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FUNDAMENTAL GROUPOIDS OF DIGRAPHS AND GRAPHS

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Abstract. We introduce the notion of fundamental groupoid of a digraph and prove its basic properties. In particular, we obtain a product theorem and an analogue of the Van Kampen theorem. Considering the category of (undirected) graphs as the full subcategory of digraphs, we transfer the results to the category of graphs. As a corollary we obtain the corresponding results for the fundamental groups of digraphs and graphs. We give an application to graph coloring.

Keywords: digraph; fundamental group; fundamental groupoid; product of graphs

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1. Introduction

In this paper we develop further the homotopy theory for digraphs (= directed graphs) initiated in [9], [8], and [10]. In the category of digraphs, the homology and the homotopy theories were introduced in [8] in such a way that the homology groups are homotopy invariant and the first homology group of a connected digraph is isomorphic to the abelization of its fundamental group. In a natural way we can consider the category of nondirected graphs as a full subcategory of digraphs. Thus, the homology and homotopy theories of digraph can be transferred to the category of nondirected graphs, thus leading to similar results for the latter category.

In the case of undirected graphs the fundamental group was first introduced in papers [3] and [4], where they described the relation of the fundamental group of graph to the Atkin homotopy theory [1], [2]. Note that for undirected graphs the notions of fundamental groups of [8] and [3], [4] coincide.

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In the present paper we introduce the notion of the fundamental groupoid of a digraph that is a natural generalization of the notion of fundamental group of digraph from [8]. Our definition of groupoid has essentially the origin in the discrete nature of graphs and is not related to the notion of fundamental groupoid of a graph as a topological space from [5] and [13].

We prove basic properties of the fundamental groupoid of digraphs, in particular, a product formula for the fundamental groupoids for various notions of product of digraphs as well as an analogue of the Van Kampen theorem for groupoids. Considering the category of nondirected graphs as a full subcategory of the category of digraphs we transfer these results to the category of nondirected graphs. Note that the Van Kampen theorem for the fundamental group of graphs was obtained also in [3] and [4].

The paper is organized as follows. In Section 2, we give a preliminary material, necessary definitions, and some useful constructions in the category of digraphs based on [8], [9], and [12].

In Section 3, we define the fundamental groupoid of a digraph and describe its basic properties. In fact, we define a functor from the category of digraphs to the category of groupoids. We prove the results concerning fundamental groupoids for various products of digraphs. We also give application to the first homology group of the products.

In Section 4, we construct a functor Δ (geometrical realization) from the category of digraphs to the category of 2-dimensional CW-complexes, that provides a natural equivalence of the corresponding fundamental groupoids on the vertices of digraphs. As a consequence of the geometric realization we obtain an analogue of the Van Kampen theorem for groupoids of digraphs.

In Section 5, we transfer the aforementioned results to the category of nondirected graphs and compare our results with those in [3], [4].

In Section 6, we give an application to coloring of graphs.

2. Category of digraphs and homotopy theory

In this section we give necessary definitions and preliminary material (see [9] and [8]) which we need in the following sections. We prove also several technical results.

Definition 2.1. A *directed graph* (*digraph*) G is a pair (V_G, E_G) consisting of a set V_G of vertices and a subset $E_G \subset \{V_G \times V_G \setminus \mathrm{diag}\}$ of ordered pairs. The elements of E_G are called *arrows* and are denoted by $v \to w$, where the vertex $v = \mathrm{orig}(v \to w)$ is the *origin of the arrow* and the vertex $w = \mathrm{end}(v \to w)$ is the *end of the arrow.*

A *based digraph* $G^* = (G, *)$ is a digraph G together with a *based vertex* $v = * \in V_G$.

If there is an arrow from v to w, then we write $v \to w$. For two vertices $v, w \in V_G$ we write $v \,\overrightarrow{=}\, w$ if either $v = w$ or $v \to w$.

Definition 2.2. A digraph H is called a *subdigraph of* G if $V_H \subset V_G$ and $E_H \subset E_G$.

Definition 2.3. A *digraph map* (or simply *map*) from a digraph G to a digraph H is a map $f\colon V_G \to V_H$ such that $v \to w$ on G implies $f(v) \,\overrightarrow{=}\, f(w)$ on H. A digraph map f is *non-degenerate* if $v \to w$ on G implies $f(v) \to f(w)$ on H.

A digraph map of based digraphs $f\colon (G, v) \to (H, w)$ has additional property: $f(v) = w$.

The set of all digraphs with digraph maps form a *category of digraphs* that will be denoted by $\mathcal{D}$. The set of all based digraphs with based digraph maps form a *category of based digraphs* that will be denoted by $\mathcal{D}^*$.

For two digraphs G and H we denote by $\mathrm{Hom}(G, H)$ the set of all digraph maps from G to H. For two based digraphs G^* and H^* we denote by $\mathrm{Hom}(G^*, H^*)$ the set of all based digraph maps from G^* to H^*.

Definition 2.4. For digraphs G, H define two notions of their product.

(i) Define a $\Box$*-product* $\Pi = G \,\Box\, H$ as a digraph with a set of vertices $V_\Pi = V_G \times V_H$ and a set of arrows E_Π given by the rule

$$(x, y) \to (x', y') \quad \text{if } x = x' \text{ and } y \to y', \quad \text{or} \quad x \to x' \text{ and } y = y',$$

where $x, x' \in V_G$ and $y, y' \in V_H$. The $\Box$-product is also referred to as the Cartesian product.

(ii) Define a $\rtimes\!\!\!\ltimes$*-product* $P = G \rtimes\!\!\!\ltimes H$ as a digraph with a set of vertices $V_P = V_G \times V_H$ and a set of arrows E_P given by the rule

$$(x, y) \to (x', y') \text{ if } x = x' \text{ and } y \to y', \text{ or } x \to x' \text{ and } y = y', \text{ or } x \to x' \text{ and } y \to y'.$$

Let G and H be digraphs. For any vertex $v \in V_H$ there are natural inclusions $i_v\colon G \to P$ and $j_v\colon G \to \Pi$ given on the set of vertices by the rules

$$i_v(x) = (x, v) \in V_P, \quad j_v(x) = (x, v) \in V_\Pi \quad \text{for } x \in V_G.$$

Similarly, there are natural inclusions $i_w\colon H \to P$ and $j_w\colon H \to \Pi$ for any $w \in V_G$.

Also we have natural projections $p\colon\ P \to G$, $q\colon\ P \to H$ given on the set of vertices by the rule

$$p(x,y) = x \in V_G, \quad q(x,y) = y \in V_H \quad \text{for } x \in V_G,\ y \in V_H.$$

Similarly, there are projections $\Pi \to G$ and $\Pi \to H$.

In what follows we use the sign $\dot\cup$ to denote a disjoint union.

Definition 2.5. (i) Let $f\colon\ G \to H$ be a digraph map of digraphs G, H. Define a digraph $\mathrm{C}_f = (V_\mathrm{C}, E_\mathrm{C})$ as

$$V_\mathrm{C} = V_G \,\dot\cup\, V_H, \quad E_\mathrm{C} = E_G \,\dot\cup\, E_H \,\dot\cup\, E_I, \quad \text{where } E_I = \{(v \to f(v))\colon\ v \in V_G\}.$$

The digraph C_f is called the *direct cylinder of the map* f. The *inverse cylinder* C_f^- of the map f has the same set of vertices V_C as C_f and the set of arrows

$$E_{\mathrm{C}^-} = E_G \,\dot\cup\, E_H \,\dot\cup\, E_{I^-}, \quad \text{where } E_{I^-} = \{(f(v) \to v)\colon\ v \in V_G\}.$$

Let us recall now the basic notions of the homotopy theory of [8]. Let I_n, $n \geqslant 0$, denote a digraph with the set of vertices $V_n = \{0, 1, \dots, n\}$ and the set of arrows E_{I_n} that contains exactly one of the arrows $i \to (i+1)$ and $(i+1) \to i$ for any $i = 0, 1, \dots, n-1$, and no other arrow. The digraph I_n is called a *line digraph.* There are only two line digraphs with two vertices, which will be denoted by $I = (0 \to 1)$ and $I^- = (1 \to 0)$.

Denote by I_n^* the based digraph $(I_n, 0)$. Let $\mathcal{I}_n$ (or $\mathcal{I}_n^*$) be the set of all line digraphs (or based line digraphs) with the vertex set V_n and set

$$\mathcal{I} = \bigcup_{n \geqslant 0} \mathcal{I}_n, \quad \mathcal{I}^* = \bigcup_{n \geqslant 0} \mathcal{I}_n^*.$$

Definition 2.6. Let G, H be digraphs.

(i) Two digraph maps $f_i\colon\ G \to H$, $i = 0, 1$, are called *homotopic* if there exists a line digraph $I_n \in \mathcal{I}$ and a digraph map $F\colon\ G \,\Box\, I_n \to H$ such that

$$F|_{G \Box \{0\}} = f_0\colon\ G \,\Box\, \{0\} \to H, \quad F|_{G \Box \{n\}} = f_1\colon\ G \,\Box\, \{n\} \to H.$$

In this case we shall write $f_0 \simeq f_1$. If $I_n = I_1$, then we shall refer to F as a *one-step homotopy from* f_0 to f_1 and to the maps f_i as *one-step homotopic.*

(ii) Two digraphs G and H are *homotopy equivalent* if there exist digraph maps

$$f\colon\ G \to H, \quad g\colon\ H \to G$$

such that

$$f \circ g \simeq \mathrm{Id}_H, \quad g \circ f \simeq \mathrm{Id}_G.$$

In this case, we write $H \simeq G$, and the maps f and g are called *homotopy inverses* to each other.

(iii) A digraph G is *contractible* if it is homotopy equivalent to the one-vertex digraph.

Thus, we obtain a well defined category $\mathcal{D}'$ of digraphs with the classes of homotopic maps as digraph maps in $\mathcal{D}'$.

A homotopy between two based digraph maps $f, g\colon G^* \to H^*$ is defined as in Definition 2.6 with additional requirement that $F|_{\{*\}\Box I_n} = *$. Then we obtain a homotopy category $\mathcal{D}^{*\prime}$ of based digraphs.

For any $I_n \in \mathcal{I}_n$ define the line digraph $\hat{I}_n \in \mathcal{I}_n$ as:

$$i \to j \ \text{ in } \hat{I}_n \Leftrightarrow (n-i) \to (n-j) \ \text{ in } I_n.$$

For any two line digraphs I_n and I_m, define the line digraph $I_{n+m} = I_n \vee I_m \in \mathcal{I}_{n+m}$ by identification of the vertices $n \in I_n$ and $0 \in I_m$ and keeping the arrows in I_n, I_m.

Definition 2.7. (i) A *path-map* in a digraph G is any digraph map $\varphi\colon I_n \to G$, where $I_n \in \mathcal{I}_n$. A *based path-map* on a based digraph G^* is a based digraph map $\varphi\colon I_n^* \to G^*$. A *loop* on a based digraph G^* is a based path-map $\varphi\colon I_n^* \to G^*$ such that $\varphi(n) = *$.

(ii) For a path-map $\varphi\colon I_n \to G$ define the *inverse path-map* $\widehat{\varphi}\colon \hat{I}_n \to G$ by $\widehat{\varphi}(i) = \varphi(n-i)$.

(iii) For two path-maps $\varphi\colon I_n \to G$ and $\psi\colon I_m \to G$ with $\varphi(n) = \psi(0)$ define the *concatenation path-map* $\varphi \vee \psi\colon I_{n+m} \to G$ as

$$\varphi \vee \psi(i) = \begin{cases} \varphi(i), & 0 \leqslant i \leqslant n, \\ \psi(i-n), & n \leqslant i \leqslant n+m. \end{cases}$$

Definition 2.8. A digraph map $h\colon I_n \to I_m$ is called a *shrinking map* if $h(0) = 0$, $h(n) = m$, and $h(i) \leqslant h(j)$ whenever $i \leqslant j$.

Definition 2.9. Consider two path-maps

$$\varphi\colon I_n \to G, \quad \psi\colon I_m \to G \quad \text{such that} \quad \varphi(0) = \psi(0),\ \varphi(n) = \psi(m). \tag{2.1}$$

A *one-step direct C_∂-homotopy* from φ to ψ is a pair (h, F), where $h\colon I_n \to I_m$ is a shrinking map and $F\colon \mathrm{C}_h \to G$ is a digraph map such that

$$F|_{I_n} = \varphi \quad \text{and} \quad F|_{I_m} = \psi. \tag{2.2}$$

If the same is true with C_h replaced everywhere by C_h^-, then we refer to a one-step *inverse C_∂*-homotopy.

Now we define an equivalence relation on the set of path-maps of a digraph G.

Definition 2.10. Let φ, ψ be path-maps as in (2.1). We call these path-maps *$C\partial$-homotopic* and write $\varphi \overset{C\partial}{\simeq} \psi$ if there exists a finite sequence $\{\varphi_k\}_{k=0}^{m}$ of path-maps such that $\varphi_0 = \varphi$, $\varphi_m = \psi$ and for any $k = 0, \dots, m-1$, φ_k is one-step $C\partial$-homotopic to φ_{k+1} or inverse φ_{k+1} is one-step $C\partial$-homotopic to φ_k.

As follows from Definition 2.10, the relation $\varphi \overset{C\partial}{\simeq} \psi$ is an equivalence relation. Note that for the based loops in a based digraph G^*, our notion of $C\partial$-homotopy from Definition 2.10 coincides with the notion of C-homotopy of [8], Definition 4.10.

Theorem 2.11 ([8]). *Let $\pi_1(G^*)$ be the set of equivalence classes under $C\partial$-homotopy of based loops of a digraph G^*. The $C\partial$-homotopy class of a based loop φ will be denoted by $[\varphi]$. Then $\pi_1(G^*)$ is a group with the neutral element $[e]$, where $e\colon I_0^* \to G^*$ is the trivial loop, the inverse element of $[\varphi]$ is $[\widehat{\varphi}]$, and the product is given by concatenation of the loops $[\varphi][\psi] = [\varphi \vee \psi]$.*

Now we discuss the properties of the $\rtimes$-product of digraphs.

Proposition 2.12. *For any line digraph I_n and any digraph G*

$$G \rtimes I_n \simeq G.$$

P r o o f. Consider the case $n = 1$ and the digraph $G \rtimes I$. We have a natural inclusion

$$j\colon\ G \to G \rtimes I, \quad j(v) = v \rtimes \{0\}, \quad v \in V_G$$

and a natural projection $p\colon\ G \rtimes I \to G$ such that the composition $p \circ j\colon\ G \to G$ is the identity map. Now we prove that the composition $j \circ p$ is homotopic to the identity map $\mathrm{Id}_{G \rtimes I}$. Define a homotopy

$$H\colon\ (G \rtimes I) \,\Box\, I^- \to G \rtimes I$$

as:

$$H_0 = \mathrm{Id}_{G \rtimes I}\colon\ (G \rtimes I) \,\Box\, \{0\} \to G \rtimes I, \quad H_0(v, t, 0) = (v, t, 0), \quad v \in V_G,\, t \in V_I,$$

on the bottom, and the composition

$$j \circ p\colon\ (G \rtimes I) \,\Box\, \{1\} \to G \rtimes \{0\}, \quad H_1(v, t, 1) = (v, 0), \quad v \in V_G,\, t \in V_I,\, 1 \in V_{I^-}$$

on the top. The map H is a well defined digraph map of digraphs.

The case of $G \rtimes I^-$ is similar, which settles the claim for $n = 1$. The claim for general n is proved by induction on n. □

Let D, G, H be arbitrary digraphs. For a given digraph map

$$f\colon D \to G \rtimes H$$

consider the digraph maps

$$f_1 = p \circ f\colon D \to G, \quad f_2 = q \circ f\colon D \to H,$$

where $p\colon G \rtimes H \to G$, $q\colon G \rtimes H \to H$ are natural projections.

Proposition 2.13. *There exists a one to one correspondence between the sets* $\mathrm{Hom}(D, G \rtimes H)$ *and* $\mathrm{Hom}(D, G) \times \mathrm{Hom}(D, H)$, *given by the rule*

$$f \leftrightarrow (f_1, f_2).$$

P r o o f. Let r be the map of sets

$$\mathrm{Hom}(D, G \rtimes H) \to \mathrm{Hom}(D, G) \times \mathrm{Hom}(D, H), \quad r(f) = (f_1, f_2). \tag{2.3}$$

Let $f \neq g \in \mathrm{Hom}(D, G \rtimes H)$. Since the digraph maps f and g are defined on the set of vertices, there exists a vertex $v \in V_D$ such that

$$f(v) = (v_1, v_2) \neq g(v) = (w_1, w_2), \quad \text{where } (v_1, v_2), (w_1, w_2) \in V_{G \rtimes H}.$$

Hence, at least one inequality $v_1 \neq w_1$, $v_2 \neq w_2$ is true. Hence, $(f_1, f_2)(v) \neq (g_1, g_2)(v)$ since $f_i(v) = v_i$, $g_i(v) = w_i$. Thus, the map r is a one-to-one inclusion. The map r is a surjection since any two maps $f_1 \in \mathrm{Hom}(D, G)$, $f_2 \in \mathrm{Hom}(D, H)$ are defined by the maps of vertices

$$f_1\colon V_D \to V_G, \quad f_2\colon V_D \to V_H,$$

which define a map of vertices

$$f = (f_1, f_2)\colon V_D \to V_{G \rtimes H} = V_G \times V_H,$$

which is a well-defined digraph map of digraphs $f\colon D \to G \rtimes H$ for which $r(f) = (f_1, f_2)$. $\square$

Lemma 2.14. *Consider a path map* $\varphi\colon I_s \to I_n \rtimes I_n$ *such that* $\varphi(0) = (0, 0)$ *and* $\varphi(k) = (n, n)$. *Then* φ *is* C_∂*-homotopic to the diagonal path map* $\Delta\colon I_n \to I_n \rtimes I_n$ *given by* $\Delta(i) = (i, i)$.

P r o o f. Using [8], Proposition 3.6, it is easy to construct a deformation retraction r from $I_n \rtimes I_n$ onto its diagonal diag which leads to a homotopy

$$F\colon (I_n \rtimes I_n) \,\square\, I_k \to I_n \rtimes I_n$$

such that $F|_{(I_n \rtimes I_n)\square\{0\}} = \mathrm{id}$, $F|_{(I_n \rtimes I_n)\square\{k\}} = r$ and additionally

$$F|_{\mathrm{diag}\square\{i\}} = \mathrm{id}_{\mathrm{diag}} \tag{2.4}$$

for any $i \in I_k$. For any path-map $\varphi\colon I_s \to I_n \rtimes I_n$ define a digraph map

$$\varphi \,\square\, \mathrm{id}_{I_k}\colon I_s \,\square\, I_k \to (I_n \rtimes I_n) \,\square\, I_k.$$

Then the composition

$$\Phi := F \circ (\varphi \,\square\, \mathrm{id}_{I_k})\colon I_s \,\square\, I_k \to I_n \rtimes I_n$$

has the following properties: $\Phi|_{I_s\square\{0\}} = \varphi$ and $\Phi|_{I_s\square\{k\}}$ is the digraph map onto diag such that $\Phi(0,k) = (0,0)$, $\Phi(s,k) = (n,n)$. Now by (2.4), $\Phi|_{I_s\square\{0\}} = \varphi$ and $\Phi|_{I_s\square\{k\}}$ are homotopic and hence, C_∂-homotopic. It remains to observe that the path-maps

$$\Phi|_{I_s\square\{k\}}\colon I_s \to \mathrm{diag}$$

and $\Delta\colon I_n \to \mathrm{diag}$ are C_∂-homotopic (for example, using [8], Theorem 4.13). $\square$

Definition 2.15. Let $\varphi\colon I_m \to G$ be a path-map. An *extension* φ^E of φ is any path-map

$$\varphi^E\colon I_n \to G, \quad I_n \in \mathcal{I}$$

that is given by the composition $\varphi \circ h$, where $h\colon I_n \to I_m$ is a shrinking map.

Note that any extension φ^E of φ by means of shrinking map $h\colon I_n \to I_m$ satisfies the conditions

$$\varphi^E(0) = \varphi(0), \quad \varphi^E(n) = \varphi(m).$$

The following technical result will be used in Section 3 to describe the fundamental groupoid of the product of digraphs.

Proposition 2.16. *Let $\psi = (\psi_1, \psi_2)\colon I_m \to G \rtimes H$ be a path-map and $h_1, h_2\colon I_n \to I_m$ be shrinking maps that induce extensions $\psi_1^E\colon I_n \to G$ and $\psi_2^E\colon I_n \to H$. Consider the digraph map*

$$\psi' := (\psi_1^E, \psi_2^E)\colon I_n \to G \rtimes H.$$

Then $\psi \overset{C_\partial}{\simeq} \psi'$.

P r o o f. Consider the commutative diagram

$$\begin{tikzcd}
I_n \arrow[r, equal] \arrow[d, "\Delta_n"] & I_n \arrow[d, "\delta"] \arrow[dr, "\psi'"] & \\
I_n \rtimes I_n \arrow[r, "h_1 \rtimes h_2"] & I_m \rtimes I_m \arrow[r, "\psi_1 \rtimes \psi_2"] & G \rtimes H \\
& I_m \arrow[u, "\Delta_m"] \arrow[ur, "\psi"'] &
\end{tikzcd}$$

in which Δ_i denotes the natural diagonal inclusions, and $\delta = (h_1 \rtimes h_2) \circ \Delta_n$. By Lemma 2.14 the path-maps $\delta\colon I_n \to I_m \rtimes I_n$ and $\Delta_m\colon I_m \to I_m \rtimes I_m$ are $C\partial$-homotopic. From commutativity of the diagram it follows that $\psi \overset{C\partial}{\simeq} \psi'$. $\square$

For two digraphs G, H define a digraph $\mathrm{Dhom}(G, H)$ with the set of vertices

$$V_{\mathrm{Dhom}(G,H)} = \mathrm{Hom}(G, H)$$

and $f \to g$ in $\mathrm{Dhom}(G, H)$ if there is a *one-step homotopy* such as

$$F\colon G \,\square\, I \to H, \quad F|_{G\square\{0\}} = f, \quad F|_{G\square\{1\}} = g. \tag{2.5}$$

Theorem 2.17. *For digraphs D, G, H there is a natural isomorphism of digraphs*

$$\mathrm{Dhom}(D, G \rtimes H) \cong \mathrm{Dhom}(D, G) \rtimes \mathrm{Dhom}(D, H).$$

P r o o f. By the proof of Proposition 2.13, the map r from (2.3) defines a bijective map of vertices

$$V_{\mathrm{Dhom}(D,G\rtimes H)} \to V_{\mathrm{Dhom}(D,G)} \times V_{\mathrm{Dhom}(D,H)}.$$

Let F be the homotopy of (2.5) that gives an arrow $f \to g$ in $\mathrm{Dhom}(G, H)$. Then

$$p \circ F\colon D \,\square\, I \to G$$

provides a homotopy between $p \circ f$ and $p \circ g$, and

$$q \circ F\colon D \,\square\, I \to H$$

provides a homotopy between $q \circ f$ and $q \circ g$. Hence, the map r maps arrows to arrows, and it is an injective map on arrows.

Now we prove that it is surjective. Consider a part of the digraph $\mathrm{Dhom}(D,G) \rtimes \mathrm{Dhom}(D,H)$

$$
\begin{tikzcd}
 & f_1 \arrow[rr] & & g_1 \\
g_2 & (f_1,g_2) \arrow[rr, "a_0"] & & (g_1,g_2) \\
f_2 \arrow[u] & (f_1,f_2) \arrow[u, "a_1"] \arrow[rru, "a_2"] \arrow[rr, "a_4"'] & & (g_1,f_2), \arrow[u, "a_3"']
\end{tikzcd}
\tag{2.6}
$$

which is obtained by the $\rtimes$-product of the arrows $f_1 \to g_1$ and $f_2 \to g_2$. Let us show that a_i belongs to the image of the map r on arrow for any $i = 0, \ldots, 4$.

Consider, at first, the case $i = 0$. By definition of the digraphs $\mathrm{Dhom}(D,G)$ and $\mathrm{Dhom}(D,H)$ it follows from (2.6) that there is a homotopy $F_1\colon D \,\Box\, I \to G$ between f_1 and g_1, and there is a homotopy $F_2\colon D \,\Box\, I \to H$ between f_2 and g_2. Let $d\colon D \,\Box\, I \to D$ be the natural projection. The map

$$(F_1, g_2 \circ d)\colon D \,\Box\, I \to G \rtimes H$$

gives a homotopy between the map $(f_1,g_2)\colon D \to G \rtimes H$ and the map $(g_1,g_2)\colon D \to G \rtimes H$. The homotopy $(F, g_2 \circ d)$ represents an arrow in $\mathrm{Dhom}(D, G \rtimes H)$ that maps by means of r to the arrow a_0 in (2.6).

The cases $i = 1,3,4$ are similar. Consider the case $i = 2$. Let Ψ denote the composition

$$D \,\Box\, I \overset{F_1 \Box F_2}{\longrightarrow} G \,\Box\, H \to G \rtimes H,$$

where the second map is the natural inclusion. This map gives a homotopy between the map $(f_1,f_2)\colon D \to G \rtimes H$ and the map $(g_1,g_2)\colon D \to G \rtimes H$, and hence represents an arrow in $\mathrm{Dhom}(D, G \rtimes H)$ that maps by means of r to the arrow a_2 in (2.6). The theorem is proved. $\Box$

For two based digraphs G^*, H^* define a based digraph $\mathrm{Dhom}(G^*,H^*)$ with the set of vertices $V_{\mathrm{Dhom}(G^*,H^*)} = \mathrm{Hom}(G^*,H^*)$ consisting of based maps, and the base point is given by the trivial map $*\colon G \to * \in H$. There is an arrow $f \to g$ in $\mathrm{Dhom}(G^*,H^*)$ if there is a one-step homotopy

$$F\colon G^* \,\Box\, I^* \to H^*, \quad * = 0 \in I, \quad F|_{G\Box\{0\}} = f, \quad F|_{G\Box\{1\}} = g. \tag{2.7}$$

The products $\Box$ and $\rtimes$ of digraphs are defined naturally in the category $\mathcal{D}^*$ of based digraphs, where $* = * \,\Box\, * \in G \,\Box\, H$ is a based vertex and, similarly, $* = * \rtimes * \in G \rtimes H$.

Corollary 2.18. *For based digraphs D^*, G^*, H^* there is a natural isomorphism of based digraphs*

$$\mathrm{Dhom}(D^*, G^* \rtimes H^*) \cong \mathrm{Dhom}(D^*, G^*) \rtimes \mathrm{Dhom}(D^*, H^*).$$

Proof. The result follows from Theorem 2.17 since the correspondence $f \leftrightarrow (f_1, f_2)$ given in Proposition 2.13 preserves the based maps. $\square$

3. Fundamental groupoids of digraphs

In this section we define a notion of the fundamental groupoid of a digraph and describe its basic properties. We prove the theorem about the fundamental groupoid of the products of digraphs. As a corollary we obtain the corresponding results for the fundamental groups of digraphs. Our definition is motivated by the classical definition of a groupoid from [13], Chapter 1, Section 7, and Chapter 3, Sections 6, 7, 8.

A *groupoid* is a small category in which every morphism is an equivalence.

Definition 3.1. (i) An *edge* of a digraph $G = (V, E)$ is an ordered pair (v, w) of vertices such that either $v = w$ or there is at least one of the arrows $v \to w$ or $v \leftarrow w$.

(ii) An *edge-path* ξ of a digraph G is a finite nonempty sequence

$$(v_0, v_1)(v_1, v_2) \dots (v_{n-2}, v_{n-1})(v_{n-1}, v_n) \tag{3.1}$$

of edges of the digraph G, where n is any natural number. The vertex v_0 is called the *tail* of the edge-path ξ and v_n the *head* of ξ. We shall write $v_0 = t(\xi)$ and $v_n = h(\xi)$.

(iii) A *closed edge-path* at the vertex $v_0 \in V_G$ is an edge-path ξ such that $t(\xi) = h(\xi) = v_0$.

(iv) If ξ_1 and ξ_2 are two edge paths with $h(\xi_1) = t(\xi_2)$, then we define the *product edge-path* $\xi_1\xi_2$ consisting of the sequence of edges ξ_1 followed by the edges of ξ_2.

(v) For any edge-path ξ from (3.1) define the inverse edge-path ξ^{-1} as

$$\xi^{-1} := (v_n, v_{n-1})(v_{n-1}, v_{n-2}) \dots (v_1, v_0).$$

We collect some obvious properties of edge-paths in the next statement.

Lemma 3.2. *The edge-paths of a digraph G satisfy the following properties:*
- ▷ $(\xi_1\xi_2)\xi_3 = \xi_1(\xi_2\xi_3)$,
- ▷ $(\xi^{-1})^{-1} = \xi$,
- ▷ $t(\xi_1\xi_2) = t(\xi_1)$, $h(\xi_1\xi_2) = h(\xi_2)$,
- ▷ $t(\xi) = h(\xi^{-1})$, $h(\xi) = t(\xi^{-1})$,

where we assume that all the products are well-defined.

Definition 3.3. (i) We shall say that the sequence of three vertices (v_0, v_1, v_2) of a digraph G forms a *triangle* if there is a permutation π of (v_0, v_1, v_2) such that the map $i \mapsto \pi(v_i)$, $i = 0, 1, 2$, provides the isomorphism from the following *triangle*

$$\begin{tikzcd} 0 \arrow[r] \arrow[dr] & 1 \arrow[d] \\ & 2 \end{tikzcd}$$

to the subdigraph of G with the vertices $\pi(v_0)$, $\pi(v_1)$, $\pi(v_2)$.

(ii) We shall say that the sequence of four vertices (v_0, v_1, v_2, v_3) of a digraph G forms a *square* if there is a cyclic permutation π of (v_0, v_1, v_2, v_3) such that the map $i \mapsto \pi(v_i)$, $i = 0, 1, 2, 3$, provides the isomorphism of the following *square*

$$\begin{tikzcd} 1 \arrow[r] & 3 \\ 0 \arrow[u] \arrow[r] & 2 \arrow[u] \end{tikzcd}$$

to the subdigraph of G with the vertices $\pi(v_0)$, $\pi(v_1)$, $\pi(v_2)$, $\pi(v_3)$.

Now we introduce the *edge-path groupoid of a digraph*.

Definition 3.4. Two edge-paths ξ_1 and ξ_2 are called *equivalent* (and we write $\xi_1 \sim \xi_2$) if ξ_1 can be obtained from ξ_2 by a finite sequence of local transformations of following types or their inverses (where the dots "..." denote the unchanged parts of the edge-paths):

(i) $\dots(v_0, v_1)(v_1, v_2)\dots \mapsto \dots(v_0, v_2)\dots$ provided (v_0, v_1, v_2) forms a triangle in G;

(ii) $\dots(v_0, v_1)(v_1, v_3)\dots \mapsto \dots(v_0, v_2)(v_2, v_3)\dots$ provided (v_0, v_1, v_2, v_3) forms a square in G;

(iii) $\dots(v_0, v_1)(v_1, v_3)(v_3, v_2)\dots \mapsto \dots(v_0, v_2)\dots$ provided (v_0, v_1, v_2, v_3) forms a square in G;

(iv) $\dots(v_0, v_1)(v_1, v_0)\dots \to \dots(v_0, v_0)\dots$ provided $v_0 \to v_1$ or $v_1 \to v_0$ or $v_0 = v_1$;

(v) $\dots(v_0, v_0)(v_0, v_1)\dots \mapsto \dots(v_0, v_1)\dots$

Using transformation (iv) and (v), we obtain also that

(vi) $\dots(v_0, v_1)(v_1, v_1)\dots \mapsto \dots(v_0, v_1)\dots$

It follows directly from the definition that the relation $\sim$ has the following properties.

Proposition 3.5. *The relation "$\sim$" is an equivalence relation on the set of edge-paths of the digraph G. It has the following properties:*

(i) *If* $\xi_1 \sim \xi_2$, *then* $t(\xi_1) = t(\xi_2)$, $h(\xi_1) = h(\xi_2)$.
(ii) *If* $\xi_1 \sim \xi_1'$, $\xi_2 \sim \xi_2'$ *and* $t(\xi_2) = h(\xi_1)$, *then* $\xi_1\xi_2 \sim \xi_1'\xi_2'$.
(iii) *Let* $t(\xi) = v_0$, $h(\xi) = v_1$, *then* (v_0, v_0), $\xi \sim \xi \sim \xi(v_1, v_1)$.
(iv) *If* $\xi_1 \sim \xi_2$, *then* $\xi_1^{-1} \sim \xi_2^{-1}$.

For a path-map $\varphi\colon I_n \to G$ with $v_i = \varphi(i) \in V$ we have for any $i = 0, \dots, n-1$ at least one of the following relations:

$$v_i = v_{i+1}, \quad v_i \to v_{i+1}, \quad v_{i+1} \to v_i.$$

Hence, the path-map φ determines the following edge-path in G:

$$\xi_\varphi = (\varphi(0), \varphi(0))(\varphi(0), \varphi(1)) \dots (\varphi(n-1), \varphi(n)).$$

Theorem 3.6. *Two path-maps* $\varphi\colon I_n \to G$ *and* $\psi\colon I_m \to G$ *with* $\varphi(0) = \psi(0)$, $\varphi(n) = \psi(m)$ *are* C_∂*-homotopic if and only if* $\xi_\psi \sim \xi_\varphi$.

Proof. The proof is similar to [8], Theorem 4.13, where the case of loops was treated. □

Proposition 3.7. *The following identities are true for path-maps* φ *and* ψ *on* G*:*

$$(\xi_\varphi)^{-1} \sim \xi_{\widehat{\varphi}}, \quad \xi_{\varphi\vee\psi} \sim \xi_\varphi\xi_\psi,$$

where $\widehat{\varphi}$ *is the inverse path-map and* $\varphi \vee \psi$ *is the concatenation of* φ *and* ψ *assuming that it is well-defined.*

The proof is trivial.

Denote by $[\xi]$ the equivalence class of the edge-path ξ under the relation "$\sim$". As follows from Proposition 3.5, the following notations make sense:

$$t([\xi]) := t(\xi), \quad h([\xi]) := h(\xi)$$

and

$$[\xi]^{-1} := [\xi^{-1}], \quad [\xi_1] \circ [\xi_2] := [\xi_1\xi_2]$$

provided $\xi_1\xi_2$ is well-defined. The following statement follows from Lemma 3.2 and Proposition 3.5.

Theorem 3.8. *For any digraph* G *the vertex set of* G *as the set of objects and the set of the equivalence classes of edge-paths* ξ *as morphisms from* $t(\xi)$ *to* $h(\xi)$ *form a category* $\mathcal{E}(G)$ *that is a groupoid. The composition of two morphisms* $[\xi_1]$ *and* $[\xi_2]$ *is given by* $[\xi_1] \circ [\xi_2]$, *and the inverse morphism of* $[\xi]$ *is* $[\xi]^{-1}$.

The groupoid $\mathcal{E}(G)$ is called the *fundamental groupoid of the digraph G*. We shall denote by $\mathrm{Hom}_{\mathcal{E}(G)}(v, w)$ the set of morphisms from $v \in V$ to $w \in V$ in the category $\mathcal{E}(G)$, or simply $\mathrm{Hom}(v, w)$ if the digraph G is clear from the context.

Let $v \in V_G$ be a vertex in a digraph G. Consider the edge-paths ξ in G with $t(\xi) = h(\xi) = v$. These edges-paths form a group with the neutral element (v, v) and with the product of edge-paths. Denote this group by $\mathrm{E}(G, v)$.

Proposition 3.9. *We have an isomorphism*

$$\mathrm{E}(G, v) \cong \pi_1(G^v).$$

P r o o f. For any path-map $\varphi\colon I_n \to G$ with $\varphi(0) = \varphi(n) = v$ we already define an edge-path ξ_φ with $t(\xi_\varphi) = h(\xi_\varphi) = v$. By Theorem 3.6, the map

$$\Theta\colon \pi_1(G, v) \to \mathrm{E}(G, v),$$
$$\Theta([\varphi]) = [\xi_\varphi]$$

is well-defined and preserves the group operations by Proposition 3.7. The map Θ is an epimorphism and a monomorphism as follows from Theorem 3.6. $\square$

Let $\mathcal{G}$ and $\mathcal{H}$ be groupoids. We shall consider a functor $\mathcal{F}\colon \mathcal{G} \to \mathcal{H}$ as a morphism of groupoids. Thus, we obtain the category $\mathcal{G}rpd$ of groupoids and morphisms of groupoids.

Proposition 3.10. *The fundamental groupoid is a functor*

$$\mathcal{E}\colon \mathcal{D} \to \mathcal{G}rpd.$$

P r o o f. Let $f\colon G \to H$ be a digraph map. For any edge-path

$$\xi = (v_0, v_1) \dots (v_{n-1}, v_n)$$

of the digraph G define an edge-path $f_*(\xi)$ of the digraph H by the rule

$$f_*(\xi) = (f(v_0), f(v_1)) \dots (f(v_{n-1}), f(v_n)).$$

By Definitions 2.3 and 3.1 the edge-path $f_*(\xi)$ is well-defined. Using Definition 3.4 it is an easy exercise to check that $\xi_1 \sim \xi_2$ implies $f_*(\xi_1) \sim f_*(\xi_2)$. Thus, we obtain a well-defined function $f_\sharp\colon \mathcal{E}(G) \to \mathcal{E}(H)$ that satisfies the relations $f_\sharp(1_v) = 1_{f(v)}$, $v \in V_G$ and $f_\sharp(\xi_1 \circ \xi_2) = f_\sharp(\xi_1) \circ f_\sharp(\xi_2)$. $\square$

Now we recall the definition of product of groupoids (see [5], Section 6.4). The product $\mathcal{C}_1 \times \mathcal{C}_2$ of two groupoids $\mathcal{C}_1$ and $\mathcal{C}_2$ is a groupoid with the set of objects $Ob(\mathcal{C}_1 \times \mathcal{C}_2)$ consisting of all ordered pairs (A_1, A_2), where $A_1 \in Ob(\mathcal{C}_1), A_2 \in Ob(\mathcal{C}_2)$. The set $Mor((A_1, A_2), (B_1, B_2))$ consists of ordered pairs of morphisms (f_1, f_2), where $f_1\colon A_1 \to B_1, f_2\colon A_2 \to B_2$ are the morphisms of the categories $\mathcal{C}_1$ and $\mathcal{C}_2$, respectively. The composition of morphisms and the inverse morphism in $\mathcal{C}_1 \times \mathcal{C}_2$ are defined in a natural way:

$$(g_1, g_2) \circ (f_1, f_2) = (g_1 f_1, g_2 f_2), \quad (f_1, f_2)^{-1} = (f_1^{-1}, f_2^{-1}).$$

We have the natural projection functors

$$\pi_1\colon \mathcal{C}_1 \times \mathcal{C}_2 \to \mathcal{C}_1, \quad \pi_2\colon \mathcal{C}_1 \times \mathcal{C}_2 \to \mathcal{C}_2$$

such that for any functors $f_1\colon \mathcal{B} \to \mathcal{C}_1$, $f_2\colon \mathcal{B} \to \mathcal{C}_2$ there is a unique functor $f\colon \mathcal{B} \to \mathcal{C}_1 \times \mathcal{C}_2$ such that $\pi_1 f = f_1$, $\pi_2 f = f_2$.

Theorem 3.11. *Let G, H be digraphs. Then the groupoid $\mathcal{E}(G \rtimes H)$ is isomorphic to $\mathcal{E}(G) \times \mathcal{E}(H)$.*

P r o o f. The natural projections of digraphs $p\colon G \rtimes H \to G$, $q\colon G \rtimes H \to H$ induce morphisms of groupoids

$$\mathcal{E}(p)\colon \mathcal{E}(G \rtimes H) \to \mathcal{E}(G), \quad \mathcal{E}(q)\colon \mathcal{E}(G \rtimes H) \to \mathcal{E}(H),$$

which determines a morphism of groupoids

$$f\colon \mathcal{E}(G \rtimes H) \to \mathcal{E}(G) \times \mathcal{E}(H).$$

Recall that $Ob(\mathcal{E}(G \rtimes H)) = Ob(\mathcal{E}(G) \times \mathcal{E}(H)) = V_G \times V_H$. The morphism f is the identity map on the set of objects $V_G \times V_H$, and for any morphism in $\mathcal{E}(G \rtimes H)$ that is given by a class $[\xi]$ of an edge-path ξ we have

$$f([\xi]) = ([p_\sharp(\xi)], [q_\sharp(\xi)]).$$

We prove, at first, that the map f is surjective. For an edge-path $\xi_1 = (v_0, v_1) \dots (v_{n-1}, v_n)$ in G and an edge-path $\xi_2 = (w_0, w_1) \dots (w_{m-1}, w_m)$ in H we define an edge-path ξ in $G \rtimes H$ such that

$$f([\xi]) = ([p_\sharp(\xi)], [q_\sharp(\xi)]) = ([\xi_1], [\xi_2]). \tag{3.2}$$

Without loss of generality we can suppose that $n \geqslant m$. By Definition 3.4, we have

$$\xi_2 \sim \xi_2' := (w_0, w_1) \dots (w_{m-1}, w_m) \underbrace{(w_m, w_m) \dots (w_m, w_m)}_{n-m \text{ times}}.$$

Define an edge-path ξ in $G \rtimes H$ as

$$\xi = ((v_0, w_0), (v_1, w_1)) \dots ((v_{m-1}, w_{m-1}), (v_m, w_m)) \dots ((v_{n-1}, w_m), (v_n, w_m)).$$

By the definition of $\rtimes$-product this is, indeed, an edge-path and condition (3.2) is satisfied. Hence the map f is surjective.

Now we prove that the map f is injective. Let ξ_1 and ξ_2 be two edge-paths in $G \rtimes H$ such that

$$t(\xi_1) = t(\xi_2) = (v_0, w_0), \quad h(\xi_1) = h(\xi_2) = (v_n, w_n)$$

and

$$p_\sharp(\xi_1) \sim p_\sharp(\xi_2), \quad q_\sharp(\xi_1) \sim q_\sharp(\xi_2). \tag{3.3}$$

Define path-maps $\varphi\colon I_n \to G \rtimes H$ and $\psi\colon I_m \to G \rtimes H$ in such a way that $\xi_1 = \xi_\varphi$, $\xi_2 = \xi_\psi$. Note that these path-maps do not have to be unique. From the definition of the projections p and q and Theorem 3.6 we obtain

$$p_\sharp(\xi_1) = \xi_{p\varphi}, \quad p_\sharp(\xi_2) = \xi_{p\psi}, \quad q_\sharp(\xi_1) = \xi_{q\varphi}, \quad q_\sharp(\xi_2) = \xi_{q\psi}$$

and

$$p\varphi \overset{C_\partial}{\cong} p\psi \quad \text{in } G, \tag{3.4}$$

$$q\varphi \overset{C_\partial}{\cong} q\psi \quad \text{in } H. \tag{3.5}$$

We would like to conclude from (3.4)–(3.5) that $\varphi \overset{C_\partial}{\cong} \psi$. Then by Theorem 3.6, $\xi_1 = \xi_\varphi \sim \xi_\psi = \xi_2$, and hence the map f in (3.2) is injective. It is sufficient to prove $\varphi \overset{C_\partial}{\cong} \psi$ in the following cases:

(1) in (3.4) we have a one-step direct C_∂-homotopy and in (3.5) the equality;

(2) in (3.4) we have a one-step inverse C_∂-homotopy and in (3.5) the equality;

(3) in (3.4) and in (3.5) we have a one-step direct C_∂-homotopy;

(4) in (3.4) and in (3.5) we have a one-step inverse C_∂-homotopy;

(5) in (3.4) we have a one-step direct C_∂-homotopy and in (3.5) a one-step inverse C_∂-homotopy.

From these cases the general case follows. Note that cases (1) and (2) follow directly from cases (3) and (4). We consider only case (5). In other cases the argument is similar and simpler.

Let (h_1, F_1) be a one-step direct C_∂-homotopy from $p\varphi$ to $p\psi$ that is given by a shrinking map $h_1\colon I_n \to I_m$ and the commutative diagram

$$\begin{tikzcd} I_n \arrow[r] \arrow[d, "p\varphi"] & \mathrm{C}_{h_1} \arrow[d, "F_1"] & I_m \arrow[l] \arrow[d, "p\psi"] \\ G \arrow[r, equal] & G \arrow[r, equal] & G. \end{tikzcd} \tag{3.6}$$

This diagram extends to the commutative diagram

$$\begin{tikzcd} I_n \arrow[r, "="] \arrow[d] & I_n \arrow[r, "p\varphi"] \arrow[d] & G \arrow[d, equal] \\ I_n \mathbin{\square} I^- \arrow[r, "S_1"] & \mathrm{C}_{h_1} \arrow[r, "F_1"] & G \arrow[d, equal] \\ I_n \arrow[r, "h_1"] \arrow[u] & I_m \arrow[r, "p\psi"] \arrow[u] & G. \end{tikzcd} \tag{3.7}$$

It follows from (3.7) that

$$p\varphi \simeq p\psi h_1 \quad \text{in } G, \tag{3.8}$$

which implies

$$(p\varphi, q\psi h_2) \simeq (p\psi h_1, q\psi h_2) \quad \text{in } G \rtimes H. \tag{3.9}$$

Let (h_2, F_2) be a one-step inverse C_∂-homotopy from $q\varphi$ to $q\psi$ that is given by a shrinking map $h_2\colon I_n \to I_m$ and the commutative diagram

$$\begin{tikzcd} I_n \arrow[r] \arrow[d, "q\varphi"] & \mathrm{C}^-_{h_2} \arrow[d, "F_1"] & I_m \arrow[l] \arrow[d, "q\psi"] \\ H \arrow[r, equal] & H \arrow[r, equal] & H. \end{tikzcd} \tag{3.10}$$

This diagram extends to the commutative diagram

$$
\begin{tikzcd}
I_n \arrow[r, "="] \arrow[d] & I_n \arrow[r, "q\varphi"] \arrow[d] & H \arrow[d, equal] \\
I_n \,\Box\, I \arrow[r, "S_2"] & C^-_{h_2} \arrow[r, "F_2"] & H \\
I_n \arrow[r, "h_2"] \arrow[u] & I_m \arrow[r, "q\psi"] \arrow[u] & H. \arrow[u, equal]
\end{tikzcd}
\tag{3.11}
$$

It follows that

$$q\varphi \simeq q\psi h_2 \quad \text{in } H$$

and hence,

$$(p\varphi, q\varphi) \simeq (p\varphi, q\psi h_2) \quad \text{in } G \rtimes H.$$

Together with (3.9) this yields

$$(p\varphi, q\varphi) \simeq (p\psi h_1, q\psi h_2) \quad \text{in } G \rtimes H.$$

By Proposition 2.16 we have

$$(p\psi h_1, q\psi h_2) \overset{C_\partial}{\simeq} (p\psi, q\psi) \quad \text{in } G \rtimes H,$$

which implies

$$\varphi = (p\varphi, q\varphi) \overset{C_\partial}{\simeq} (p\psi, q\psi) = \psi \quad \text{in } G \rtimes H,$$

which was to be proved. $\Box$

Corollary 3.12. *For based digraphs G^* and H^* there is a natural isomorphism*

$$\pi_1(G^* \rtimes H^*) \cong \pi_1(G^*) \times \pi_1(H^*),$$

where $\pi_1(G^*) \times \pi_1(H^*)$ is the direct product of fundamental groups.

Proof. Follows from Proposition 3.9 and Theorem 3.11. $\Box$

Theorem 3.13. *For digraphs G and H, the natural inclusion $\sigma\colon\ G \,\Box\, H \to G \rtimes H$ induces an isomorphism of fundamental groupoids*

$$\mathcal{E}(G \,\Box\, H) \cong \mathcal{E}(G \rtimes H).$$

In particular, for the based digraphs, this map induces an isomorphism

$$\pi_1(G^* \,\Box\, H^*) \cong \pi_1(G^* \rtimes H^*) \cong \pi_1(G^*) \times \pi_1(H^*)$$

of fundamental groups.

P r o o f. The inclusion σ induces a morphism $\sigma_\sharp\colon \mathcal{E}(G \Box H) \to \mathcal{E}(G \rtimes H)$ of groupoids. We will prove that it is surjective and injective.

For any edge-path ξ in $G \rtimes H$, define an edge-path $\xi^\Box$ in $G \Box H$ such that $\xi \sim \xi^\Box$ in $G \rtimes H$. To that end we transform any diagonal edge $((v_1, w_1), (v_2, w_2))$ of ξ in $G \rtimes H$ to the edge path

$$((v_1, w_1), (v_1, w_2))((v_1, w_2), (v_2, w_2)), \tag{3.12}$$

that lies in $G \Box H$, using transformation (i) of Definition 3.4 in $G \rtimes H$. Doing that to all diagonal edges of ξ, we obtain an edge-path $\xi^\Box$ as was claimed above. This implies immediately that $\sigma_\sharp$ is surjective, since $\sigma_\sharp([\xi^\Box]) = [\xi]$.

Now let us prove the following claim: if ξ, η are edge-paths in $G \rtimes H$ which are equivalent in $G \rtimes H$, then $\xi^\Box \sim \eta^\Box$ in $G \Box H$. If this is already known, then for any two edge-paths ξ and η in $G \Box H$ such that $\xi \sim \eta$ in $G \rtimes H$ we have $\xi^\Box = \xi$, $\eta^\Box = \eta$, and hence, $\xi \sim \eta$ in $G \Box H$, which implies the injectivity of $\sigma_\sharp$.

To prove the above claim it suffices to assume that η is obtained from ξ by one elementary transformation in $G \rtimes H$. By Definition 3.4 any elementary transformation is done along an embedded digraph $S \subset G \rtimes H$, where S is isomorphic to one of the following digraphs: a single vertex digraph, $0 \to 1$, $0 \leftrightarrows 1$, the triangle, the square. Let P be a projection of S onto G and Q be a projection of S onto H. Then $P \Box Q$ is a subgraph of $G \Box H$. By inspecting all the above cases of S, one sees that $P \Box Q$ is always contractible. By the assumption that η is obtained from ξ by one elementary transformation, we have

$$\xi = \gamma_1 \alpha \gamma_2, \quad \eta = \gamma_1 \beta \gamma_2,$$

where γ_1, γ_2 are edge-paths in $G \rtimes H$, α, β are edge-paths in $P \rtimes Q$, and $t(\alpha) = t(\beta)$, $h(\alpha) = h(\beta)$, where α is transformed to β along S. By the definition of the operation $\xi \to \xi^\Box$, we obtain

$$\xi^\Box = \gamma_1^\Box \alpha^\Box \gamma_2^\Box, \quad \eta^\Box = \gamma_1^\Box \beta^\Box \gamma_2^\Box,$$

where

$$t(\alpha^\Box) = t(\beta^\Box), \quad h(\alpha^\Box) = h(\beta^\Box).$$

By the contractibility of $P \Box Q$, the edge-paths $\alpha^\Box$, $\beta^\Box$ are equivalent in $P \Box Q$. Hence, $\xi^\Box \sim \eta^\Box$ in $G \Box H$, which finishes the proof. $\Box$

The notion of homology groups $H_p(G, \mathbb{Z})$ of digraphs was introduced in [10] (see also [6], [7], [9]). The physical applications of homology (cohomology) theory of digraphs requires development of effective methods of computing of these groups.

Using isomorphism between the first homology group and the abelization of the fundamental group for digraphs [8], Theorem 4.23, and applying Theorem 3.13, we obtain the following result.

Theorem 3.14. *For any two connected digraphs G, H we have*

$$H_1(G \,\Box\, H, \mathbb{Z}) \cong H_1(G \rtimes H, \mathbb{Z}) \cong H_1(G, \mathbb{Z}) \oplus H_1(H, \mathbb{Z}).$$

4. Geometric realization and Van Kampen theorem

In this section, for any finite digraph $G = (V, E)$ we construct a 2-dimensional finite CW-complex $K = \Delta(G)$ (with topological space $|K|$) for which the set of 0-dimensional cells coincides with the set of vertices V. We prove the functoriality of Δ and obtain an isomorphism

$$\mathrm{Hom}_{\mathcal{E}(G)}(v, w) \cong \mathrm{Hom}_{\mathcal{P}(|K|)}(v, w), \quad v, w \in V,$$

where $\mathrm{Hom}_{\mathcal{E}(G)}(v, w)$ is the set of morphisms from v to w of the groupoid $\mathcal{E}(G)$ and $\mathrm{Hom}_{\mathcal{P}(|K|)}(v, w)$ is the set of morphisms from v to w of the fundamental groupoid $\mathcal{P}(|K|)$ of the topological space $|K|$ (see [13], Chapter 1, Section 7). This implies, in particular, that for any vertex $v \in V$

$$\pi_1(G, v) \cong \pi_1(|K|, v).$$

Then we obtain a Van Kampen theorem for the fundamental groupoids of digraphs and provide several examples which illustrate this theorem.

At first we need several technical definitions and lemmas.

Definition 4.1. Let $\{G_i\}_{i\in A}$ be a family of subdigraphs of one digraph, where A is any index set.

(i) The *union* $G = \bigcup\limits_{i\in A} G_i$ *of digraphs* G_i is a digraph G such that

$$V_G = \bigcup_{i\in A} V_{G_i}, \quad E_G = \bigcup_{i\in A} E_{G_i}.$$

(ii) The intersection $G = \bigcap\limits_{i\in A} G_i$ is a digraph G such that

$$V_G = \bigcap_{i\in A} V_{G_i}, \quad E_G = \bigcap_{i\in A} E_{G_i}.$$

Now, for any finite digraph $G = (V, E)$ we construct functorialy a 2-dimensional cell complex $K = \Delta(G)$.

The 0-dimensional skeleton K^0 of K consists of the set of vertices V. Let $D^1 = [0, 1]$ denote the standard closed unit interval which is a closed 1-cell with the boundary $\partial D^1 = \{0, 1\}$.

Let P be the set of all ordered pairs (v, w), where $v, w \in V$, such that $v \to w$; if also $w \to v$, then we choose in P only one of the pairs (v, w), (w, v). For any pair $(v, w) \in P$ we attach a one-dimensional cell D^1 to K^0, using attaching map

$$\varphi_{v,w} \colon \partial D^1 \to K^0, \quad \varphi_{v,w}(0) = v, \quad \varphi_{v,w}(1) = w.$$

Now, we define 1-dimensional skeleton K^1 of K by attaching to K^0 1-dimensional cells D^1 according to the maps $\varphi_{v,w}$ for all $(v, w) \in P$.

Let T be the set of subdigraphs of G that are isomorphic to the triangle from Definition 3.3 (i). For any subdigraph

$$\tau = \begin{tikzcd} v_0 \arrow[r] \arrow[dr] & v_1 \arrow[d] \\ & v_2 \end{tikzcd} \tag{4.1}$$

from T we attach to K^1 a standard triangle $D^2 \subset \mathbb{R}^2$ with the vertices $\{a_0, a_1, a_2\}$ and with boundary $\partial D^2 = [a_0, a_1] \cup [a_1, a_2] \cup [a_0, a_2]$ using attaching map

$$\varphi_\tau \colon \partial D^2 \to K^1, \quad \varphi_\tau([a_i, a_j]) = [v_i, v_j].$$

Let S be the set of all subdigraphs of G that are isomorphic to the square. For any subdigraph

$$\sigma = \begin{tikzcd} v_0 \arrow[r] \arrow[d] & v_1 \arrow[d] \\ v_2 \arrow[r] & v_3 \end{tikzcd} \tag{4.2}$$

from S we attach to K^1 a standard square $D^2 \subset \mathbb{R}^2$ with the vertices $\{a_0, a_1, a_2, a_3\}$ with boundary $\partial D^2 = [a_0, a_1] \cup [a_0, a_2] \cup [a_1, a_3] \cup [a_2, a_3]$ using attaching map

$$\varphi_\sigma \colon \partial D^2 \to K^1, \quad \varphi_\sigma([a_i, a_j]) = [v_i, v_j]. \tag{4.3}$$

Now we define $\Delta(G) = K = K^2$ as the cell complex that is obtained from K^1 by attaching all the triangles and squares as above.

Proposition 4.2. *For any digraph map $f\colon G \to H$ we can define a cellular map*

$$\Delta_f\colon \Delta(G) \to \Delta(H)$$

which coincides with f on the set of 0-dimensional cells (that is, with V_G) in such a way that we obtain a functor Δ from the category of digraphs $\mathcal{D}$ to the category of CW-complexes (with cellular maps).

P r o o f. By the definition of a digraph map, f can map triangles to triangles or edges or vertices, and squares to squares or triangles, or edges, or vertices. Now, it follows that the map Δ_f, that is firstly defined on vertices as f, extends uniquely to a cellular map $\Delta(G) \to \Delta(H)$. $\square$

For a digraph $G = (V, E)$ let $\mathcal{P}(|K|)$ denote the fundamental groupoid of the topological space $|K|$, where $K = \Delta(G)$. The class of the path $\varphi\colon [0,1] \to |K|$ in $\mathcal{P}(|K|)$ will be denoted by $[\varphi]$. For the points $v, w \in |K|$ we denote by $\mathrm{Hom}_{\mathcal{P}(|K|)}(v, w)$ the set of morphisms from v to w in $\mathcal{P}(|K|)$. Any vertex $v \in V$ determines a 0-dimensional cell in K and a point in $|K|$, which we continue denoting by v.

Let J_n be the CW-complex that is the subdivision of the closed unit interval $[0, 1]$ in n equal parts (1-cells) by 0-cells $i_0 = 0, \dots, i_n = 1$. For any edge-path $\xi = (v_0, v_1) \dots (v_{n-1}, v_n)$ in the digraph G define a cellular map $\varphi_\xi\colon J_n \to K$ by $\varphi_\xi(i_k) = v_k$ on the set of 0-cells, and

$$\varphi_\xi[i_k, i_{k+1}] = [v_k, v_{k+1}]$$

on the 1-cells. This map defines a path in $|K|$ by

$$|\varphi_\xi|\colon [0,1] \to |K|, \quad |\varphi_\xi|(0) = v_0 = t(\xi), \quad |\varphi_\xi|(1) = v_n = h(\xi).$$

Lemma 4.3.

(i) *Let $\xi_1 \sim \xi_2$ be edge-paths in a digraph G. Then the maps $|\varphi_{\xi_1}|$ and $|\varphi_{\xi_2}|$ are homotopic relative to the boundary.*

(ii) *If $h(\xi_1) = t(\xi_2)$, then $|\varphi_{\xi_1\xi_2}|$ is homotopic to the path $|\varphi_{\xi_1}| * |\varphi_{\xi_2}|$ relative to the boundary.*

P r o o f. Follows from Definition 3.4 and the construction of $\Delta(G)$ (this result is a cellular analogue of the simplicial case, see [13], Chapter 3, Sections 6, 9–11). $\square$

It follows from Lemma 4.3 that for any two vertices $v, w \in V$ the map

$$\varrho\colon \mathrm{Hom}_{\mathcal{E}(G)}(v, w) \to \mathrm{Hom}_{\mathcal{P}(K)}(v, w), \quad \varrho([\xi]) = [|\varphi_\xi|] \tag{4.4}$$

is well-defined.

Proposition 4.4. *For any two vertices $v, w \in V$ the map ϱ in (4.4) is a bijection.*

P r o o f. This is a cellular version of the simplicial theorem (see [13], Chapter 3, Section 6, Theorem 16). The proof is standard, using cellular approximation theorem (see [11], Chapter 4.1, Theorem 4.8). $\square$

Corollary 4.5. *For any digraph $G = (V, E)$ and $v \in V$ we have isomorphisms*

$$\pi_1(G, v) \cong E(G, v) \cong \pi_1(|\Delta(G)|, v).$$

Now we recall several notions from the category theory (see, for example, [5], Chapter 6.6). Let $\mathcal{C}$ be a category. A commutative square $\mathbf{C}$

$$\begin{tikzcd} C_0 \arrow[r, "i_1"] \arrow[d, "i_2"] & C_1 \arrow[d, "u_1"] \\ C_2 \arrow[r, "u_2"] & C \end{tikzcd} \tag{4.5}$$

in the category $\mathcal{C}$ is called a *pushout* if for any commutative diagram

$$\begin{tikzcd} C_0 \arrow[r, "i_1"] \arrow[d, "i_2"] & C_1 \arrow[d, "u_1'"] \\ C_2 \arrow[r, "u_2'"] & C' \end{tikzcd}$$

in the category $\mathcal{C}$ there is a unique morphism $c\colon C \to C'$ such that $cu_i = u_i'$, $i = 1, 2$.

Now let X be a CW-complex with CW-subcomplexes X_1, X_2 such that $X = X_1 \cup X_2$, and set $X_0 = X_1 \cap X_2$. Then we obtain a pushout $\mathbf{X}$ of natural inclusions

$$\begin{tikzcd} {|X_0|} \arrow[r, "i_1"] \arrow[d, "i_2"] & {|X_1|} \arrow[d, "u_1"] \\ {|X_2|} \arrow[r, "u_2"] & {|X|} \end{tikzcd} \tag{4.6}$$

in the category of topological spaces (see [5], Chapters 4 and 6).

Let $A \subset X$ be a subset of a topological space X. Then we can define a full subgroupoid $\mathcal{P}_A(X)$ of the fundamental groupoid $\mathcal{P}(X)$ in the following way [5], Chapter 6.3. The elements of $\mathcal{P}_A(X)$ are all classes of homotopy paths relative to the boundary in the space X, joining points of A. Thus, for example, $\mathcal{P}_*(X) = \pi_1(X, *)$, where $*$ is a base point. Any inclusion of topological spaces $j\colon Y \to X$ induces a morphism of groupoids $j_*\colon \mathcal{P}_A(Y) \to \mathcal{P}_A(X)$. A set A is called *representative in X* if A meets each path-component of the space X. We need the following result.

Theorem 4.6 (Van Kampen theorem [5], Chapter 6.7.2)**.** *Let X be a path-connected space and let $\mathbf{X}$ be pushout* (4.6)*. If the set $A \subset X$ is representative in X_0, X_1, X_2, then the square*

$$
\begin{tikzcd}
\mathcal{P}_A(X_0) \arrow[r, "i_{1*}"] \arrow[d, "i_{2*}"] & \mathcal{P}_A(X_1) \arrow[d, "u_{1*}"] \\
\mathcal{P}_A(X_2) \arrow[r, "u_{2*}"] & \mathcal{P}_A(X)
\end{tikzcd}
\tag{4.7}
$$

is a pushout square in the category of groupoids.

Definition 4.7. We shall call any of the following subdigraphs a *cell* of a digraph G:

(i) any subdigraph that consists of two adjacent vertices of G with all arrows between them;

(ii) any subdigraph that is a triangle;

(iii) any subdigraph that is a square (see Definition 3.3).

Theorem 4.8 (Van Kampen theorem for digraphs)**.** *Let a connected digraph G be a union of two subdigraphs $G = G_1 \cup G_2$ such that any cell of the digraph G lies at least in one of the subdigraphs G_i, $i = 1, 2$, and let $G_0 = G_1 \cap G_2$. Then the square*

$$
\begin{tikzcd}
\mathcal{E}(G_0) \arrow[r] \arrow[d] & \mathcal{E}(G_1) \arrow[d] \\
\mathcal{E}(G_2) \arrow[r] & \mathcal{E}(G),
\end{tikzcd}
\tag{4.8}
$$

in which all morphisms are induced by natural inclusions, is a pushout in the category of groupoids.

P r o o f. The inclusions of digraphs induce the inclusion of topological spaces of their CW-complexes

$$
\begin{tikzcd}
|\Delta(G_0)| \arrow[r] \arrow[d] & |\Delta(G_1)| \arrow[d] \\
|\Delta(G_2)| \arrow[r] & |\Delta(G)|.
\end{tikzcd}
\tag{4.9}
$$

Now the result follows from Theorem 4.6 and Proposition 4.4 since the set of vertices V is representative in $|\Delta(G_0)|$, $|\Delta(G_1)|$, and $|\Delta(G_2)|$. $\square$

Corollary 4.9. *Let G^* be a based connected digraph with connected based subdigraphs G_i^*, $i = 1, 2$, such that $G = G_1 \cup G_2$ and $G_0 = G_1 \cap G_2$ is connected. Under the assumptions of Theorem* 4.8,

$$\pi_1(G^*) = \pi_1(G_1^*) * \pi_1(G_2^*)/N, \tag{4.10}$$

where N is the normal subgroup of the free product generated by all the elements of the form $[x] * [x]^{-1}$, where x is a based loop in G_0.

In the following examples we show that the conditions of Theorem 4.8 cannot be relaxed.

Example 4.10. (i) Consider the following based digraph G^*

$$\begin{tikzcd}
1 \arrow[rr] \arrow[dd] & & 2 \arrow[dl] \arrow[dd] \\
& * \arrow[ul] \arrow[dl] & \\
3 \arrow[rr] & & 4 \arrow[ul]
\end{tikzcd} \tag{4.11}$$

and let G_1 be the subdigraph that is obtained from G by removing vertex 4 with adjacent arrows, and G_2 is obtained similarly removing vertex 1. Clearly, $G = G_1 \cup G_2$ and the intersection $G_0 = G_1 \cap G_2$ is the following line digraph

$$2 \to * \to 3.$$

There are deformation retractions of G_1^*, G_2^*, and G^* to the following cyclic subdigraphs, respectively,

$$\begin{tikzcd}
1 \arrow[rr] & & 2 \arrow[dl] \\
& * \arrow[ul] &
\end{tikzcd}
\qquad
\begin{tikzcd}
* & * \arrow[dl] & \\
3 \arrow[rr] & & 4 \arrow[ul]
\end{tikzcd}
\quad \text{and} \quad
\begin{tikzcd}
1 \arrow[rr] & & 2 \arrow[dl] \\
& * \arrow[ul] &
\end{tikzcd}$$

(see [8], Example 3.14). Hence, by [8],

$$\pi_1(G_1^*) \cong \pi_1(G_2^*) \cong \pi_1(G^*) \cong \mathbb{Z}, \quad \pi_1(G_0^*) = \{e\}, \tag{4.12}$$

which implies that (4.10) is not satisfied. In this case Corollary 4.9 does not apply since the cell given by the square $\{1, 2, 3, 4\}$ lies neither in G_1 nor in G_2.

(ii) For the based digraph G^*

$$\begin{tikzcd} 3 \arrow[r] \arrow[d] & 2 \arrow[d] \\ 1 \arrow[r, shift left] & * \arrow[l, shift left] \arrow[ul] \end{tikzcd}$$

there is a deformation retraction of G^* onto $(* \rightleftarrows 1)$. Hence by [8], $\pi_1(G^*) = \{e\}$. The digraph G is the union of two digraphs

$$\text{(4.13)} \qquad G_1 = \begin{tikzcd} 3 \arrow[r] \arrow[d] & 2 \arrow[d] \\ 1 \arrow[r, shift right] & * \arrow[l, shift right] \end{tikzcd} \quad \text{and} \quad G_2 = \begin{tikzcd} 3 \arrow[r] & 2 \arrow[d] \\ & * \arrow[ul] \end{tikzcd} .$$

Then $G_0 = G_1 \cap G_2 = (3 \to 2 \to *)$ and

$$\pi_1(G^*) = \pi_1(G_1^*) = \pi_1(G^*) = \{e\}, \quad \pi_1(G_2^*) \cong \mathbb{Z},$$

so (4.10) fails. In this case the cell

$$\begin{tikzcd} 3 \arrow[d] & \\ 1 & * \arrow[l] \arrow[ul] \end{tikzcd}$$

does not lie in G_1 or in G_2 and Corollary 4.9 is not applicable.

(iii) Consider a digraph G^*

$$\text{(4.14)} \qquad \begin{tikzcd} & 1 \arrow[d, shift right] \arrow[dr] & \\ 2 \arrow[ur] \arrow[r] & * \arrow[u, shift right] & 3 \arrow[l] \end{tikzcd} .$$

There is an evident deformation retraction of G^* onto $(* \rightleftarrows 1)$, hence $\pi_1(G^*) = 0$. We can present G^* as the union of two digraphs:

$$\text{(4.15)} \qquad G_1 = \begin{tikzcd} & 1 \arrow[d] \\ 2 \arrow[ur] \arrow[r] & * \end{tikzcd} \quad \text{and} \quad G_2 = \begin{tikzcd} & 1 \arrow[dr] & \\ 2 \arrow[ur] \arrow[r] & * \arrow[u] & 3 \arrow[l] \end{tikzcd} .$$

Then $G_0 = G_1 \cap G_2 = (1 \leftarrow 2 \to *)$ and

$$\pi_1(G^*) = \pi_1(G_1^*) = \pi_1(G_0^*) = \{e\}, \quad \pi_1(G_2^*) = \mathbb{Z}.$$

In this case the cell $(* \rightleftarrows 1)$ does not lie in G_1 or in G_2, Corollary 4.9 is not applicable, and (4.10) fails.

5. Fundamental groupoids of graphs

The deep connection between Atkin homotopy theory and a homotopy theory for graphs was exhibited in [3] and [4]. In particular, the new notion of the fundamental group for undirected graphs was introduced there. In [8] the notion of the fundamental group for digraphs was introduced, and it was transferred to the category of graphs, using isomorphism between the category of graphs and the full subcategory of symmetric digraphs. The so obtained fundamental group is isomorphic to the fundamental group from [3].

In this section we transfer the results about fundamental groupoids of digraphs to that of undirected graphs, similarly to [8].

We recall shortly the notation from [8], Section 6, that we shall use in this section with minimal changes. To denote graphs and the graph maps we shall use bold font, for example, $\mathbf{G} = (\mathbf{V_G}, \mathbf{E_G})$, $\mathbf{f}\colon \mathbf{G} \to \mathbf{H}$.

Definition 5.1. A *graph* $\mathbf{G} = (\mathbf{V_G}, \mathbf{E_G})$ is a pair of a set $\mathbf{V_G}$ of *vertices* and a subset $\mathbf{E_G} \subset \{\mathbf{V_G} \times \mathbf{V_G} \setminus \mathrm{diag}\}$ of non-ordered pairs of vertices that are called *edges*. We shall write $v \sim w$ for $(v, w) \in \mathbf{E_G}$.

A *graph map* from a graph $\mathbf{G} = (\mathbf{V_G}, \mathbf{E_G})$ to a graph $\mathbf{H} = (\mathbf{V_H}, \mathbf{E_H})$ is a map

$$\mathbf{f}\colon \mathbf{V_G} \to \mathbf{V_H}$$

such that for any edge $v \sim w$ on $\mathbf{G}$ we have either $\mathbf{f}(v) = \mathbf{f}(w)$ or $\mathbf{f}(v) \sim \mathbf{f}(w)$.

As usually, a *based graph* $\mathbf{G}^*$ is the graph $\mathbf{G}$ with a fixed vertex $*$ and a based graph map preserves base vertexes.

The set of all graphs with graph maps forms a category $\mathcal{G}$. Let us associate to each graph $\mathbf{G} = (\mathbf{V_G}, \mathbf{E_G})$ a symmetric digraph $\mathcal{O}(\mathbf{G}) = G = (V_G, E_G)$, where $V_G = \mathbf{V_G}$ and E_G is defined by the condition $v \to w \Leftrightarrow v \sim w$. Thus, we obtain a functor $\mathcal{O}$ that provides an isomorphism of the category $\mathcal{G}$ and the full subcategory of symmetric digraphs of the category $\mathcal{D}$.

The functor $\mathcal{O}$ allows us to transfer the notions and results obtained in category $\mathcal{D}$ to category $\mathcal{G}$. In particular, we obtain in this way the definition of the fundamental groupoid of a graph as below.

Definition 5.2. (i) A *formal edge* of a graph $\mathbf{G} = (\mathbf{V}, \mathbf{E})$ is an ordered pair (v, w) of vertices such that $v \sim w$ or $v = w$.

(ii) An *edge-path* ξ of a graph $\mathbf{G}$ is a finite nonempty sequence

$$(v_0 v_1)(v_1, v_2) \ldots (v_{n-1}, v_n) \tag{5.1}$$

of formal edges of the graph $\mathbf{G}$. The vertex v_0 is called the *tail* of the edge-path ξ and v_n the *head* of the edge-path ξ. We write $v_0 = t(\xi)$, $v_n = h(\xi)$.

(iii) A *closed edge-path* at the vertex $v_0 \in \mathbf{V}$ is an edge-path ξ such that $t(\xi) = h(\xi) = v_0$.

(iv) For two edge-paths ξ_1 and ξ_2 with $h(\xi_1) = t(\xi_2)$ we define a *product edge-path* $\xi_1\xi_2$ consisting of the sequence of formal edges ξ_1 followed by the formal edges of ξ_2.

(v) For any edge-path ξ from (5.1) define the inverse edge-path ξ^{-1} as

$$\xi^{-1} := (v_n, v_{n-1})(v_{n-1}, v_{n-2}) \dots (v_1, v_0).$$

It follows directly from Definition 5.2 that the edge-paths of a graph $\mathbf{G}$ satisfy the following properties:

▷ $t(\xi_1\xi_2) = t(\xi_1)$, $h(\xi_1\xi_2) = h(\xi_2)$,
▷ $t(\xi) = h(\xi^{-1})$, $h(\xi) = t(\xi^{-1})$,
▷ $(\xi_1\xi_2)\xi_3 = \xi_1(\xi_2\xi_3)$,
▷ $(\xi^{-1})^{-1} = \xi$,

where we suppose that all products are defined.

Define an *edge-path groupoid of a graph* similarly as in Section 3.

Definition 5.3. Two edge-paths ξ_1 and ξ_2 in $\mathbf{G} = (\mathbf{V}, \mathbf{E})$ are called *equivalent* (and we write $\xi_1 \sim \xi_2$) if ξ_1 can be obtained from ξ_2 by a finite sequence of the following *local transformations* or their inverses (where the dots "..." denote the unchanged parts of the edge-paths):

(i) $\dots(v_0, v_1)(v_1, v_2)\dots \mapsto \dots(v_0, v_2)\dots$, where $v_0 \sim v_2$ or $v_0 = v_2$;

(ii) $\dots(v_0, v_1)(v_1, v_2)\dots \mapsto \dots(v_0, v_3)(v_3, v_2)\dots$, where the vertices v_0, v_1, v_2, v_3 are different and $v_0 \sim v_3$ and $v_3 \sim v_2$;

(iii) $\dots(v_0, v_1)(v_1, v_2)(v_2, v_3)\dots \mapsto \dots(v_0, v_3)\dots$, where the vertices v_0, v_1, v_2, v_3 are different and $v_0 \sim v_3$.

Note that the list of local transformations in Definition 5.3 follows from Definition 3.4 using inverse functor $\mathcal{O}^{-1}$ on the subcategory of symmetric digraphs, which allows to simplify this list.

The relation "$\sim$" on the set of edge paths of a graph $\mathbf{G}$ is an equivalence relation. We shall denote by $[\xi]$ the equivalence class of the edge-path ξ. For equivalence classes the following notations and operations are well-defined:

$$t([\xi]){:=}t(\xi), \quad h([\xi]){:=}h(\xi), \quad \text{for } t(\xi_1) = h(\xi_1) \quad [\xi_1] \circ [\xi_2]{:=}[\xi_1\xi_2], \quad [\xi]^{-1} = [\xi^{-1}].$$

Theorem 5.4. *For any graph* $\mathbf{G}$ *the vertex set of* $\mathbf{G}$ *as the set of objects and the set of the equivalence classes of edge-paths* ξ *as morphisms from* $t(\xi)$ *to* $h(\xi)$, *form a category* $\mathcal{E}(\mathbf{G})$ *that is a groupoid. The composition of two morphisms* $[\xi_1]$ *and* $[\xi_2]$ *is given by* $[\xi_1] \circ [\xi_2]$, *and the inverse morphism of* $[\xi]$ *is* $[\xi]^{-1}$.

The groupoid $\mathcal{E}(\mathbf{G})$ is called the *fundamental groupoid* of the graph $\mathbf{G}$.

We denote by $\mathrm{Hom}_{\mathcal{E}(\mathbf{G})}(v,w)$ the set of morphisms from $v \in \mathbf{V}$ to $w \in \mathbf{V}$ in the category $\mathcal{E}(\mathbf{G})$, or simply $\mathrm{Hom}(v,w)$ if the graph $\mathbf{G}$ is clear from the context.

Let $v \in \mathbf{V}$ be a vertex in a graph $\mathbf{G}$. Consider the set of equivalence classes $[\xi]$ of edge-paths ξ of $\mathbf{G}$ such that $t(\xi) = h(\xi) = v$. This set is a group with the neutral element $[(v,v)]$ and with the groupoid product of $\mathcal{E}(\mathbf{G})$. Denote this group by $\mathrm{E}(\mathbf{G},v)$. Note that the fundamental group $\pi_1(\mathbf{G}^*)$ of a based graph $\mathbf{G}^*$ was introduced in [3], and [4], Proposition 5.6. It follows from [8] that

$$\mathrm{E}(\mathbf{G},v) \cong \pi_1(\mathbf{G}^v).$$

Definition 5.5. Let $\mathbf{G} = (\mathbf{V_G}, \mathbf{E_G})$ and $\mathbf{H} = (\mathbf{V_H}, \mathbf{E_H})$ be two graphs.

(i) Define the *Cartesian product* $\mathbf{\Pi} = \mathbf{G} \,\square\, \mathbf{H}$ as a graph with the set of vertices $\mathbf{V_\Pi} = \mathbf{V_G} \times \mathbf{V_H}$ and with the set of edges $\mathbf{E_\Pi}$ such that $(x,y) \sim (x',y')$ if and only if

$$\text{either } x' = x \;\text{ and }\; y \sim y', \qquad \text{or } x \sim x' \;\text{ and }\; y = y'.$$

(ii) Define a $\rtimes$-product $\mathbf{P} = \mathbf{G} \rtimes \mathbf{H}$ as a graph with the set of vertices $\mathbf{V_P} = \mathbf{V_G} \times \mathbf{V_H}$ and there is an edge

$$(x,y) \sim (x',y') \quad \text{for } x,x' \in \mathbf{V_G};\; y,y' \in \mathbf{V_H}$$

if one of the following conditions is satisfied:

$$x' = x,\; y \sim y'; \quad \text{or} \quad y' = y,\; x \sim x'; \quad \text{or} \quad x \sim x',\; y \sim y'.$$

Theorem 5.6. *We have an isomorphism of groupoids*

$$\mathcal{E}(\mathbf{G} \,\square\, \mathbf{H}) \cong \mathcal{E}(\mathbf{G} \rtimes \mathbf{H}) \cong \mathcal{E}(\mathbf{G}) \times \mathcal{E}(\mathbf{H}).$$

In particular, for based graphs we have an isomorphism of fundamental groups

$$\pi_1(\mathbf{G}^* \,\square\, \mathbf{H}^*) \cong \pi_1(\mathbf{G}^* \rtimes \mathbf{H}^*) \cong \pi_1(\mathbf{G}^*) \times \pi_1(\mathbf{H}^*).$$

This property of fundamental groups of graphs is new. We think that the direct proof of this result, using the definition of π_1 from [3] and [4], can be very nontrivial.

Now we state the Van Kampen theorem for the fundamental groupoids of graphs. For the fundamental group of graph it was proved in [4].

The union and intersection of subgraphs is defined in the same way as those for digraphs in Definition 4.1.

Definition 5.7. We shall call any of the following subgraphs a *cell* of a graph $\mathbf{G}$:
(i) a full subgraph consisting of three vertices (triangle);
(ii) a subgraph consisting of four vertices whose edges form a square.

Theorem 5.8 (Van Kampen theorem for graphs)**.** *Let $\mathbf{G} = \mathbf{G}_1 \cup \mathbf{G}_2$ be a connected graph such that any cell of $\mathbf{G}$ lies in one of the subgraphs $\mathbf{G}_1, \mathbf{G}_2$. Set $\mathbf{G}_0 = \mathbf{G}_1 \cap \mathbf{G}_2$. Then the square*

$$\begin{tikzcd} \mathcal{E}(\mathbf{G}_0) \arrow[r] \arrow[d] & \mathcal{E}(\mathbf{G}_1) \arrow[d] \\ \mathcal{E}(\mathbf{G}_2) \arrow[r] & \mathcal{E}(\mathbf{G}), \end{tikzcd} \tag{5.2}$$

in which all morphisms are induced by natural inclusions, is a pushout in the category of groupoids.

Corollary 5.9 ([4])**.** *Let $\mathbf{G}^*$ be a based connected graph with connected based subdigraphs $\mathbf{G}_i^*$, $i = 1, 2$, such that $\mathbf{G} = \mathbf{G}_1 \cup \mathbf{G}_2$ and $\mathbf{G}_0 = \mathbf{G}_1 \cap \mathbf{G}_2$ is connected. Under the assumptions of Theorem* 5.8 *we have*

$$\pi_1(\mathbf{G}^*) = \pi_1(\mathbf{G}_1^*) * \pi_1(\mathbf{G}_2^*)/N,$$

where N is the normal subgroup of the free product generated by all the elements of the form $[x] * [x]^{-1}$, where x is a based loop in $\mathbf{G}_0$.

6. An application to coloring

Now we formulate and prove a natural generalization of the classical Sperner lemma, using the results of Section 3.

Let $\mathbf{G} = (\mathbf{V}, \mathbf{E})$ be a planar (nondirected) finite connected graph which provides a simplicial triangulation of a simply-connected closed domain $D \subset \mathbb{R}^2$. Let $\mathbf{H}$ be the subdigraph of $\mathbf{G}$ that lies on the boundary ∂D. Let any vertex of $\mathbf{G}$ be colored by one of three colors, say $\{0, 1, 2\}$. Define a digraph $G = (V, E)$ by putting $V = \mathbf{V}$ and defining the set E of arrows according to the colors of vertices as follows:

$$0 \to 1, \quad 1 \to 2, \quad 2 \to 0, \quad 0 \leftrightarrows 0, \quad 1 \leftrightarrows 1, \quad 2 \leftrightarrows 2.$$

In particular, we obtain a subdigraph $H = (V_H, E_H)$ of G that lies on ∂D. Let us fix a vertex $* \in V_H$ and set $n = |V_H|$. Going along ∂D clockwise, starting and ending at $*$, we obtain a loop $\varphi\colon\ I_n^* \to H^* \subset G^*$.

Theorem 6.1.

(i) *If* $[\varphi] \neq [e]$ *in* $\pi_1(G^*)$, *then there is at least one* 3*-color triangle in the triangulation of* D.

(ii) *If* $\operatorname{rank} \pi_1(G^*) = r$, *then there are at least* r 3*-color triangles in the triangulation of* D.

P r o o f. Follows from the description of local transformations in Section 3 and the method of [8], Theorem 4.20. □

Corollary 6.2. *The number of* 3*-color triangles in the triangulation of* D *is at least* $\operatorname{rank} H_1(G, \mathbb{Z})$.

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