebraically via the alphabet $\mathbb{A}$. For nonbalanced words, units of the corresponding 3-diagram can come to the boundary without joining to other units. $\square$

Outline of the proof of Theorem 2. All relations (1)–(6) can readily be realized by an isotopy in $\mathbb{R}^3$. This isotopy can be carried out in the two-dimensional complex $\mathbb{T}$ obtained from $\mathbb{Y}$ by attaching a half-plane P_4 to $P_1 \cup P_2$ along a line perpendicular to α. Any 3-diagram can be reduced to a special one according to the following assertion (its proof is similar to that of Proposition 2 in [1]).

Lemma 1. *For any $i \in \mathbb{Z}_3$, any balanced word can be decomposed into the subwords a_i, b_i, c_i, d_i, e_i, $b_{i-1}b_id_{i-1}$, and $b_{i-1}d_id_{i-1}$ by means of relations* (1)–(6). $\square$

It remains to show that relations (1)–(6) are sufficient to realize any isotopy of graphs. Introduce the semigroup *Sit* of infinite tangles. Take two horizontal positive axes $\mathbb{R}_+$ in $\mathbb{R}^3$ one of which is above the other and denote by V the three-dimensional layer between the horizontal planes containing these axes. Consider a 3-valent graph T with finitely many 3-valent vertices and countably many isolated segments. By an *infinite tangle* we mean an embedding of the graph T in the above layer V such that the end vertices of the graph T coincide with positive integer points on the axes $\mathbb{R}_+$. Assume that, at a rather large distance from the zero border, all segments of the tangle are parallel to one another (but can be not vertical). The equivalence relation for such graphs is an ambient isotopy on V that is the identity mapping on the boundary of the layer. The *product* T_1T_2 of tangles is obtained by attaching the upper axis $\mathbb{R}_+$ of T_2 to the lower axis $\mathbb{R}_+$ of T_1. We thus obtain the structure of a semigroup on *Sit* with identity element 1 consisting of the vertical segments. The next lemma can be proved similarly to the Reidemeister theorem. Geometrically, relations (7)–(15) correspond to a passage through singularities of codimension one in the space of all infinite tangles with self-intersections.

Lemma 2. *The semigroup Sit can be presented by the generators u_k, v_k, $\sigma_k^{\pm 1}$, λ_k, and y_k,*



u_k v_k σ_k σ_k^{-1} λ_k y_k

and the defining relations $(k+1 < l)$

$$
(7)\begin{cases} u_k u_l = u_{l+2} u_k, \quad u_k v_l = v_{l+2} u_k, \quad u_k \sigma_l = \sigma_{l+2} u_k, \quad u_k \lambda_l = \lambda_{l+2} u_k, \quad u_k y_l = y_{l+2} u_k, \\ v_k v_l = v_{l-2} v_k, \quad v_k \sigma_l = \sigma_{l-2} v_k, \quad v_k \lambda_l = \lambda_{l-2} v_k, \quad v_k y_l = y_{l-2} v_k, \quad \lambda_k \sigma_l = \sigma_{l-1} \lambda_k, \\ \lambda_k \lambda_l = \lambda_{l-1} \lambda_k, \quad \lambda_k y_l = y_{l-1} \lambda_k, \quad y_k \sigma_l = \sigma_{l+1} y_k, \quad y_k y_l = y_{l+1} y_k, \quad \sigma_k \sigma_l = \sigma_l \sigma_k, \end{cases}
$$

$$
(8) \quad v_{k+1} u_k = 1 = v_k u_{k+1}, \qquad (11) \quad v_k \sigma_k = v_k, \quad \sigma_k u_k = u_k,
$$

$$
(9) \quad \lambda_k = v_{k+1} y_k, \quad y_k = \lambda_k u_{k+1}, \qquad (12) \quad \sigma_k \sigma_k^{-1} = 1 = \sigma_k^{-1} \sigma_k,
$$

$$
(10) \quad v_{k+2} \sigma_{k+1} u_k = \sigma_k^{-1} = v_k \sigma_{k+1} u_{k+2}, \qquad (13) \quad \sigma_k \sigma_{k+1} \sigma_k = \sigma_{k+1} \sigma_k \sigma_{k+1},
$$

$$
(14) \quad \lambda_k \sigma_{k+1} \sigma_k = \sigma_k \lambda_{k+1}, \; \sigma_k \sigma_{k+1} y_k = y_{k+1} \sigma_k, \; \sigma_k \lambda_k = \lambda_{k+1} \sigma_k \sigma_{k+1}, \; y_k \sigma_k = \sigma_{k+1} \sigma_k y_{k+1},
$$

$$
(15) \quad \lambda_k \sigma_k = \lambda_k, \quad \sigma_k y_k = y_k. \quad \square
$$

One can convert any infinite tangle into a 3-diagram by erecting the axes $\mathbb{R}_+$ vertically, attaching two half-planes to the lower bound $\mathbb{R} \times 0$ thus obtained, and moving the crossings and the 3-valent vertices to the axis $\mathbb{R} \times 0$. This defines an embedding of the semigroup *Sit* of infinite tangles in the semigroup *Stg*. In particular, the above generators are taken to the so-called *elementary* words: $u_k = d_3^k c_3 b_3^{k-1}$, $v_k = d_3^{k-1} a_3 b_3^k$, $\sigma_k = d_3^{k-1} b_2 d_3 d_2 b_3^k$, $\lambda_k = d_3^{k-1} e_3 b_3^k$, and $y_k = d_3^k f_3 b_3^{k-1}$. Any balanced word can be decomposed into elementary ones, and this is similar to that in [12], i.e., a balanced word defines an infinite tangle. Since any spatial graph is represented by a balanced word, it follows that an infinite tangle can be assigned to such a graph, and to isotopic spatial graphs there correspond isotopic infinite tangles. To complete the proof of Theorem 2, it remains to derive relations (7)–(15) of the semigroup *Sit* from relations (1)–(6) of the semigroup *Stg*. The decomposition into elementary words and the proof of the relations are similar to those in [12]. $\square$

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