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## **ON THE SOMBOR INDEX OF CHEMICAL TREES**

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**Summary.** We give sharp bounds on the Sombor index of chemical trees and characterize the cases of the equalities. We stated conjectures regarding second maximal chemical trees of order *n* with respect to Sombor index, when  $n \equiv 0 \pmod{3}$  and  $n \equiv 1 \pmod{3}$ .

### **1 INTRODUCTION**

Molecular descriptors are mathematical values used in evaluation and prediction of properties of chemical compounds. They are used to describe the structure and shape of molecules of even more not yet synthesized compounds and so play significant role in mathematical chemistry and pharmacology [11, 13]. Topological indices are type of molecular descriptors calculated on the graphs associated to molecules of chemical compounds. In the literature of mathematical chemistry several dozens of topological indices have been introduced and studied [4-8,12].

Let *G* be a graph with the vertex set V(G) and the edge set E(G). For a vertex  $v \in V(G)$ , the degree of *v* is denoted by  $d_G(v)$ , or simply d(v) whenever the graph is clear from the context. The Sombor index is defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d^2(u) + d^2(v)}.$$
 (1)

This index, abbreviated as SO index, has been proposed recently by Gutman in [8]. The contribution of the edge  $uv \in E(G)$  to SO(G) is

$$s_G(uv) = \sqrt{d^2(u) + d^2(v)}$$
 (2)

and we will use the next form of equation (1)

$$SO(G) = \sum_{e \in E(G)} s_G(e).$$
(3)

A tree is connected graph with no cycles. The problem of finding extreme values of topological indices over chemical trees, that is trees with vertex degrees less or equal 4, has attracted

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considerable attention in the mathematical-chemistry literature [1-3,9,12-14]. In this paper we consider the problem of extreme values of SO index among chemical trees with *n*-vertices. We stated conjectures regarding second maximal chemical trees with respect to Sombor index, when  $n \equiv 0 \pmod{3}$  and  $n \equiv 1 \pmod{3}$ .

#### **2** DEFINITIONS AND PRELIMINARIES

Let *T* be a chemical tree of order *n*. Throughout the paper, the number of vertices with degree *i* is denoted by  $n_i$ , for every  $i = \overline{1,4}$ , and for every  $1 \le i \le j \le n-1$ ,  $m_{ij}$  denotes the number of edges of *T* between a vertex with degree *i* and a vertex with degree *j*. Now, in this notation, formula (1) takes the form

$$SO(T) = \sum_{1 \le i \le j \le n-1} m_{ij} \sqrt{i^2 + j^2}.$$
(4)

which will be used, for the most part.

It has be shown by Gutman [8] that the path graph and the star graph are the graphs with extremal values of SO index among all *n*-vertex trees. Since the path is chemical tree, the minimum of the SO index in the set of chemical trees with a constant number of vertices is achieved for path graphs, while the maximum is achieved for star graphs only for  $n \le 5$ . Our goal here is to characterize the chemical trees of order  $n \ge 6$  that maximize SO index.

#### **3** ON THE BOUNDS OF TNE NUMBERS $n_i$ AND $m_{ii}$

In this section we are going to present and prove two statements that will be crucial in proving the final theorem that gives the upper bound of SO index and complete characterization of the chemical trees on which SO index attains the maximum value.

**Lemma 1.** Let T be a n-vertex,  $n \ge 6$ , chemical tree with maximum value of SO-index. Then, in T holds the following:

$$m_{22} = 0, m_{23} = 0, m_{33} = 0, m_{12} \le 1.$$

*Proof.* Let us prove the first claim  $m_{22} = 0$ . In the contrary, suppose that there is an edge  $e = uv \in E(T)$  whose endpoints u and v have degrees 2. Let  $uu_1$  and  $vv_1$  be the remaining edges incident with vertices u and v, respectively, and let  $T' = T - vv_1 + uv_1$ . Note that, since T is acyclic,  $u_1$  and  $v_1$  are distinct vertices. Therefore, due to (3),

$$SO(T') - SO(T) = (s_{T'}(uu_1) + s_{T'}(uv) + s_{T'}(uv_1)) - (s_T(uu_1) + s_T(uv) + s_T(vv_1))$$

To obtain the contradiction with the assumption that *T* is maximal, we need to prove that this difference is positive. Since  $d_T(u) = d_T(v) = 2$ ,  $d_{T'}(u) = 3$  and  $d_{T'}(v) = 1$ , it holds:  $s_T(uu_1) < s_{T'}(uu_1)$ ,  $s_T(uv) = \sqrt{8} < \sqrt{10} = s_{T'}(uv)$  and  $s_T(vv_1) < s_{T'}(vv_1)$ , that is SO(T') > SO(T).

The next claim,  $m_{23} = 0$ , will be proved in the same manner, by the similar graph transformation. Suppose to the contrary that in *T* there is an edge  $e_0 = uv \in E(T)$  such that d(u) = 3and d(v) = 2. Let  $e_1 = vw$  be the remaining edge incident with vertex *v* and let  $e_2, e_3$  be the remaining edges incident with vertex u. Now, for the graph T' = T - vw + uw holds

$$SO(T') - SO(T) = \sum_{i=0}^{3} s_{T'}(e_i) - \sum_{i=0}^{3} s_T(e_i),$$

and  $s_{T'}(e_0) = \sqrt{17} < \sqrt{13} = s_T(e_0)$ . Since, vertex degree of the only one of two endpoints of edge  $e_i$  is increased and the other one is unchanged, we obtain that  $s_{T'}(e_i) > s_T(e_i)$ , for each  $i = \overline{1,3}$ . Hence, SO(T') > SO(T).

The claim,  $m_{33} = 0$ , is going to be proved similarly. Let us suppose that  $e_0 = uv \in E(T)$  is an edge whose the both endpoints have degrees 3. Further, let  $e_1 = vw_1$  and  $e_2 = vw_2$  be the remaining edges incident with vertex v and  $e_3$  and  $e_4$  be the remaining edges incident with vertex u. Without losing the generality, suppose that  $d(w_1) \leq d(w_2)$  and let us construct a new chemical tree T' from T, by relocating its edge  $e_1$  as follows:  $T' = T - vw_1 + uw_1$ . Then,

$$SO(T') - SO(T) = \sum_{i=0}^{4} s_{T'}(e_i) - \sum_{i=0}^{4} s_T(e_i)$$

In view of the definition of graph T',  $d_T(u) = d_T(v) = 3$ ,  $d_{T'}(u) = 4$  and  $d_{T'}(v) = 2$ , so  $s_{T'}(e_i) > s_T(e_i)$  for  $i \in \{0, 3, 4\}$ . It remains to be seen how the sum of contributions of the edges  $e_1$  and  $e_2$  has been changed.

$$s_T(e_1) + s_T(e_2) = \sqrt{9 + d_{w_1}^2} + \sqrt{9 + d_{w_2}^2}$$
$$s_{T'}(e_1) + s_{T'}(e_2) = \sqrt{16 + d_{w_1}^2} + \sqrt{4 + d_{w_2}^2}$$

Using the assumption that  $d(w_1) \le d(w_2)$  and  $d(w_1), d(w_2) \in \{1, \dots, 4\}$ , by checking of ten cases, we obtain that  $s_T(e_1) + s_T(e_2) < s_{T'}(e_1) + s_{T'}(e_2)$ . It follows that SO(T') > SO(T).

At the end, we want to argue that  $m_{12} \le 1$ . Assume for contradiction that, in some maximal tree T of order  $n \ge 6$ , there are two edges e = uv and g = ab whose endpoints have vertex degrees 2 and 1, that is d(u) = d(a) = 2 and d(v) = d(b) = 1. Because of assumption  $n \ge 6$ , u and a are distinct vertices. Let us denote by w and c the remaining vertices adjacent with the vertices u and a, respectively, and let T' = T - uv + av. Due to previously proved claims, w and c are vertices, not necessarily distinct, with degree 4 and so

$$s_T(uw) = s_T(ac) = \sqrt{20}, s_T(uv) = s_T(ab) = \sqrt{5},$$
  
$$s_{T'}(uw) = \sqrt{17}, s_{T'}(ac) = 5, s_{T'}(ab) = \sqrt{10}, s_{T'}(av) = \sqrt{10}$$

Hence, graph T' is a new chemical tree whose SO-index is greater than SO(T), because of

$$SO(T') - SO(T) = (\sqrt{17} + 5 + 2\sqrt{10}) - 2(\sqrt{20} + \sqrt{5}) \approx 2.031 > 0$$

**Lemma 2.** Let T be a chemical tree with maximum value of SO-index. Then, in T holds the following:  $n_2 \le 1$ ,  $n_3 \le 1$ ,  $n_2 = 1 \Rightarrow n_3 = 0$  and  $n_3 = 1 \Rightarrow n_2 = 0$ .

#### Proof.

**Proof of the claim**  $n_2 \le 1$ : Assume that *u* and *a* are two vertices of chemical tree *T* with degree 2, a let us denote by  $v_1$ ,  $v_2$  and  $b_1$ ,  $b_2$  their first neighbors, respectively. Due to Lemma 1,

degrees of the each of the four vertices  $v_i$ ,  $b_i$ , i = 1, 2 belongs to  $\{1,4\}$ . Since *T* is connected graph, the both first neighbors of *u* can not be pendant vertices, that is at least on of its first neighbors has degree 4. The same holds for the vertex *a*. Without losing the generality suppose that  $d(v_1) = d(b_1) = 4$ . Vertices  $v_1$  and  $b_1$  are not necessarily distinct. Now we construct a graph *T'* by removing edge  $uv_2$  from graph *T* and inserting a new edge among *a* and  $v_2$ , that is  $T' = T - uv_2 + av_2$ . The following holds

$$\begin{split} s_T(uv_1) &= s_T(ab_1) = \sqrt{20}, \\ s_T(uv_2) &= \sqrt{4 + d(v_2)^2}, \\ s_{T'}(uv_1) &= \sqrt{17}, \\ s_{T'}(ab_2) &= \sqrt{9 + d(b_2)^2}, \\ \end{split}$$

Hence,

$$\begin{split} SO(T') - SO(T) = & (5 + \sqrt{17} + \sqrt{9 + d(b_2)^2} + \sqrt{9 + d(v_2)^2} \\ & -(2\sqrt{20} + \sqrt{4 + d(v_2)^2} + \sqrt{4 + d(b_2)^2} \\ & > 5 + \sqrt{17} - 2\sqrt{20} \\ & \approx 0.1788337156 > 0 \end{split}$$

This is opposite with the assumption that T is a chemical tree with maximum value of Sombor index.

**Proof of the claim**  $n_3 \le 1$ : Assume for contradiction that there are two vertices  $u, a \in V(T)$  with degree 3, and let  $v_i$  and  $b_i$ ,  $i = \overline{1,3}$  be their first neighbors, respectively. Due to Lemma 1, u and a are not adjacent vertices and degrees  $d(v_i)$ ,  $d(b_i)$ , for each  $i = \overline{1,3}$ , belongs to  $\{1,4\}$ . As in the proof of the previous claim, assume that  $d(v_1) = d(b_1) = 4$  Now, we distinguished the next three cases:

**Case 1:**  $d(v_2) = d(v_3) = d(b_2) = d(b_3) = 4$ .

In this case, we transform graph T to a new on T' as follows:  $T' = T - uv_2 + av_2$ . The next is worth

$$s_T(uv_i) = s_T(ab_i) = 5, i = \overline{1,3} s_{T'}(uv_1) = s_{T'}(uv_3) = 2\sqrt{5}, s_{T'}(av_2) = s_{T'}(ab_i) = 4\sqrt{2}, i = \overline{1,3}.$$

that is

$$SO(T') - SO(T) = (4\sqrt{5} + 16\sqrt{2}) - 30 \approx 1.571688908 > 0.$$

So, *T* is not a chemical tree with maximum value of Sombor index. Case 2: The both of vertices  $v_2$ ,  $v_3$  have degrees 1, or the both of vertices  $b_2$ ,  $b_3$  have degrees 1. Without losing generality, let us assume that  $d(v_2) = d(v_3) = 1$ . Let  $T' = T - uv_2 + av_2$ . Then,

$$s_{T}(uv_{1}) = s_{T}(ab_{1}) = 5,$$
  

$$s_{T}(uv_{2}) = s_{T}(uv_{3}) = \sqrt{10},$$
  

$$s_{T}(ab_{i}) < s_{T'}(ab_{i}), \quad i = \overline{1,2},$$
  

$$s_{T'}(uv_{1}) = 2\sqrt{5}, \quad s_{T'}(uv_{3}) = \sqrt{5},$$
  

$$s_{T'}(ab_{1}) = 4\sqrt{2}, \quad s_{T'}(av_{2}) = \sqrt{17}$$

It follows that

$$SO(T') - SO(T) > (3\sqrt{5} + 4\sqrt{2} + \sqrt{17}) - (10 + 2\sqrt{10}) \approx 0.1636 > 0,$$

and again *T* is not maximal.

**Case 3:** Previous two cases have not been satisfied. In this case, without losing generality, we may assume that  $d(v_2) = 4$  and  $d(v_3) = 1$ . Since in this, third case, the both of vertices  $b_2$ ,  $b_3$  are not pendant, let as suppose that  $d(b_2) = 4$ . Denote by T' chemical tree obtained from T on the same way as in the previous, that is  $T' = T - uv_2 + av_2$ . We obtain

$$s_{T}(uv_{1}) = s_{T}(uv_{2}) = 5, \qquad s_{T}(uv_{3}) = \sqrt{10}$$
  

$$s_{T}(ab_{1}) = s_{T}(ab_{2}) = 5, \qquad s_{T}(ab_{3}) = \sqrt{9 + d(b_{3})^{2}}$$
  

$$s_{T'}(uv_{1}) = 2\sqrt{5}, \qquad s_{T'}(uv_{3}) = \sqrt{5},$$
  

$$s_{T'}(av_{2}) = s_{T'}(ab_{i}) = 4\sqrt{2}, \qquad i = 1, 2.$$
  

$$s_{T'}(ab_{3}) = \sqrt{16 + d(b_{3})^{2}}$$

and conclude that

$$SO(T') - SO(T) > (12\sqrt{2} + 3\sqrt{5}) - (20 + \sqrt{10}) \approx 0.51649 > 0,$$

that is *T* is not maximal.

**Proof of the claim**  $n_2 = 1 \Rightarrow n_3 = 0$ : Assume for the contradiction that u and a are the vertices of T such that d(u) = 2 and d(a) = 3. In the same manner as in the previous, u and a are not the first neighbors and there are vertices  $u_1$  and  $b_1$  with degrees 4, adjecent with the vertices u and b, respectively. Since d(u) = 2, denote by  $v_2$  remaining vertex adjacent with u and by by  $b_2$ ,  $b_3$  remaining vertices adjacent with a. We do the same graph transformation  $T' = T - uv_2 + av_2$  as in the previous two cases, and obtain the following values

$$s_{T}(uv_{1}) = 2\sqrt{5}, \qquad s_{T}(uv_{2}) = \sqrt{4 + v_{2}^{2}}$$
  

$$s_{T}(ab_{1}) = 5, \qquad s_{T}(ab_{i}) = \sqrt{9 + d(b_{i})^{2}}, i = 2, 3$$
  

$$s_{T'}(uv_{1}) = \sqrt{17}, \qquad s_{T'}(ab_{1}) = 4\sqrt{2},$$
  

$$s_{T'}(av_{2}) = \sqrt{16 + v_{2}^{2}} \qquad s_{T'}(ab_{i}) = \sqrt{16 + d(b_{i})^{2}}, i = 2, 3$$

Hence,

$$SO(T') - SO(T) > (\sqrt{17} + 4\sqrt{2}) - (5 + 2\sqrt{5}) \approx 0.3078239 > 0,$$

and the claim is proven.

**Proof of the claim**  $n_3 = 1 \Rightarrow n_2 = 0$ : This claim is direct consequence of the first and the previous one.

#### 4 CHEMICAL TREES WITH EXTREME VALUES OF SOMBOR INDEX

For n = 3k,  $k \ge 2$ , let  $\mathscr{T}_n$  be the family of chemical trees with *n* vertices such that: k - 1 vertices have degree 4, one vertex has degree 2, remaining vertices are pendant and its single vertex with degree 2 is adjacent to the vertices of degree 4, in the case  $k \ge 3$ . In the case k = 2, that is n = 6, there is only one graph in  $\mathscr{T}_6$  and its single vertex with degree 2 is adjacent with one pendant vertex and one vertex with degree 4.

For n = 3k + 1,  $k \ge 2$ , denote by  $\mathscr{T}_n$  the family of chemical trees with *n* vertices such that: k - 1 vertices have degree 4, one vertex has degree 3, all other vertices are pendant and, in the case  $k \ge 4$ , its single vertex with degree 3 is adjacent with vertices of degree 4. In the case k = 2, that is n = 7, there is only one graph in  $\mathscr{T}_7$  and its single vertex with degree 3 is adjacent with two pendant vertices and one vertex with degree 4. In the case k = 3, that is n = 10, there is only one graph in  $\mathscr{T}_{10}$  and its single vertex with degree 3 is adjacent with one pendant vertex and two vertices with degree 4.

For  $n = 3k + 2 \ge 5$ ,  $\mathscr{T}_n$  is the family of chemical trees with *n* vertices such that: *k* vertices have degree 4 and remaining are pendant.

Our the main result is presented through the next three theorems, in which the following easy observation will be important:

Let T be a chemical tree with n. Then,

$$n_1 + n_2 + n_3 + n_4 = n \tag{5}$$

and from handshaking lemma

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1).$$
(6)

From (5) and (6) we conclude that

$$n_2 + 2n_3 + 3n_4 = n - 2. \tag{7}$$

**Theorem 1.** Let *T* be chemical tree of order  $n \ge 6$ , such that  $n \equiv 0 \pmod{3}$ . Then

$$SO(T) \leq 2\frac{n}{3}(\sqrt{17} + 2\sqrt{2}) + \\ + \begin{cases} 4\sqrt{5} - 12\sqrt{2}, & n \ge 9\\ 3\sqrt{5} - \sqrt{17} - 8\sqrt{2} & n = 6 \end{cases}$$

*The equality is attained if and only if*  $T \in \mathcal{T}_n$ *.* 

*Proof.* Let us suppose that n = 3k, for some  $k \ge 2$ . In this case, equality (7) implies that  $n_4 \le k-1$ .

First, let's see what's going on when  $n_4$  takes values less then k - 1. Substituting  $n_4 \le k - 2$  into (7) gives  $n_2 + 2n_3 \ge 4$ . This is impossible because of first two claims from Lemma 2.

Otherwise, when  $n_4 = k - 1$ , (7) gives  $n_2 + 2n_3 = 1$ , that is  $n_2 = 1$  and  $n_3 = 0$ . This implies that, for  $k \ge 3$ , there are two possibilities, that is two potential types of maximal graphs:

**Type 1:** Chemical tree in which k - 1 vertices have degree 4, one vertex has degree 2, remaining vertices are pendant and the both first neighbors of its single vertex with degree 2 have degree 4

**Type 2:** Chemical tree in which k - 1 vertices have degree 4, one vertex has degree 2, remaining vertices are pendant and only one of the first neighbors of its single vertex with degree 2 has degree 4 but the other one is pendant.

Denote by  $G_1$  graph of the first type and by  $G_2$  the graph of the second type. We will prove that  $SO(G_1) > SO(G_2)$ .

In the both of  $G_1$  and  $G_2$  holds  $n_1 = n - n_4 - 1 = 2k$ . Further, in  $G_1$  holds:

$$SO(G_1) = m_{24}\sqrt{20} + m_{14}\sqrt{17} + m_{44}\sqrt{32}$$
  
=  $2k(\sqrt{17} + 2\sqrt{2}) + 4\sqrt{5} - 12\sqrt{2}$  (8)

$$\approx 2k(\sqrt{17+2\sqrt{2}}) - 8.0262908, \tag{9}$$

since in this type of graphs  $m_{24} = 2$ ,  $m_{14} = n_1 = 2k$ ,  $m_{44} = k - 3$  and  $m_{ij} = 0$  for all other values of *i* and *j*.

On the other side, in  $G_2$  holds:

$$SO(G_2) = m_{12}\sqrt{5} + m_{24}\sqrt{20} + m_{14}\sqrt{17} + m_{14}\sqrt{32}$$
  
=  $2k(\sqrt{17} + 2\sqrt{2}) + 3\sqrt{5} - \sqrt{17} - 8\sqrt{2}$  (10)

$$\approx 2k(\sqrt{17} + 2\sqrt{2}) - 8.728610192, \tag{11}$$

since in this type of graphs  $m_{12} = 1$ ,  $m_{24} = 1$ ,  $m_{14} = n_1 - 1 = 2k - 1$ ,  $m_{44} = k - 2$ . From (9) and (11) follows that  $SO(G_1) > SO(G_2)$ .

In the case when k = 2, that is n = 6, there is no graph type 1. Moreover there is only one graph  $G_2$  type 2 and from (10) we obtain that its SO index is equal  $4(\sqrt{17} + 2\sqrt{2}) + 3\sqrt{5} - \sqrt{17} - 8\sqrt{2}$ .

**Theorem 2.** Let *T* be chemical tree of order  $n \ge 7$ , such that  $n \equiv 1 \pmod{3}$ . Then

$$SO(T) \leq 2\lfloor \frac{n}{3} \rfloor (\sqrt{17} + 2\sqrt{2}) + \\ + \begin{cases} 15 + \sqrt{17} - 16\sqrt{2}, & n \geq 13\\ 10 + \sqrt{10} - 12\sqrt{2}, & n = 10\\ 5 + 2\sqrt{10} - \sqrt{17} - 8\sqrt{2}, & n = 7 \end{cases}$$

The equality is attained if and only if  $T \in \mathcal{T}_n$ .

*Proof.* Let n = 3k + 1, for some  $k \ge 2$ . As in the previous, equality (7) implies that  $n_4 \le k - 1$ . If  $n_4$  takes values less then k - 1, substituting into (7) gives  $n_2 + 2n_3 \ge 5$ , which is impossible by Lemma 2.

Let  $n_4 = k - 1$ . From (7) follows that  $n_2 + 2n_3 = 2$ , that is  $n_2 = 0$  and  $n_3 = 1$ . Now, for  $k \ge 4$ , we distinguish three cases, that is tree potential types of maximal trees, regarding the degrees of the first neighbors of its single vertrex with degree 3:

**Type 1:** Chemical tree in which k - 1 vertices have degree 4, one vertex has degree 3, remaining vertices are pendant and each of the first neighbors of its single vertex with degree 3 have degree 4.

**Type 2:** Chemical tree in which k - 1 vertices have degree 4, one vertex has degree 3, remaining vertices are pendant and two of the first neighbors of its single vertex with degree 3 have degree 4 and third one is pendant.

**Type 3:** Chemical tree in which k - 1 vertices have degree 4, one vertex has degree 3, remaining vertices are pendant and only one the first neighbors of its single vertex with degree 3 has degree 4 and the two are pendants.

In the case k = 3, that is n = 10, there is no graph type 3 and for k = 2, what is equivalent with n = 7, there is only graph type 1.

Denote by  $G_1$  the graph of the first type, by  $G_2$  the graph of the second type and by  $G_3$  the graph of the third type. We are going to prove that

$$SO(G_1) > SO(G_2) > SO(G_3) \tag{12}$$

The number  $n_1$  of pendant vertices in each of this graphs is the same  $n_1 = n - n_4 - 1 = 2k + 1$ . In  $G_1$  holds

$$SO(G_1) = m_{34}\sqrt{25} + m_{14}\sqrt{17} + m_{44}\sqrt{32}$$
  
=  $2k(\sqrt{17} + 2\sqrt{2}) + 15 + \sqrt{17} - 16\sqrt{2}$  (13)

$$\approx 2k(\sqrt{17} + 2\sqrt{2}) - 3.504311372, \tag{14}$$

since in the graphs of type 1 is valid:  $m_{34} = 3$ ,  $m_{14} = n_1 = 2k + 1$ ,  $m_{44} = k - 4$  and  $m_{ij} = 0$  for all other values of *i* and *j*.

In G<sub>2</sub> numbers  $m_{ij}$  take the values:  $m_{13} = 1, m_{34} = 2, m_{14} = 2k, m_{44} = k - 3$ , so it follows

$$SO(G_2) = m_{13}\sqrt{10} + m_{34}\sqrt{25} + m_{14}\sqrt{17} + m_{44}\sqrt{32}$$
  
=  $2k(\sqrt{17} + 2\sqrt{2}) + 10 + \sqrt{10} - 12\sqrt{2}$  (15)

$$\approx \qquad 2k(\sqrt{17} + 2\sqrt{2}) - 3.808285088 \tag{16}$$

Finally, in  $G_3$  nonzero numbers  $m_{ij}$  take the values:  $m_{13} = 2, m_{34} = 1, m_{14} = 2k - 1, m_{44} = k - 2$ , so

$$SO(G_3) = m_{13}\sqrt{10} + m_{34}\sqrt{25} + m_{14}\sqrt{17} + m_{44}\sqrt{32}$$
  
=  $2k(\sqrt{17} + 2\sqrt{2}) + 5 + 2\sqrt{10} - \sqrt{17} - 8\sqrt{2}$  (17)

$$\approx 2k(\sqrt{17}+2\sqrt{2})-4.112258804.$$
 (18)

Thefore, we get to be valid  $SO(G_1) > SO(G_2) > SO(G_3)$ .

The assertion of the theorem follows.

**Theorem 3.** Let *T* be chemical tree of order *n*, such that  $n \equiv 2 \pmod{3}$ . Then

$$SO(T) \le 2\frac{n-2}{3}(\sqrt{17}+2\sqrt{2})+2\sqrt{17}-4\sqrt{2}.$$

*The equality is attained if and only if*  $T \in \mathcal{T}_n$ *.* 

*Proof.* Let n = 3k + 2, for some  $k \ge 1$ . In this case, equality (7) implies that  $n_4 \le k$ . When  $n_4 < k$ , from (7) follows  $n_2 + 2n_3 \ge 3$ . Based on the first two claims of Lemma 2, this is valid only for  $n_2 = n_3 = 1$ , but this is impossible due to the last claims of the same Lemma.

Let us assume that  $n_4 = k$ . Equality (7) gives  $n_2 + 2n_3 = 0$ , that is  $n_2 = n_3 = 0$ . It follows that is in this graph numbers  $m_{ij}$  take the next values:  $m_{14} = n_1 = 2k + 2$ ,  $m_{44} = k - 1$ , and  $m_{ij} = 0$  for all other values of *i* and *j*. Hence,

$$SO(G_1) = m_{14}\sqrt{17} + m_{44}\sqrt{32} = 2k(\sqrt{17} + 2\sqrt{2}) + 2\sqrt{17} - 4\sqrt{2}$$
(19)

$$= 2\frac{n-2}{3}(\sqrt{17}+2\sqrt{2})+2\sqrt{17}-4\sqrt{2}.$$
 (20)

The proof is completed.

#### **5 CONCLUDING REMARKS AND FURTHER WORK**

Sombor index is a recently introduced vertex-degree-based topological index. This paper is one of the several studies ([3], [12]) produced immediately after [7] became available. In

this paper we consider its bounds of over the chemical trees and characterize the appropriate extreme cases.

Based on the proofs of Theorem 1 and Theorem 2 we have the following conjectures

**Conjecture 1.** *Let T* be a chemical tree of order  $n \ge 9$ , such that  $n \equiv 0 \pmod{3}$ , with the second maximum of SO index. Then,

$$SO(T) \le 2\frac{n}{3}\left(\sqrt{17} + 2\sqrt{2}\right) + 3\sqrt{5} - \sqrt{17} - 8\sqrt{2}.$$

The equality is attained if and only if T is chemical tree in which  $\frac{n}{3} - 1$  vertices have degree 4, one vertex has degree 2, remaining vertices are pendant and only one of the first neighbors of its single vertex with degree 2 has degree 4 but the other one is pendant.

**Conjecture 2.** Let T be a chemical tree of order  $n \ge 10$ , such that  $n \equiv 1 \pmod{3}$ , with the second maximum of SO index. Then,

$$SO(T) \le 2\frac{n-1}{3}\left(\sqrt{17}+2\sqrt{2}\right)+10+\sqrt{10}-12\sqrt{2}.$$

The equality is attained if and only if T is chemical tree in which  $\frac{n-1}{3} - 1$  vertices have degree 4, one vertex has degree 3, remaining vertices are pendant and two of the first neighbors of its single vertex with degree 3 has degree 4 but the third one is pendant.

#### REFERENCES

- [1] B. Borovićanin, K.C. Das, B. Furtula, I. Gutman, "Zagreb indices: Bounds and extremal graphs", *MATCH Commun. Math. Comput. Chem.*, **78**, 67-153 (2017).
- [2] R. Cruz, J. Monsalve, J. Rada, "Extremal values of vertex-degree-based topological indices of chemical trees", App. Math and Comp., 380(C), 125281 (2020).
- [3] R. Cruz, I. Gutman, J. Rada, "Sombor index of chemical graphs", Appl. Math. Comput. 399, 126018 (2021).
- [4] K.C. Das, "Maximizing the sum of the squares of the degrees of a graph", *Discrete Math.*, 285, 57-66 (2004).
- [5] K.C. Das, K. Xu, I. Gutman, "On Zagreb and Harary indices", MATCH Commun. Math. Comput. Chem, 70, 301-314 (2013).
- [6] B. Furtula, A. Graovac, D. Vukičević, "Atom-bond connectivity index of trees", *Discret. Appl. Math.* 157, 2828-2835 (2009)
- [7] I. Gutman, O. Miljković, G. Caporossi, P. Hansen, "Alkanes with small and large Randić connectivity indices", *Chem. Phys. Lett.* **306**, 366-372 (1999).
- [8] I. Gutman, "Geometric Aproach to Degree-Based Topologocal Indices: Sombor Idices", MATCH Commun. Math. Comput. Chem, 86, 11-16 (2021).
- [9] I. Gutman, K.C. Das, "The first Zagreb index 30 years after", MATCH Commun. Math. Comput. Chem, 50, 83-92 (2004).
- [10] Ž. Kovijanić Vukićević, G. Popivoda, "Chemical Trees with Extreme Values of Zagreb Indices and Coindices", *Iranial Journa of Math. Chem.*, 5, 19-29 (2014).
- [11] V. R. Kulli, Graph indices, in:M. Pal, S. Samanta, A. Pal (Eds.), *Handbook of Research of Advanced Applications of Graph Theory in Modern Society*, Global, Hershey, 66-91.
- [12] I. Redzepovic, "Chemical applicability of Sombor indices", J. Serb. Chem. Soc., https://doi.org/10.2298/JSC201215006R
- [13] R. Todeschini, V. Consonni, Molecular Descriptors for Chemoinformatics, Wiley-VCH, Weinheim, (2009).
- [14] K. Xu, Y. Alizadeh, K.C.Das, "On two eccentricity-based topological indices of graphs", *Discrete Appl. Math.*, 233, 240–251 (2017).

- [15] K. Xu, K.C. Das, H. Liu, "Some extremal results on the connective eccentricity index of graphs", *J. Math. Anal. Appl.*, **433**, 803-817 (2016).
- [16] B. Zhou, N. Trinajstić, "On a novel connectivity index", J. Math. Chem. 46 1252-1270 (2009).

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## COMPLEX NUMBERS SIMILAR TO THE GENERALIZED BERNOULLI NUMBERS AND THEIR APPLICATIONS BRAHIM MITTOU<sup>1\*</sup> and ABDALLAH DERBAL<sup>2</sup>

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Summary. Let  $\chi$  be a primitive Dirichlet character modulo  $k \ge 3$ . In this paper, we define complex numbers associated with  $\chi$ , which we denote by  $C_r(\chi)(r = 0, 1, ...)$ , and we discuss their properties and their relationships with the generalized Bernoulli numbers.

#### **1. INTRODUCTION**

Let  $\chi$  be a Dirichlet character modulo  $k \ge 3$ . Then the classical generalized Bernoulli numbers  $B_m(\chi)$  for (m = 0, 1, ...) are defined by:

$$\sum_{l=1}^{k} \chi(l) \frac{z e^{lz}}{e^{kz} - 1} = \sum_{m=0}^{+\infty} B_m(\chi) \frac{z^m}{m!}, \qquad |z| < \frac{2\pi}{k}$$

They can be expressed in terms of Bernoulli polynomials as (see [2, formula (4.1)]):

$$B_m(\chi) = k^{m-1} \sum_{l=1}^{\kappa} \chi(l) B_m\left(\frac{l}{k}\right),$$

where the Bernoulli polynomials  $B_m(x)$  are defined by:

$$\frac{ze^{xz}}{e^z - 1} = \sum_{m=0}^{+\infty} B_m(x) \frac{z^m}{m!}, \qquad |z| < 2\pi.$$

The Dirichlet L-function corresponding to  $\chi$  is defined by:

$$L(s,\chi) = \sum_{n=1}^{+\infty} \frac{\chi(n)}{n^s}, \qquad \Re(s) > 1.$$

Now, let  $\chi$  be a primitive character. It is well known [2, Theorem 9.10] that the values of  $L(s, \chi)$  at s = -n, (n = 0, 1, ...) can be expressed by the generalized Bernoulli numbers as:

$$L(-n,\chi) = -\frac{B_{n+1}(\chi)}{n+1}.$$
 (1.1)

Also from [2, Theorem 9.6] if  $\chi(-1) = (-1)^n (n = 1, 2, ...)$ , then the special values of  $L(s, \chi)$  at s = n are given by:

$$L(n,\chi) = (-1)^{n-1} \frac{\tau(\chi)}{2n!} \left(\frac{2\pi i}{k}\right)^n B_n(\bar{\chi}),$$
(1.2)

where  $\tau(\chi) = \sum_{a=1}^{k} \chi(a) e^{\frac{2\pi i a}{k}}$  is the Gaussian sum associated with  $\chi$ .

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Key words and Phrases: Dirichlet L-function, Primitive character, Generalized Bernoulli number, Fourier series expansion.

In this paper, based on a definition given by Davies and Haselgrove in [4], we rewrite the formulas (1.1) and (1.2) in terms of the numbers  $C_r(\chi)$ . We also give some results, properties and applications of these numbers, and their relationship with the generalized Bernoulli numbers.

#### 2. DEFINITION AND LEMMAS

In order to prove our main results, we give the following definition and we need the later lemmas.

**Definition 2.1** Let  $\chi$  be a non-principal character modulo  $k \ge 3$ . For an integer  $r \ge 0$  we define the function  $p_r(x, \chi)$  for  $x \in \mathbb{R}_+$  as follows:

$$p_{0}(x,\chi) = S(x,\chi) + C_{0}(\chi), \text{ where } S(x,\chi) = \sum_{n \le x} \chi(n),$$

$$p_{r+1}(x,\chi) = \int_{0}^{x} p_{r}(t,\chi) dt + C_{r+1}(\chi),$$

$$\int_{0}^{k} p_{r}(x,\chi) dx = 0.$$
(2.1)

**Lemma 2.2** Let  $\chi$  be a non-principal character modulo  $k \ge 3$ . Then

- 1. The function  $S(x, \chi)$  is k-periodic.
- 2. For any function f defined from [0, k) to C which has an antiderivative g we have

$$\int_{0}^{k} S(t,\chi) f(t) dt = -\sum_{m=1}^{k-1} g(m) \chi(m)$$

3. If  $\chi$  is primitive, then the Fourier series expansion of  $S(x, \chi)$  is given by:

$$S(x,\chi) = \frac{1}{k} \sum_{m=1}^{k-1} m \chi(m) + \frac{E(\chi)}{\pi} \sum_{n=1}^{+\infty} \frac{\overline{\chi}(n)}{n} \sin\left(\frac{2n\pi x}{k}\right) \text{ if } \chi(-1) = +1,$$

$$S(x,\chi) = \frac{1}{k} \sum_{m=1}^{k-1} m \chi(m) - \frac{E(\chi)}{\pi} \sum_{n=1}^{+\infty} \frac{\overline{\chi}(n)}{n} \cos\left(\frac{2n\pi x}{k}\right) \text{ if } \chi(-1) = -1,$$
(2.2)

where

$$E(\chi) = \sum_{m=1}^{k} \chi(m) \frac{\cos\left(\frac{2m\pi}{k}\right)}{\sin\left(\frac{2m\pi}{k}\right)} \text{ if } \chi(-1) = \pm 1.$$

**Proof.** 1. For any integer *N*, we have

$$S(x+Nk,\chi) = \sum_{n \leq x+Nk} \chi(n) = \sum_{n \leq x} \chi(n+Nk) = \sum_{n \leq x} \chi(n) = S(x,\chi),$$

so  $S(x, \chi)$  is k-periodic.

2. This follows at once from the integration by parts and the fact that  $\sum_{m=1}^{k-1} \chi(m) = 0$  (see e.g. [1, p. 30]).

3. The Fourier series expansion of  $S(x, \chi)$  is given by:

$$a_0 + \sum_{n=1}^{+\infty} \left( a_n \cos\left(\frac{2n\pi x}{k}\right) + b_n \sin\left(\frac{2n\pi x}{k}\right) \right),$$

where

$$a_{0} = \frac{1}{k} \int_{0}^{k} S(t,\chi) dt = \frac{-1}{k} \sum_{m=1}^{k-1} m\chi(m),$$

$$a_{n} = \frac{2}{k} \int_{0}^{k} S(t,\chi) \cos\left(\frac{2n\pi t}{k}\right) dt = \frac{-1}{n\pi} \sum_{m=1}^{k-1} \chi(m) \sin\left(\frac{2m\pi x}{k}\right) \text{ for } n \ge 1,$$

$$b_{n} = \frac{2}{k} \int_{0}^{k} S(t,\chi) \sin\left(\frac{2n\pi t}{k}\right) dt = \frac{1}{n\pi} \sum_{m=1}^{k-1} \chi(m) \cos\left(\frac{2m\pi x}{k}\right) \text{ for } n \ge 1.$$

$$a_{n} = \frac{1}{k} \sum_{k=1}^{k} \int_{0}^{k} S(t,\chi) \sin\left(\frac{2n\pi t}{k}\right) dt = \frac{1}{n\pi} \sum_{m=1}^{k-1} \chi(m) \cos\left(\frac{2m\pi x}{k}\right) \text{ for } n \ge 1.$$

If  $\chi(-1) = +1$ , we put  $\theta = \frac{2n\pi}{k}$  and we show that  $a_n = 0$  for  $n \ge 1$ . Indeed

$$a_n = \frac{-1}{n\pi} \sum_{m=1}^{k-1} \chi(m) \sin(m\theta) = \frac{-1}{n\pi} \sum_{\substack{m=1\\k-1}}^{k-1} \chi(k-m) \sin((k-m)\theta)$$
$$= \frac{1}{n\pi} \sum_{m=1}^{k-1} \chi(m) \sin(m\theta) = -a_n.$$

Also  $a_0 = 0$ , since

$$\sum_{m=1}^{k-1} m\chi(m) = \sum_{m=1}^{k-1} (k-m)\chi(k-m) = k \sum_{m=1}^{k-1} \chi(m) - \sum_{m=1}^{k-1} m\chi(m) = -\sum_{m=1}^{k-1} m\chi(m).$$
  
If  $\chi(-1) = -1$ , we show by the same way that  $b_n = 0$  for  $n \ge 1$ .

According to [1, Theorem 8.15] we have

$$\bar{\chi}(n)E(\chi) = \sum_{m=1}^{k} \chi(m) \frac{\cos\left(\frac{2mn\pi}{k}\right)}{\sin\left(\frac{2mn\pi}{k}\right)} \text{ if } \chi(-1) = \pm 1,$$

from which we can write for  $n \ge 1$ :

$$b_n = \frac{1}{n\pi} \times E(\chi)\overline{\chi}(n)$$
 if  $\chi(-1) = +1$ , and  $a_n = \frac{-1}{n\pi} \times E(\chi)\overline{\chi}(n)$  if  $\chi(-1) = -1$ .  
s completes the proof.

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**Lemma 2.3** Let  $\chi$  be a primitive character modulo  $k \ge 3$ . Then

- 1. For  $r \ge 1$ , the function  $p_r(x, \chi)$  is continuous and *k*-periodic.
- 2. The Fourier series expansion of  $p_r(x, \chi)$  is given by:

$$p_0(x,\chi) = \pm \frac{E(\chi)}{\pi} \sum_{n=1}^{+\infty} \frac{\bar{\chi}(n)}{n} \frac{\sin\left(\frac{2n\pi x}{k}\right)}{\cos\left(\frac{2n\pi x}{k}\right)} \text{ if } \chi(-1) = \pm 1.$$
(2.3)

For  $r \ge 1$  and  $\chi(-1) = +1$ , we have

$$p_{2r-1}(x,\chi) = (-1)^r \frac{E(\chi)}{\pi} \left(\frac{k}{2\pi}\right)^{2r-1} \sum_{n=1}^{+\infty} \frac{\bar{\chi}(n)}{n^{2r}} \cos\left(\frac{2n\pi x}{k}\right),$$

$$p_{2r}(x,\chi) = (-1)^r \frac{E(\chi)}{\pi} \left(\frac{k}{2\pi}\right)^{2r} \sum_{n=1}^{+\infty} \frac{\bar{\chi}(n)}{n^{2r+1}} \sin\left(\frac{2n\pi x}{k}\right).$$
(2.4)

For  $r \ge 1$  and  $\chi(-1) = -1$ , we have

$$p_{2r-1}(x,\chi) = (-1)^r \frac{E(\chi)}{\pi} \left(\frac{k}{2\pi}\right)^{2r-1} \sum_{n=1}^{+\infty} \frac{\bar{\chi}(n)}{n^{2r}} \sin\left(\frac{2n\pi x}{k}\right),$$

$$p_{2r}(x,\chi) = (-1)^{r+1} \frac{E(\chi)}{\pi} \left(\frac{k}{2\pi}\right)^{2r} \sum_{n=1}^{+\infty} \frac{\bar{\chi}(n)}{n^{2r+1}} \cos\left(\frac{2n\pi x}{k}\right).$$
(2.5)

**Proof.** 1. It is clear that, for  $r \ge 1$  the function  $p_r(x, \chi)$  is continuous, since it is the primitive of piece-wise continuous function. The properties of the Dirichlet characters and formulas (2.1) allow us to show by induction that, for any  $N \in \mathbb{Z}$  and  $r \in \mathbb{N}$ :

$$\int_{Nk}^{(N+1)k} p_r(x,\chi) dx = 0, \text{ and } p_r(x+Nk,\chi) = p_r(x,\chi),$$

from which the periodicity of  $p_r(x, \chi)$  follows.

2. The formulas (2.3), (2.4) and (2.5) are obtained by successive integrations of (2.2), taking into consideration the formulas (2.1). The lemma is proved.

#### **3. MAIN RESULTS**

In this section we give our main results. Let us start by the explicit formulas for the numbers  $C_r(\chi)$ .

**Theorem 3.1** Let  $\chi$  be a primitive character modulo  $k \ge 3$ . Then the numbers  $C_r(\chi)$  are explicit as follows:

If 
$$\chi(-1) = +1$$
,

$$C_1(\chi) = \frac{-1}{2k} \sum_{m=1}^{k-1} m^2 \chi(m), \quad C_{2r}(\chi) = 0 \ (r \ge 0),$$

$$C_{2r-1}(\chi) = -\sum_{m=1}^{r-1} \frac{k^{2r-2m}}{(2r-2m+1)!} C_{2m-1}(\chi) - \frac{1}{k(2r)!} \sum_{m=1}^{k-1} m^{2r} \chi(m) \ (r \ge 2).$$
(3.1)

If  $\chi(-1) = -1$ ,

$$C_{0}(\chi) = \frac{1}{k} \sum_{m=1}^{k-1} m\chi(m), \quad C_{2r-1}(\chi) = 0 \ (r \ge 1),$$

$$C_{2r}(\chi) = -\sum_{m=0}^{r-1} \frac{k^{2r-2m}}{(2r-2m+1)!} C_{2m}(\chi) + \frac{1}{k(2r+1)!} \sum_{m=1}^{k-1} m^{2r+1}\chi(m) \ (r \ge 1).$$
(3.2)

**Proof.** The first formula of (2.4) and the last formula of (2.5) show that for  $r \ge 1$ :

 $C_{2r}(\chi) = p_{2r}(0,\chi) = 0$  if  $\chi(-1) = +1$ , and  $C_{2r-1}(\chi) = p_{2r-1}(0,\chi) = 0$  if  $\chi(-1) = -1$ . According to the last formula of (2.1), we have

$$C_0(\chi) = \frac{1}{k} \sum_{m=1}^{k-1} m\chi(m)$$
, and  $C_1(\chi) = \frac{k}{2} C_0(\chi) - \frac{1}{2k} \sum_{m=1}^{k-1} m^2 \chi(m)$ .

Also for  $\alpha \geq 2$ ,

$$C_{\alpha}(\chi) = \frac{1}{k} \int_0^k x p_{\alpha-1}(x,\chi) dx.$$

Integration by parts  $\alpha - 1$  times gives us

$$C_{\alpha}(\chi) = \left(\sum_{m=2}^{\alpha} \frac{(-1)^m k^m}{m!} C_{\alpha-m+1}(\chi) + \frac{(-1)^{\alpha+1}}{\alpha!} \int_0^k x^{\alpha} p_0(x,\chi) dx\right).$$

But

$$\int_{0}^{k} x^{\alpha} p_{0}(x,\chi) dx = C_{\alpha}(\chi) \frac{k^{\alpha+1}}{\alpha+1} - \frac{1}{\alpha+1} \sum_{m=1}^{k-1} m^{\alpha+1} \chi(m),$$

from which we find

$$C_{\alpha}(\chi) = \sum_{m=2}^{\alpha+1} \frac{(-1)^m k^{m-1}}{m!} C_{\alpha-m+1}(\chi) + \frac{(-1)^{\alpha}}{k(\alpha+1)!} \sum_{m=1}^{k-1} m^{\alpha+1} \chi(m).$$
(3.3)

If  $\chi(-1) = +1$ , to obtain the formulas (3.1), we simply take  $\alpha = 2r - 1$  with  $(r \ge 2)$  in (3.3), taking into consideration that  $C_{2r}(\chi) = 0$ .

If  $\chi(-1) = -1$ , to obtain the formulas (3.2), we simply take  $\alpha = 2r$  with  $(r \ge 1)$  in (3.3), taking into consideration that  $C_{2r-1}(\chi) = 0$ . The theorem is proved.

**Corollary 3.2** For any primitive character  $\chi$  modulo  $k \ge 3$ , we have  $C_r(\overline{\chi}) = \overline{C_r(\chi)}$  for  $(r \ge 0)$ .

**Proof.** The result follows directly by using induction on *r*.

**Example 3.3** 1. Let  $\chi_3$  and  $\chi_4$  be the non-principal Dirichlet characters modulo 3 and 4, respectively. Then we have  $C_{2r+1}(\chi_3) = C_{2r+1}(\chi_4) = 0$  ( $r \ge 0$ ), since  $\chi_3$  and  $\chi_4$  are odd characters. Also, it follows by using Theorem 3.1 the following table:

	<i>C</i> <sub>0</sub>	<i>C</i> <sub>2</sub>	<i>C</i> <sub>4</sub>	<i>C</i> <sub>6</sub>	<i>C</i> <sub>8</sub>	<i>C</i> <sub>10</sub>	<i>C</i> <sub>12</sub>
<i>Х</i> з	$-\frac{1}{3}$	$\frac{1}{9}$	$-\frac{1}{36}$	7 1080	$-\frac{809}{544320}$	1847 5443200	$-\frac{7943}{102643200}$
<b>X</b> 4	$-\frac{1}{2}$	$\frac{1}{4}$	$-\frac{5}{48}$	$\frac{61}{1440}$	$-\frac{277}{16128}$	50521 7257600	$-\frac{540553}{19160040}$

Table 1. The first values of  $C_r$  (r = 0, 2, ..., 12) for  $\chi_3$  and  $\chi_4$ .

2. Let  $\chi_{1,5}$ ,  $\chi_{2,5}$ , and  $\chi_{3,5}$  be the Dirichlet character modulo 5 such that  $\chi_{1,5}(2) = -1$ ,  $\chi_{2,5}(2) = i$ , and  $\chi_{3,5} = \overline{\chi_{2,5}}$ . Then we have  $C_{2r}(\chi_{1,5}) = 0$   $(r \ge 0)$ , since  $\chi_{1,5}$  is even character. Also, by using Theorem 3.1 we obtain the following:

	<i>C</i> <sub>1</sub>	<i>C</i> <sub>3</sub>	<i>C</i> <sub>5</sub>	<i>C</i> <sub>7</sub>	C <sub>9</sub>	<i>C</i> <sub>11</sub>	<i>C</i> <sub>13</sub>
X1,5	$-\frac{2}{5}$	$\frac{1}{3}$	$-\frac{67}{300}$	$\frac{361}{2520}$	$-\frac{412751}{4536000}$	1150921 19958400	$\frac{568591843}{15567552000}$

Table 2. The first values of  $C_r$  (r = 1, 3, ..., 13) for  $\chi_{1.5}$ .

On the other hand, since  $\chi_{2,5}$  and  $\chi_{3,5}$  are odd, we have  $C_{2r+1}(\chi_{2,5}) = C_{2r+1}(\chi_{3,5}) = 0$  ( $r \ge 0$ ). Finally, Theorem 3.1 and Corollary 3.2 allow us to get

	<i>C</i> <sub>0</sub>	<i>C</i> <sub>2</sub>	$C_4$	<i>C</i> <sub>6</sub>	<i>C</i> <sub>8</sub>	<i>C</i> <sub>10</sub>
X <sub>2,5</sub> X <sub>3,5</sub>	$-\frac{3}{5}+\frac{1}{5}i$	$\frac{2}{5}\pm\frac{1}{5}i$	$-\frac{37}{150}+\frac{43}{300}i$	$\frac{139}{900} \pm \frac{169}{1800}i$	$-\frac{4913}{50400}\mp\frac{6047}{100800}i$	$\frac{279763}{4536000} \pm \frac{345433}{9072000}i$

Table 3. The first values of  $C_r$  (r = 0, 2, ..., 10) for  $\chi_{2,5}$  and  $\chi_{3,5}$ .

**Theorem 3.4** Let  $\chi$  be a primitive character modulo  $k \ge 3$ . Then for all  $x \in \mathbb{R}_+$  we have 1. If  $\chi(-1) = +1$  and  $r \ge 1$ :

$$|p_{2r-1}(x,\chi)| \le |\mathcal{C}_{2r-1}(\chi)|$$

2. If  $\chi(-1) = -1$  and  $r \ge 0$ :

$$|p_{2r}(x,\chi)| \le |\mathcal{C}_{2r}(\chi)|.$$

**Proof.** 1. Let  $\chi(-1) = +1$ ,  $r \ge 1$  and  $x \in \mathbb{R}_+$ . Then from the first formula of (2.4) we have

$$|p_{2r-1}(x,\chi)| = \frac{|E(\chi)|}{\pi} \left(\frac{k}{2\pi}\right)^{2r-1} \left| \sum_{n=1}^{+\infty} \frac{\bar{\chi}(n)}{n^{2r}} \cos\left(\frac{2n\pi x}{k}\right) \right|.$$

If we put  $\bar{\chi}(n) = a(n) + ib(n)$  for  $(n \ge 1)$ , then we get

$$\sum_{n=1}^{+\infty} \frac{\bar{\chi}(n)}{n^{2r}} \cos\left(\frac{2n\pi x}{k}\right) = f(x) + ig(x),$$

where

$$f(x) = \sum_{n=1}^{+\infty} \frac{a(n)}{n^{2r}} \cos\left(\frac{2n\pi x}{k}\right), \text{ and } g(x) = \sum_{n=1}^{+\infty} \frac{b(n)}{n^{2r}} \cos\left(\frac{2n\pi x}{k}\right),$$

from which we can write

$$|p_{2r-1}(x,\chi)| = \frac{|E(\chi)|}{\pi} \left(\frac{k}{2\pi}\right)^{2r-1} \sqrt{\left(f(x)\right)^2 + \left(g(x)\right)^2}.$$

On the other hand we have

$$\begin{aligned} |p_{2r-1}(0,\chi)| &= \frac{|E(\chi)|}{\pi} \left(\frac{k}{2\pi}\right)^{2r-1} \left|\sum_{n=1}^{+\infty} \frac{\bar{\chi}(n)}{n^{2r}}\right| = \frac{|E(\chi)|}{\pi} \left(\frac{k}{2\pi}\right)^{2r-1} \left|\sum_{n=1}^{+\infty} \frac{a(n)}{n^{2r}} + i\sum_{n=1}^{+\infty} \frac{b(n)}{n^{2r}}\right| \\ &= \frac{|E(\chi)|}{\pi} \left(\frac{k}{2\pi}\right)^{2r-1} \sqrt{\left(\sum_{n=1}^{+\infty} \frac{a(n)}{n^{2r}}\right)^2 + \left(\sum_{n=1}^{+\infty} \frac{b(n)}{n^{2r}}\right)^2}.\end{aligned}$$

Now, we wish to prove that

$$(f(x))^2 \le \left(\sum_{n=1}^{+\infty} \frac{a(n)}{n^{2r}}\right)^2$$
, and  $(g(x))^2 \le \left(\sum_{n=1}^{+\infty} \frac{b(n)}{n^{2r}}\right)^2$ .

Let  $X = \sum_{n=1}^{+\infty} \frac{a(n)}{n^{2r}}$ . Then  $(f(x))^2 - X^2 = (f(x) - X)(f(x) + X)$ , so that

$$f(x) - X = \sum_{n=1}^{+\infty} \left( \frac{a(n)}{n^{2r}} \left( \cos\left(\frac{2n\pi x}{k}\right) - 1 \right) \right), f(x) + X = \sum_{n=1}^{+\infty} \left( \frac{a(n)}{n^{2r}} \left( \cos\left(\frac{2n\pi x}{k}\right) + 1 \right) \right)$$

which are absolutely convergent series, i.e.

$$(f(x))^2 - X^2 = \sum_{n=1}^{+\infty} \left\{ \left( \frac{a(n)}{n^{2r}} \right)^2 \left( \cos^2 \left( \frac{2n\pi x}{k} \right) - 1 \right) \right\} \le 0.$$

By the same, we can show that  $(g(x))^2 \le (\sum_{n=1}^{+\infty} \frac{b(n)}{n^{2r}})^2$ . Thus  $|p_{2r-1}(x,\chi)| \le |p_{2r-1}(0,\chi)| = |C_{2r-1}(\chi)|.$  2. Let  $\chi(-1) = -1$  and  $r \ge 0$ . Then by the same reasoning as above we get the second formula.

Now, let us rewrite the formula (1.2) by using the numbers  $C_r(\chi)$ .

**Theorem 3.5** Let  $\chi$  be a primitive character modulo  $k \ge 3$ .

1. If  $\chi(-1) = +1$  and  $r \ge 1$  then:

$$L(2r, \bar{\chi}) = (-1)^r \frac{\pi}{E(\chi)} \left(\frac{2\pi}{k}\right)^{2r-1} C_{2r-1}(\chi).$$

2. If  $\chi(-1) = -1$  and  $r \ge 0$  then:

$$L(2r+1,\bar{\chi}) = (-1)^{r+1} \frac{\pi}{E(\chi)} \left(\frac{2\pi}{k}\right)^{2r} C_{2r}(\chi).$$

**Proof.** This follows directly by taking x = 0 in the first formula of (2.4) and x = 0 in the last formula of (2.5), taking into consideration that  $p_r(0, \chi) = C_r(\chi)$ .

The following corollary gives the relationship between the numbers  $C_{r-1}(\chi)$  and the generalized Bernoulli numbers  $B_r(\chi)$ .

**Corollary 3.6** Let  $\chi$  be a primitive character modulo  $k \ge 3$ .

1. If  $\chi(-1) = +1$  and  $r \ge 1$  then:

$$C_{2r-1}(\chi) = \frac{-1}{(2r)!} B_{2r}(\chi).$$

2. If  $\chi(-1) = -1$  and  $r \ge 0$  then:

$$C_{2r}(\chi) = \frac{1}{(2r+1)!} B_{2r+1}(\chi).$$

**Proof.** This follows directly from Theorem 3.5 and the formula (1.2).

The above corollary allows us to rewrite the formula (1.1) as:

**Corollary 3.7** Let  $\chi$  be a primitive character modulo  $k \ge 3$ .

1. If  $\chi(-1) = +1$  and  $r \ge 0$  then:

$$L(-(2r+1),\chi) = (2r+1)! C_{2r+1}(\chi).$$

2. If  $\chi(-1) = -1$  and  $r \ge 0$  then:

$$L(-2r, \chi) = -(2r)! C_{2r}(\chi).$$

As an application, the following theorem gives explicit formulas for sums related to the generalized Bernoulli numbers.

**Theorem 3.8** Let  $\chi$  be a primitive character modulo  $k \ge 3$ .

1. If  $\chi(-1) = +1$  and  $r \ge 1$  then:

$$\sum_{m=1}^{r} \frac{k^{2r-2m}}{2r-2m+1} {2r \choose 2m} B_{2m}(\chi) = \frac{1}{k} \sum_{m=1}^{k} m^{2r} \chi(m).$$

2. If  $\chi(-1) = -1$  and  $r \ge 0$  then:

$$\sum_{m=0}^{r} \frac{k^{2r-2m}}{2r-2m+1} {2r+1 \choose 2m+1} B_{2m+1}(\chi) = \frac{1}{k} \sum_{m=1}^{k} m^{2r+1} \chi(m),$$

**Proof.** 1. Let  $\chi(-1) = +1$  and  $r \ge 1$ . Then from the formulas (3.1) we have

$$C_{2r-1}(\chi) = -\sum_{m=1}^{r-1} \frac{k^{2r-2m}}{(2r-2m+1)!} C_{2m-1}(\chi) - \frac{1}{k(2r)!} \sum_{m=1}^{k-1} m^{2r} \chi(m).$$

The Corollary 3.6 allows us to write

$$B_{2r}(\chi) = -\sum_{m=1}^{r-1} \frac{k^{2r-2m}(2r)!}{(2m)!(2r-2m+1)!} B_{2m}(\chi) + \frac{1}{k} \sum_{m=1}^{k-1} m^{2r} \chi(m),$$

SO

$$B_{2r}(\chi) + \sum_{m=1}^{r-1} \frac{k^{2r-2m}}{(2r-2m+1)} \frac{(2r)!}{(2m)!(2r-2m)!} B_{2m}(\chi) = \frac{1}{k} \sum_{m=1}^{k-1} m^{2r} \chi(m),$$

from which

$$\sum_{m=1}^{r} \frac{k^{2r-2m}}{2r-2m+1} {2r \choose 2m} B_{2m}(\chi) = \frac{1}{k} \sum_{m=1}^{k} m^{2r} \chi(m).$$

2. Let  $\chi(-1) = -1$  and  $r \ge 0$ . Then similarly we get the second formula. This proves the theorem.

As another application, the following theorem gives asymptotic formulas for  $L(s, \chi)$  in terms of the generalized Bernoulli numbers.

**Theorem 3.9** Let  $\chi$  be a primitive character modulo  $k \ge 3$  and let  $L(s, \chi)$  be the Dirichlet *L*-function corresponding to  $\chi$ . Let *N* and *r* be positive integers such that  $\Re(s) = \sigma > 1 - 2r$  if  $\chi(-1) = +1$  and  $\sigma > -2r$  if  $\chi(-1) = -1$ . Then

$$L(s,\chi) = \sum_{n=1}^{kN} \frac{\chi(n)}{n^s} + \sum_{m=1}^r \frac{B_{2m}(\chi)}{(2m)!} \prod_{j=0}^{2m-2} \left(\frac{s+j}{(kN)^{s+1}}\right) + R_1(s) \text{ if } \chi(-1) = +1, \quad (3.4)$$

$$L(s,\chi) = \sum_{n=1}^{kN} \frac{\chi(n)}{n^s} - s \frac{B_1(\chi)}{(kN)^s} - \sum_{m=1}^r \frac{B_{2m+1}(\chi)}{(2m+1)!} \prod_{j=0}^{2m-1} \left(\frac{s+j}{(kN)^{s+1}}\right) + R_2(s) \text{ if } \chi(-1) = -1,$$
(3.5)

where

$$|R_1(s)| \le |T_{2r-1}(\chi)| \times \frac{|s+2r-1|}{\sigma+2r-1}$$
, and  $|R_2(s)| \le |T_{2r}(\chi)| \times \frac{|s+2r|}{\sigma+2r}$ 

with

$$T_{2r-1}(\chi) = C_{2r-1}(\chi) \frac{s(s+1)\cdots(s+2r-2)}{(kN)^{s+2r-1}}, \ T_{2r}(\chi) = C_{2r}(\chi) \frac{s(s+1)\cdots(s+2r-1)}{(kN)^{s+2r}}$$

Proof. First of all we can write

$$L(s,\chi) = \sum_{n=1}^{kN} \frac{\chi(n)}{n^s} + \sum_{n>kN}^{+\infty} \frac{\chi(n)}{n^s}.$$

It follows by using [5, Theorem 1.3] that:  $+\infty$ 

$$\sum_{n>kN}^{+\infty} \frac{\chi(n)}{n^s} = s \int_{kN}^{+\infty} \frac{S(t,\chi)}{t^{s+1}} dt = -s \frac{C_0(\chi)}{(kN)^s} + s \int_{kN}^{+\infty} \frac{p_0(t,\chi)}{t^{s+1}} dt.$$
(3.6)

If  $\chi(-1) = +1$ , then  $C_{2r}(\chi) = 0 (r \ge 0)$ . Integrating by parts 2r - 1 times the integral in the right hand side of (3.6), taking into consideration that  $p_r(kN,\chi) = C_r(\chi)$ , we obtain:

$$L(s,\chi) = \sum_{n=1}^{kN} \frac{\chi(n)}{n^s} - C_1(\chi) \frac{s}{(kN)^{s+1}} - C_3(\chi) \frac{s(s+1)(s+2)}{(kN)^{s+3}} - \cdots - C_{2r-1}(\chi) \frac{s(s+1)(s+2)\cdots(s+2r-2)}{(kN)^{s+2r-1}} + s(s+1)(s+2)\cdots(s+2r-1) \int_{kN}^{+\infty} \frac{p_{2r-1}(t,\chi)}{t^{s+2r}} dt.$$
(3.7)

Now Corollary 3.6 and the formula (3.7) imply the formula (3.4) with:

$$R_1(s) = s(s+1)(s+2)\cdots(s+2r-1)\int_{kN}^{+\infty} \frac{p_{2r-1}(t,\chi)}{t^{s+2r}}dt$$

According to Theorem 3.4, we have

$$R_{1}(s) \leq |s(s+1)(s+2)\cdots(s+2r-1)| \times |\mathcal{C}_{2r-1}(\chi)| \left| \int_{kN}^{+\infty} \frac{1}{t^{s+2r}} dt \right|$$
$$= \left| \frac{s(s+1)(s+2)\cdots(s+2r-1)\mathcal{C}_{2r-1}(\chi)}{(kN)^{s+2r-1}} \right| \frac{|s+2r-1|}{\sigma+2r-1}$$

$$= |T_{2r-1}(\chi)| \times \frac{|s+2r-1|}{\sigma+2r-1}$$

If  $\chi(-1) = -1$ , then  $C_{2r-1}(\chi) = 0$  ( $r \ge 1$ ). Integrating by parts 2r times the integral in the right hand side of (3.6), taking into consideration that  $p_r(kN, \chi) = C_r(\chi)$ , we obtain:

$$L(s,\chi) = \sum_{n=1}^{kN} \frac{\chi(n)}{n^s} - C_0(\chi) \frac{s}{(kN)^{s+1}} - C_2(\chi) \frac{s(s+1)}{(kN)^{s+2}} - \dots - C_{2r}(\chi) \frac{s(s+1)(s+2)\cdots(s+2r)}{(kN)^{s+2r}} + s(s+1)(s+2)\cdots(s+2r) \int_{kN}^{+\infty} \frac{p_{2r}(t,\chi)}{t^{s+2r+1}} dt.$$
(3.8)

Now Corollary 3.6 and the formula (3.8) imply the formula (3.5) with:

$$R_2(s) = s(s+1)(s+2)\cdots(s+2r)\int_{kN}^{+\infty} \frac{p_{2r}(t,\chi)}{t^{s+2r+1}}dt$$

According to Theorem 3.4, we have

$$\begin{split} R_{2}(s) &\leq |s(s+1)(s+2)\cdots(s+2r)| \times |\mathcal{C}_{2r}(\chi)| \left| \int_{kN}^{+\infty} \frac{1}{t^{s+2r+1}} dt \right| \\ &= \left| \frac{s(s+1)(s+2)\cdots(s+2r-1)\mathcal{C}_{2r}(\chi)}{(kN)^{s+2r}} \right| \frac{|s+2r|}{\sigma+2r} \\ &= |T_{2r}(\chi)| \times \frac{|s+2r|}{\sigma+2r}. \end{split}$$

This completes the proof.

**Remark 3.10** From [3, p.37] we have

$$L(s,\chi) = \prod_{p|k} \left(1 - \frac{\chi^*(p)}{p^s}\right) L(s,\chi^*),$$

where  $\chi^*$  is the unique primitive character which induces  $\chi$ . Thus  $L(s, \chi)$  can be expressed in terms of  $L(s, \chi^*)$ , so one can use this fact to generalize above theorem to an arbitrary character  $\chi$ .

**Remark 3.11** One can use the first formula of (2.4) and the last formula of (2.5) to get another upper bound of  $R_1(s)$  and of  $R_2(s)$  as follows:

$$R_1(s) \le \frac{2|s|\sqrt{k}\zeta(2r)}{(2r+\sigma-1)(2\pi)^{2r}(kN)^{\sigma}} \prod_{j=1}^{2r-1} \left(\frac{|s+j|}{N}\right),$$

and

$$R_{2}(s) \leq \frac{2|s|\sqrt{k}\zeta(2r+1)}{(2r+\sigma)(2\pi)^{2r+1}(kN)^{\sigma}} \prod_{j=1}^{2r} \left(\frac{|s+j|}{N}\right).$$

#### **3. CONCLUSION**

In this paper, we define complex numbers associated with a primitive Dirichlet character  $\chi$ , and we use them to rewrite some known results as formulas (1.1) and (1.2). Also, we use them to give explicit formulas for sums related to the generalized Bernoulli numbers, as shown by the Theorem 3.8, and to give asymptotic formulas for  $L(s,\chi)$  in terms of the generalized Bernoulli numbers, as shown by the Theorem 3.9.

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### REFERENCES

- [1] T. M. Apostol, Introduction to Analytic Number Theory, Springer-Verlage, New York (1976).
- [2] T. Arakawa, T. Ibukiyama, and M. Kaneko, *Bernoulli Numbers and Zeta Functions*, Springer Japan (2014).
- [3] H. Davenport, *Multiplicative Number Theory*, Springer-Verlage, New York (1980).
- [4] D. Davies and C.B. Haselgrove, "Evaluation of Dirichlet L-Functions", *Proc. Roy. Soc. Ser.* A, **264**, 122-132 (1961).
- [5] H.L. Montgomery and R.C. Vaghan, *Multiplicative Number Theory I. Classical Theory*, Cambridge University Press (2006).

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## **POWER CONTAMINATION AND DOMINATION ON THE GRID**

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**Summary.** The contamination game of a grid graph G(n,m) is a dynamic variant of the domination, similar to the power domination. This standard is introduced by Haynes, Hedetniemi and Henning in 2002, which is initially defined as a basic domination for a set of vertices *S* in a graph *G*, and then a propagation of this domination in all vertices of *G*, while starting with *S*. On the other hand, the contamination phenomena in G(n,m) is interpreted by an evolutionary automaton cellular, which aims to propagate viruses according to a given propagation rules. In this paper, we define a mathematical self-playing game called a contamination game based on the power domination, in which, we identify the minimum number of contaminant cells for G(n,m), called the contamination number and denoted  $\gamma$  (G(n,m)).

### **1 INTRODUCTION**

Electric power systems need to be monitored in real-time. One way to achieve this task is to place phase measurement units at selected locations in the system. The power system monitoring problem is a combinatorial optimization problem that consists of minimizing the number of measurement devices to be put in an electric power system. The power system monitoring problem has been formulated as a graph theory domination problem by Haynes, Hedetniemi, Hedetniemi, and Henning in [1]. This problem is of somehow different flavor than standard domination type problems, since putting a phase measurement unit into a vertex of a graph can have global effects. For instance, if an electric power system no matter how long is the path.

Let G = (V, E) be a connected graph. For a vertex v of G, let N(v) denote the open neighbor-hood of v, and for a subset  $S \subset V$  let  $N(S) = (\bigcup_{v \in S} N(v)) \setminus S$ . We denote by M(S) the set monitored by S, defined algorithmically as follows [2]:

Algorithm 1 Construction of a monitored set $M(S)$
Input: Graph $G = (V, E)$ and $S \subset V$ .
Output: $M(S)$ the monitored set by $S$ .
1: Initiate $M(S) \leftarrow S \cup N(S)$ ;
2: While there exists $v \in M(S)$ such that $N(v) \cap (V \setminus M(S)) = \{w\}$ do
$3: M(S) \leftarrow M(S) \cup \{w\};$
4: EndWhile;
5: Return <b>M</b> ( <b>S</b> );

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The set **S** is called a power dominating set of **G** if M(S) = V and the power domination number, denoted by  $\gamma_{\pi}(G)$ , is the minimum cardinality of a power dominating set.

Various papers have addressed the power domination number, in which they essentially concentrate on its algorithmic point of view (see [3], [4], [5], [6], [7] and [8]). This problem is proven to be NP-complete even when restricted to bipartite graphs, chordal graphs, planar graphs, circle graphs and split graphs [9]. In contrast, the problem can be solved in polynomial time for trees and interval graphs [10]. Dorfling and Henning obtained closed formulas for the power domination numbers of grid graphs [11]. This result is in striking contrast with the fact that a determination of such formulas for the usual domination number of grid graphs is an open problem [1]. Now, a natural description of a grid is a cartesian product of two paths. However, there exist other graph products such as the strong, the direct, and the lexicographic product [1]. Hence, it is natural to ask whether the power domination number can also be determined for these products of paths.

In this paper we introduce a new variant of domination characterized as a viruscontamination in grid graph G(n, m), which is defined in two steps:

(1) Local domination for a few cells of G(n, m).

(2) Propagation on all cells of G(n, m) according to a given initial contamination rules.

## **2 POWER CONTAMINATION ON THE GRID**

Let G(n, m) = (V, E) be a grid graph, and  $S \subset V$ . The set S is said to be a contaminating set if a full contamination of G(n, m) can be achieved from G(n, m) and the power contamination number  $\gamma_c(G(n, m))$  is the minimum cardinality of a power contaminating set. In the following, we will illustrate the problem as a self-playing game, in order to deal with the problem of contamination in G(n, m).

For a vertex  $\boldsymbol{v}$  of  $\boldsymbol{G}(\boldsymbol{n}, \boldsymbol{m})$ , let  $\boldsymbol{M}(\boldsymbol{v})$  and  $\boldsymbol{VN}(\boldsymbol{v})$  denote, respectively, Moore neighborhood (see Fig.1(a)) and Von Neumann neighborhood (see Fig.1(b)) of  $\boldsymbol{v}$ , extended to the cells at the edge of  $\boldsymbol{G}(\boldsymbol{n}, \boldsymbol{m})$ .



Figure 1: Moore and Von Newmann neighborhoods of the black cell.

#### 2.1 Contamination rules in G(n, m)

The contamination game of G(n, m) can be seen as a cellular automaton, or a model where each state leads automatically to the next state from predefined rules. This game takes place on G(n, m), whose cells are considered by analogy as living cells, which can take two different states "sick" or "healthy". At each step, the state of any cell is determined by the state of its eight neighbors, in regards to a given initial contamination rules. The goal of this game is to find the minimum number of initial contaminated cells  $\gamma_c(G(n, m))$ , such that the entire grid is contaminated. This kind of contamination can be seen as an evolutionary cellular automaton, which models an epidemiological phenomenon, illustrating the propagation of viruses in living cells.

The space of states is a two-dimensional grid of sick or healthy living cells. The chosen transition rule depends on the number and position of the contaminated living neighboring cells that surround a cell, it corresponds to Moore neighborhood.

A cell v is contaminated by two sick cells  $v_1$  and  $v_2$  if one of the following conditions is fulfilled:

(i)  $\boldsymbol{v}_1, \boldsymbol{v}_2 \in \boldsymbol{VN}(\boldsymbol{v}),$ 

(*ii*)  $v_1, v_2 \notin VN(v)$  and  $M(v_1) \cap M(v_2) = \{v\}$ .

The possible configurations which satisfy these conditions are given in Fig.2.



Figure 2: The contamination rules of the blue cell.

The following algorithm illustrates the contamination and spread process which yield the contaminated set *S*, according to the contamination rules:

Algorithm 2 Construction of a contaminated set $C(S)$
Input: Graph $G = (V, E)$ and $S \subset V$ .
Output: $C(S)$ the subset of vertices contaminated by $S$ .
1: Initiate $C(S) \leftarrow S$ ;
2: While there exists $v \in V \setminus C(S)$ such that (i) and (ii) are satisfied do
$3: C(S) \leftarrow C(S) \cup \{v\};$
4: EndWhile;
5: Return <i>C</i> ( <i>S</i> );

## 2.2 Mathematical model

Let  $x_{ij}^{(k)}$  be the decision variable at the step k,

$$x_{ij}^{(k)} = \begin{cases} 1 & \text{if the cell } (i,j) \text{ is contaminated in step } k; \\ 0 & else. \end{cases}$$

The goal of this game is to find the minimum number of contaminating cells  $\gamma_c(G(n, m))$  at the step 0, so that the entire grid is contaminated after  $k_0$  steps, according to Algorithm 2.

The objective is the following:

$$Min(Z) = \sum_{i=1}^{n} \sum_{j=1}^{m} x_{ij}^{(0)} \qquad (k_0 \text{ steps}) \qquad \sum_{i=1}^{n} \sum_{j=1}^{m} x_{ij}^{(k_0)} = nm,$$

according to the contamination rules presented above, which are written as follows:

$$\begin{cases} x_{ij}^{(k)} x_{i+2,j+2}^{(k)} \le x_{i+1,j+1}^{(k+1)}, & \forall i = 1, n-2, \forall j = 1, m-1 \quad (Fig. 2(a)); \\ x_{ij}^{(k)} x_{i+2,j-2}^{(k)} \le x_{i+1,j-1}^{(k+1)}, & \forall i = 1, n-2, \forall j = 1, m-1 \quad (Fig. 2(b)); \end{cases}$$

$$x_{ij}^{(k)} x_{i+2,j}^{(k)} \le x_{i+1,j}^{(k+1)}, \ \forall i = 1, n-2, \forall j = 1, m$$
 (Fig. 2(c));

$$x_{ij}^{(k)} x_{i,j+2}^{(k)} \le x_{i,j+1}^{(k+1)}, \ \forall i = 1, n, \forall j = 1, m-2$$
 (Fig. 2(d));

$$k \to k+1 \left\{ x_{ij}^{(k)} x_{i+1,j-1}^{(k)} \le x_{i+1,j}^{(k+1)}, \quad \forall i = 1, n-1, \forall j = 1, m \right.$$
 (Fig. 2(e));

$$x_{ij}^{(k)} x_{i+1,j+1}^{(k)} \le x_{i,j+1}^{(k+1)}, \ \forall i = 1, n-1, \forall j = 1, m-1 \quad (Fig. 2(f));$$

$$x_{ij}^{(k)} x_{i+1,j-1}^{(k)} \le x_{i,j-1}^{(k+1)}, \ \forall i = 1, n-1, \forall j = 1, m-1 \quad (Fig. 2(g));$$

$$\begin{cases} x_{ij}^{(k)} x_{i+1,j+1}^{(k)} \le x_{i+1,j}^{(k+1)}, & \forall i = 1, n-1, \forall j = 1, m-1 \quad (Fig. 2(h)); \\ x_{ij}^{(k)} \in \{0,1\}. \end{cases}$$

## **3 CONTAMINATION ON STRONG PRODUCT OF TWO PATHS**

A natural representation of a grid G(n, m) is as the strong product of two paths  $P_n \boxtimes P_m$ , such that (see Fig.3):

- (1) each cell of G(n, m) is represented by a vertex v in  $P_n \boxtimes P_m$ ,
- (2) the neighboring between two cells in G(n, m) is represented by an edge in  $P_n \boxtimes P_m$ .



Figure 3: G(3,4) modeled as the strong product of paths.

The number of neighboring of each cell in G(n, m) represents the degree of the corresponding vertex in  $P_n \boxtimes P_m$ , as shown in Fig.3. This implies that the virus-contamination on G(n, m) is equivalent as on  $P_n \boxtimes P_m$ .

Fig.4 represents an optimal contamination of G(3,4). The red cells (equivalently the red vertices in  $P_3 \boxtimes P_4$ ) represent the contaminated cells in step 0.



Figure 4: 
$$\gamma_c(G(3,4)) = 3$$

The evolution of the total contamination of the grid G(3,4) is shown in Fig.5.



Figure 5: The evolution of the total contamination of G(3,4).

#### **4 MAIN RESULTS**

**Lemma 4.1.** For any positive integer \$m\$, the contamination number of the path  $P_m = P_1 \boxtimes P_m$  is:

$$\gamma_c(P_m) = 1 + \left\lfloor \frac{m}{2} \right\rfloor.$$

**Proof.** Let  $v_1, ..., v_m$ , with  $d(v_1) = d(v_m) = 1$  and for  $i \in \{2, ..., m-1\}$ ,  $d(v_i) = 2$ . In order to have a full contamination of  $P_m$ , we should deploy viruses on the extremities of the path,  $v_1$  and  $v_m$ , and then we deploy the viruses alternatively on  $P_m$ , according to the contamination rule Fig.2(d). Thus, we should deployed  $2 + \lfloor \frac{m-2}{2} \rfloor$  viruses, which implies that  $\gamma_c(P_n) = 1 + \lfloor \frac{m}{2} \rfloor$  (see for instance Fig.6).



Figure 6: Optimal contamination in  $P_6$  and  $P_5$ .

**Theorem 4.2.** Let *n*, *m* be two positive integers. Then we have

$$\gamma_c(P_n \boxtimes P_m) \le \begin{cases} max\left\{\left\lfloor\frac{n}{2}\right\rfloor, \left\lfloor\frac{m}{2}\right\rfloor\right\} + 1 & \text{if } n \text{ and } m \text{ have the same parity,} \\ max\left\{\left\lceil\frac{n}{2}\right\rceil, \left\lceil\frac{m}{2}\right\rceil\right\} + 1 & \text{else.} \end{cases}$$

**Proof.** Let us first observe that the minimum number of viruses contaminating the grid G(n, m) is the same as G(m, n), simply rotate G(n, m) through  $\frac{\pi}{2}$ . For this reason, we assume throughout the proof that  $m \ge n \ge 1$ .

In the following we give a construction of a contaminant set with the given cardinality. We conjecture that the construction is optimal; therefore this upper bound gives the exact value.

If n = 1, the contamination is achieved with the given cardinality, using Lemma 1. Suppose that  $m \ge n \ge 2$  and set  $G = P_n \boxtimes P_m$ . In order to have a full contamination, it suffices to decompose G into  $G_1$  and  $G_2$ , such that  $G_1 = P_n \boxtimes P_n$  and  $G_2 = P_n \boxtimes P_{m-n}$ . The contamination of  $G_1$  and  $G_2$  induces a full contamination of G. For that, we distinguish fourth cases:

Case 1: *n* and *m* are even.

Let  $P_{n-i}^i$  be a diagonal of  $P_n \boxtimes P_n$  of order *i* and size n - i, such that  $i \in \{0, ..., n - 1\}$ . The main diagonal  $P_n^0$ , which is a path, is fully contaminated using  $\frac{n}{2} + 1$  viruses, according to Lemma 1. From the contamination rules defined above, more precisely Fig.2(f) and Fig.2(h), the parallel paths  $P_{n-i}^1$  of size n - 1 are fully contaminated. The contamination continues to spread according to the same rules until reaching the last diagonal. Thus we have a full contamination of  $G_1 = P_n \boxtimes P_n$ .

Now we move to the contamination of  $G_2$ . To contaminate this latter it suffices to alternatively deploy  $\frac{m-n}{2}$  viruses on the first path from the top of G, starting by the last vertex according to the contamination rules Fig.2(d) and Fig.2(e). Hence, we get a full contamination of  $G_2$ , and then a full contamination of  $G = P_n \boxtimes P_m$ , using  $\frac{m}{2} + 1$  viruses (see Fig.7).



Figure 7: Contamination strategy in  $P_4 \boxtimes P_{10}$ .

Case 2: *n* and *m* are odd.

The contamination of *G* is done in two steps, as seen in the first case. A full contamination of  $P_n \boxtimes P_n$  is attained by deploying alternatively  $\left\lfloor \frac{n}{2} \right\rfloor + 1$  viruses on the main diagonal of  $G_1$  using Lemma 1 and the contamination rules Fig2(a), Fig.2 (f) and Fig.2(h). The contamination of  $G_2$  is obtained by deploying alternatively  $\frac{m-n}{2}$  viruses on the first path from the top of *G*, starting by the last vertex according to the contamination rules Fig.2 (d) and Fig.2(e). Hence, we get a full contamination of  $G_2$ , and then a full contamination of  $G = P_n \boxtimes P_m$ , by using  $\left\lfloor \frac{n}{2} \right\rfloor + \frac{m-n}{2} + 1 = \left\lfloor \frac{m}{2} \right\rfloor + 1$  viruses (see Fig.8).



Figure 8: Contamination of  $P_3 \boxtimes P_9$ .

Case 3: *n* odd and *m* even.

As seen in the second case,  $G_1$  is fully contaminated by using  $\left\lfloor \frac{n}{2} \right\rfloor + 1 = \left\lfloor \frac{n}{2} \right\rfloor + 1$  viruses. To contaminate  $G_2$  it suffices to alternatively deploy  $\left\lfloor \frac{m-n}{2} \right\rfloor = \frac{m}{2} - \left\lfloor \frac{n}{2} \right\rfloor$  viruses on the first path from the top of G, starting with the second vertex of  $G_2$  then add a virus at the last vertex (see Fig.9). Hence, we have a full contamination of  $G_2$ , according to the contamination rules Fig.2(d) and Fig.2(e) and then a full contamination of  $G = P_n \boxtimes P_m$ , using  $\left\lfloor \frac{n}{2} \right\rfloor + \left\lfloor \frac{m-n}{2} \right\rfloor + 1 = \frac{m}{2} + 1$ .



Figure 9: Contamination of  $P_3 \boxtimes P_8$ .

Case 4: *n* even and *m* odd.

The graph  $G_1$  is fully contaminated by using  $\frac{n}{2} + 1$ , as seen in the first case. To contaminate  $G_2$  it suffice to alternatively deploy  $\left[\frac{m-n}{2}\right] = \left[\frac{m}{2}\right] - \frac{n}{2}$  viruses on the first path from the top of G, starting with the second vertex of  $G_2$  then add a virus at the last vertex (see Fig.10). Hence, we have a full contamination of  $G_2$ , according to the contamination rules Fig.2 (d) and Fig.2(e) and then a full

contamination of  $G = P_n \boxtimes P_m$ , using  $\frac{n}{2} + \left[\frac{m-n}{2}\right] + 1 = \left\lfloor\frac{m}{2}\right\rfloor + 1$ .  $P_4 \boxtimes P_4$   $P_4 \boxtimes P_5$ 

Figure 10: Contamination of  $P_4 \boxtimes P_9$ .

As a consequence of the above theorem, we can give the following Corollary.

**Corollary 4.3.** For any positive integer *n*, we have:

$$\gamma_c(P_n \boxtimes P_n) \le \left\lfloor \frac{n}{2} \right\rfloor + 1.$$

Our investigation therefore puts us in a position to conjecture the following result:

**Conjecture.** Let *n*, *m* be two positive integers. Then we have

$$\gamma_c(P_n \boxtimes P_m) = \begin{cases} max\left\{\left\lfloor\frac{n}{2}\right\rfloor, \left\lfloor\frac{m}{2}\right\rfloor\right\} + 1 & \text{if } n \text{ and } m \text{ have the same parity,} \\ max\left\{\left\lceil\frac{n}{2}\right\rceil, \left\lceil\frac{m}{2}\right\rceil\right\} + 1 & \text{else.} \end{cases}$$

#### **5** CONCLUSION

In this work, we have introduced a new dynamic variant of domination, which has the same principle of unfolding as power domination. This type of domination can be interpreted as a biological phenomenon or an evolutionary social phenomenon, which is called a contamination game and takes place in the grid graph G(n, m). We identified an upper bound for the minimum number of contaminant cells  $\gamma_c(G(n, m))$  and conjectured that it gives the exact value.

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#### REFERENCES

- [1] T.W. Haynes, S.M. Hedetniemi S.T. Hedetniemi and M.A. Henning, "Domination in graphs applied to electric power networks", *SIAM J. Discrete Math*, **15**(4): 519-529, (2002).
- [2] P. Dorbec, M. Mollard, S. Klavzar and S. Spacapan, "Power Domination in product graphs", *SIAM J. Discrete Math*, **22**(2): 554-567, (2008).
- [3] P. Dorbec, S. Varghese and A. Vijayakumar, "Heredity for generalized power

domination", Discrete Mathematics and Theoretical Computer Science, 18(3), (2016).

- [4] T.L. Baldwin, L. Mili, M.B. Boisen and R. Adapa, "Power system obserability wih minimal phasor measurement placement", *IEEE Trans Power System* 8(2), 707-715, (1993).
- [5] C.-S. Liao and D-T. Lee, "Power domination problem in graph", *Lecture Notes comp.Sci*, 3595, 818-828, (2005).
- [6] D. Ferrero, S. Varghese and A. Vijayakumar, "Power domination in honeycomb networks", *Journal of Discrete Mathematical Sciences and Cryptography*, **14**(6): 521-529, (2011).
- [7] J.G. Chang, P. Dorbec, M. Montassier and A. Raspaud, "Generalized power domination of graphs", *Discrete Appl. Math*, **160**(12), 1691-1698, (2012).
- [8] P. Dorbec and S. Klavzar, "Generalized power domination, Propagation radius and Sierpinski graphs", Acta Applicandae Mathematicae, 134(1), 75-86, (2014).
- [9] P. Bose, C. Pennarun and S. Verdonschot, "Power domination on triangular grids", Proceedings of 29th CCCG, 2-6, (2017).
- [10] D Gonçalves, A. Pinlou, M. Rao and S. Thomassé, "The domination number of grid", *SIAM Journal on Discrete Mathematics*, **25**(4): 1443-1453, (2011).
- [11] M. Dorfling, M.A. Henning. "A note on power domination in grid graph", *Discrete Applied Math*, **154**(6): 1023-1027, (2006).

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## SOME ASPECTS OF NEYMAN TRIANGLES AND DELANNOY ARRAYS

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**Summary.** This note considers some number theoretic properties of the orthonormal Neyman polynomials which are related to Delannoy numbers and certain complex Delannoy numbers.

#### **1 INTRODUCTION**

Rayner and Best point out that "the concept of smooth goodness of fitness tests was introduced in Neyman (1937)" [22]. Goodness of fit concepts in general usually go back to Karl Pearson [20]. Rayner [21] further pointed out that Jerzy Neyman's smooth alternative of order k to the uniform distribution on (0,1) has probability density for

$$h(y,\theta) = exp \sum_{i=1}^{\infty} \theta_i \pi_i(y) - K(\theta) \bigg\}, 0 < y < 1, k = 1, 2, \dots$$
(1.1)

where  $K(\theta)$  is a normalising constant and the  $\pi_i(y)$  are orthonormal polynomials (Freeman) related to the Legendre polynomials.

It is the purpose of this note to consider some number theoretic properties of the  $\pi_i(y)$  polynomials (i = 0,1,2,3,4 in Rayner) which, for convenience, we label as Neyman polynomials. In Deveci and Shannon [9] complex-type k-Fibonacci numbers are defined and the relationships between the k-step Fibonacci numbers and the complex-type k-Fibonacci numbers are provided together with miscellaneous properties of the complex-type k-Fibonacci sequence modulo m. Finally, they obtained the period of the complex-type 2-Fibonacci sequences in the Dihedral group  $D_{2n}$ ,  $(n \ge 2)$ .

In this paper, we define the complex-type Delannoy numbers and then give the relationships between the Delannoy numbers and the complex-type Delannoy numbers. Furthermore, we study the complex-type Delannoy sequence modulo m.

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**Key words and Phrases:** Neyman polynomials, Legendre polynomials, Delannoy numbers, Fibonacci numbers, Tribonacci triangles.

## **2 NEYMAN POLYNOMIALS**

Rayner elsewhere lists the first five such polynomials and we add some more in order to build up a picture of patterns. To help with this we have slightly modified some aspects of his notation as in Bera and Ghosh [3]:

$$\begin{aligned} \pi_0(y) &= \sqrt{1(1)} \\ \pi_1(y) &= \sqrt{3(2y-1)} \\ \pi_2(y) &= \sqrt{5(6y^2 - 6y + 1)} \\ \pi_3(y) &= \sqrt{7(20y^3 - 30y^2 + 12y - 1)} \\ \pi_4(y) &= \sqrt{9(70y^4 - 140y^3 + 90y^2 - 20y + 1)} \\ \pi_5(y) &= \sqrt{11(252y^5 - 630y^4 + 560y^3 - 210y^2 + 30y - 1)} \\ \pi_6(y) &= \sqrt{13(924y^6 - 2772y^5 + 3150y^4 - 1680y^3 + 420y^2 - 42y + 1)}. \end{aligned}$$

Blinov and Lemeshko [4] have set out corresponding Legendre polynomials as, in effect,

$$p_{0}(y) = \sqrt{1(1)}$$

$$p_{1}(y) = \sqrt{3(2y)}$$

$$p_{2}(y) = \sqrt{5(6y^{2} - 0.5)}$$

$$p_{3}(y) = \sqrt{7(20y^{3} - 3y)}$$

$$p_{4}(y) = \sqrt{9(70y^{4} - 15y^{2} + 0.375)}$$

#### **3 NEYMAN TRIANGLE**

We assemble the absolute values of the polynomial coefficients into a triangle, as the row sums are all unity if we include the signed values of the coefficients. The row sums are in the right-most column, and the pertinent OIES references [23] are in the bottom row.

1							1
2	1						3
6	6	1					13
20	30	12	1				63
70	140	90	20	1			321
252	630	560	210	30	1		1683
924	2772	3150	1680	420	42	1	8989
A000984	A002457	A002544	A007744	A106440	A013613		A001850

Table 1: Neyman triangle

The leading diagonals in this table generate the sequence  $\{1,2,7,26,101,404,1645,...\}$  which does not seem to be in OEIS, but the anti-diagonals can related to OEIS sequences in Table 2(a).

1	1	1	1	1	1	1	1	A000012
2	6	12	20	30	42	56	72	A002378
6	30	90	210	420	756	1260	1980	A033487
20	140	560	1680	4200	9240	18480	34320	A105939
70	630	3150	11550	34650	90090	210210	450450	70xA000581

Table 2(a): Anti-diagonals in Neyman triangle

The patterns are clearer when we express the Neyman anti-diagonals as multiples of the first element in each row, as in Table 2 (b). The leading diagonal here yields a known sequence (A005809) as do the anti-diagonals (A001519), the odd Fibonacci numbers as a bisection of the Fibonacci sequence, but we shall not pursue these here.

1 X	1	1	1	1	1	1	1	1	A000012
2 X	1	3	6	10	15	21	28	36	A000217
6 X	1	5	15	35	70	126	210	330	A000332
20 X	1	7	28	84	210	462	924	1716	A000579
70 X	1	9	45	165	495	1287	3003	6435	A000581
A0	00012	05408	0384	000447	53134	02299	53135	53136	

Table 2(b): Anti-diagonals in Neyman triangle

The leading diagonals in Table 2(a) generate the sequence {1,3,13,63,321,1683,8989,...} [A001850] the elements of which are the Central Delannoy numbers [2], so called because they constitute the central anti-diagonal in the infinite square Delannoy array [A008288] in Table 3. The leading anti-diagonal here is A005809.

$n\downarrow$								
$m \rightarrow$	0	1	2	3	4	5	6	7
0	1	1	1	1	1	1	1	1
1	1	3	5	7	9	11	13	15
2	1	5	13	25	41	61	85	113
3	1	7	25	63	129	231	377	575
4	1	9	41	129	321	681	1289	2241
5	1	11	61	231	681	1683	3653	7183
6	1	13	85	377	1289	3653	8989	19825
7	1	15	113	575	2241	7183	19825	48639

Table 3: Square Delannoy array

The leading diagonals in this array generate the Pell numbers  $\{1,2,5,12,29,\ldots\}$ , and, in the sense of this paper, Alladi and Hoggatt [1] further related these numbers to Tribonacci triangles. When this array is turned clockwise through  $45^{\circ}$  we have the Pell triangle.

We also see regular intersections (as common elements) among the row and column sequences, which is a topic worth exploring as in Stein [24] who found it necessary to examine the intersection of Fibonacci sequences in order to answer the question of whether every member of a variety is a quasigroup given that every finite member is [25].

The Central Delannoy numbers  $\{a_n\}, n \ge 0$ , can be expressed as
$$a_n = \sum_{k=0}^n \binom{n}{k} \binom{n+k}{k}$$
(3.1)

and

$$a_n = \frac{\pi_n(2)}{\sqrt{n}} \tag{3.2}$$

in terms of the Neyman numbers, which would appear to be new. This suggests we consider in turn

$$\frac{\pi_n(3)}{\sqrt{n}} = \{1, 5, 37, 305, 2641, 23525, \dots\}$$

which is A006442, the expansion of  $(x^2 - 10x + 1)^{-\frac{1}{2}}$ , which is also related to the Delannoy numbers. Likewise A084768 is

$$\frac{\pi_n(4)}{\sqrt{n}} = \{1,7,73,847,10321,129367,1651609,\dots\}$$

and so on.

## **4 THE COMPLEX-TYPE DELANNOY NUMBERS**

Now we define a new sequence that we call the complex-type Delannoy sequence  $\{D^i(m,n)\}$  as follows:

$$D^{i}(m,n) = \begin{cases} 1 & \text{if } m = 0 \text{ or } n = 0, \\ i \cdot D^{i}(m-1,n) + i \cdot D^{i}(m,n-1) - D^{i}(m-1,n-1) & \text{otherwise.} \end{cases}$$
(1)

Note that when m = n = a, the complex-type Delannoy sequence  $\{D^i(m,n)\}$  is reduced to the central complex-type sequence  $\{D^i(a,a)\}$ .

A table for the values of the complex-type Delannoy numbers is given by below:

n↓								
$m \rightarrow$	0	1	2	3	4	5	6	7
0	1	1	1	1	1	1	1	1
1	1	2 <i>i</i> -1	-3	-2 <i>i</i> -1	1	2 <i>i</i> -1	-3	-2 <i>i</i> -1
2	1	-3	-8 <i>i</i> +1	13	16 <i>i</i> +1	-19	-24 <i>i</i> +1	29
3	1	-2 <i>i</i> -1	13	34 <i>i</i> -1	-63	-98 <i>i</i> -1	141	194 <i>i</i> -1
4	1	1	16 <i>i</i> +1	-63	-160 <i>i</i> +1	321	560 <i>i</i> +1	-895
5	1	2 <i>i</i> -1	-19	-98 <i>i</i> -1	321	802 <i>i</i> -1	-1683	-3138 <i>i</i> -1
6	1	-3	-24 <i>i</i> +1	141	560 <i>i</i> +1	-1683	-4168 <i>i</i> +1	8989
7	1	-2 <i>i</i> -1	29	194 <i>i</i> -1	-895	-3138 <i>i</i> -1	8989	22146 <i>i</i> -1

Table 4: Square complex-type Delannoy numbers

From the definitions of the Delannoy numbers and the complex-type Delannoy numbers, we derive the following relations:

*i*. For  $m, n \ge 1$ 

$$D^{i}(m,n) = \begin{cases} 2(i)^{n} \cdot D(m-1,n-1) - D^{i}(m-1,n-1), & n \equiv 1 \pmod{4}, \\ 2(i)^{n+1} \cdot D(m-1,n-1) - D^{i}(m-1,n-1), & n \equiv 2 \pmod{4}, \\ 2(i)^{n+2} \cdot D(m-1,n-1) - D^{i}(m-1,n-1), & n \equiv 3 \pmod{4}, \\ 2(i)^{n+3} \cdot D(m-1,n-1) - D^{i}(m-1,n-1), & n \equiv 0 \pmod{4}. \end{cases}$$

*ii*. For  $m, n \ge 0$ ,  $D^{i}(m, n) = D^{i}(n, m)$ .

*iii*. For  $m, n \ge 0$ ,  $D^{i}(n+1, n) = D^{i}(n, n+1) = (-1)^{n} \cdot D(n, n)$ .

It is well-known that a sequence is periodic if, after a certain point, it consists only of repetitions of a fixed subsequence. The number of elements in the repeating subsequence is the period of the sequence.

The research on the conformity of a single term,  $a_n \pmod{p}$ , has a long history forming most known Pascal's oldest fractal problem, which was originally created by the parities of binomial coefficients  $\binom{n}{k}$ ; see for example, [5,6,7,8,10,12,14,16,17,18,29,30]. We now extend the concept to the complex-type Delannoy numbers.

Consider the sequence

$$\{D^{i}(m,n)\} = \{D^{i}(0,n), D^{i}(1,n), D^{i}(2,n), \ldots\}$$

where *n* is a fixed positive integer and m = 0, 1, 2, ...

If we reduce the sequence  $\{D^i(m,n)\}$  modulo  $\alpha$ , taking least nonnegative residues, then we can get the repeating sequence, denoted by

$$\left\{D^{i}(m,n)(\alpha)\right\} = \left\{D^{i}(0,n)(\alpha), D^{i}(1,n)(\alpha), D^{i}(2,n)(\alpha), \ldots\right\}$$

where  $D^{i}(u,n)(\alpha)$  is used to mean the *u*th element of the sequence  $\{D^{i}(m,n)(\alpha)\}$  modulo  $\alpha$  for the positive integer constant *n*.

We note here that the sequence  $\{D^i(m,n)(\alpha)\}$  has the same recurrence relation as in (1).

**Theorem 4.1.** The sequence  $\{D^i(m,n)(\alpha)\}$  is periodic.

**Proof.** It is clear that sequence  $\{D^i(m,1)(\alpha)\}$  is a constant sequence. Since the sequence  $\{D^i(m,1)(\alpha)\}$  is a constant sequence; that is, since it consists only the repetitions of a constant subsequence, we can say that the sequence  $\{D^i(m,2)(\alpha)\}$  is also a periodic sequence, using the recurrence relation in the sequence  $\{D^i(m,n)(\alpha)\}$ . Similarly, since the

sequences  $\{D^i(m,1)(\alpha)\}\$  and  $\{D^i(m,2)(\alpha)\}\$  are periodic; that is, they consist only the repetitions of constant sub-sequences, the sequence  $\{D^i(m,n)(\alpha)\}\$  is also periodic. By a similar idea, we get the repeating sequences

$$\left\{D^{i}(m,1)(\alpha)\right\}, \left\{D^{i}(m,2)(\alpha)\right\}, \ldots, \left\{D^{i}(m,n-1)(\alpha)\right\}$$

are periodic; that is, they consist only the repetitions of constant sub-sequences, using the recurrence relation in the sequence  $\{D^i(m,n)(\alpha)\}$ . Thus, this implies that the sequence  $\{D^i(m,n)(\alpha)\}$  is periodic.

**Example 2.1.** We have

$$\left\{D^{i}(m,3)(3)\right\} = \left\{\begin{array}{l}1, i-1, 1, i-1, 0, i-1, 0, 2i-1, 0, 2i-1, 1, i-1, \\1, i-1, 1, i-1, 0, i-1, 0, 2i-1, 0, 2i-1, 1, i-1, \ldots\right\}$$

and its terms repeat so we get  $L(D^{i}(m,3)(3))=12$ , where the period of the sequence  $\{D^{i}(m,n)(\alpha)\}$  is denoted by  $L(D^{i}(m,n)(\alpha))$ .

**Conjecture 4.1.** Let *p* be prime, let *n* be a fixed positive integer and m = 0, 1, 2, ... If *u* is the smallest positive integer such that  $L(D^i(m,n)(p^{u+1})) \neq L(D^i(m,n)(p^u))$ , then  $L(D^i(m,n)(p^v)) = p^{v-u} \cdot L(D^i(m,n)(p^u))$ .

**Theorem 4.2.** Let  $\alpha_1$  and  $\alpha_2$  be positive integers with  $\alpha_1, \alpha_2 \ge 2$ , then

$$L(D^{i}(m,n)(lcm(\alpha_{1},\alpha_{2}))) = lcm[L(D^{i}(m,n)(\alpha_{1})),L(D^{i}(m,n)(\alpha_{2}))].$$

**Proof.** Let  $lcm(\alpha_1, \alpha_2) = \alpha$ . Then,

$$D^{i}(m,n)\left[L(D^{i}(m,n)(\alpha))\right] \equiv D^{i}(m,n)\left[L(D^{i}(m,n)(\alpha))+1\right]$$
$$\equiv \cdots \equiv D^{i}(m,n)\left[L(D^{i}(m,n)(\alpha))+n-1\right] \equiv 0 \pmod{\alpha}$$

and

$$D^{i}(m,n)\Big[L\big(D^{i}(m,n)(\alpha_{k})\big)\Big] \equiv D^{i}(m,n)\Big[L\big(D^{i}(m,n)(\alpha_{k})\big)+1\Big]$$
$$\equiv \cdots \equiv D^{i}(m,n)\Big[L\big(D^{i}(m,n)(\alpha_{k})\big)+n-1\Big] \equiv 0\big(\operatorname{mod}\alpha_{k}\big)$$

for k = 1, 2. Using the least common multiple operation this implies that

$$D^{i}(m,n)\Big[L(D^{i}(m,n)(\alpha))\Big] \equiv D^{i}(m,n)\Big[L(D^{i}(m,n)(\alpha))+1\Big]$$
$$\equiv \cdots \equiv D^{i}(m,n)\Big[L(D^{i}(m,n)(\alpha))+n-1\Big] \equiv 0 \pmod{\alpha_{k}}$$

for 
$$k = 1, 2$$
. So we have  $L(D^{i}(m,n)(\alpha_{1}))|L(D^{i}(m,n)(\alpha))$  and  $L(D^{i}(m,n)(\alpha_{2}))|L(D^{i}(m,n)(\alpha))$ ,  
which means that  $lcm[L(D^{i}(m,n)(\alpha_{1})), L(D^{i}(m,n)(\alpha_{2}))]$  divides  
 $L(D^{i}(m,n)(lcm(\alpha_{1},\alpha_{2})))$ . We also know that  
 $D^{i}(m,n)[lcm(L(D^{i}(m,n)(\alpha_{1})), L(D^{i}(m,n)(\alpha_{2})))] \equiv D^{i}(m,n)[lcm(L(D^{i}(m,n)(\alpha_{1})), L(D^{i}(m,n)(\alpha_{2})))+1]$   
 $\equiv \cdots \equiv D^{i}(m,n)[lcm(L(D^{i}(m,n)(\alpha_{2})))+n-1] \equiv 0 \pmod{\alpha_{k}}$ 

Then,

$$D^{i}(m,n)\Big[lcm\Big(L\Big(D^{i}(m,n)(\alpha_{1})\Big),L\Big(D^{i}(m,n)(\alpha_{2})\Big)\Big)\Big] \equiv D^{i}(m,n)\Big[lcm\Big(L\Big(D^{i}(m,n)(\alpha_{1})\Big),L\Big(D^{i}(m,n)(\alpha_{2})\Big)\Big)+1\Big]$$
$$\equiv \cdots \equiv D^{i}(m,n)\Big[lcm\Big(L\Big(D^{i}(m,n)(\alpha_{1})\Big),L\Big(D^{i}(m,n)(\alpha_{2})\Big)\Big)+n-1\Big]\equiv 0 \pmod{\alpha}.$$

and it follows that  $L(D^i(m,n)(lcm(\alpha_1,\alpha_2)))$  divides  $lcm[L(D^i(m,n)(\alpha_1)), L(D^i(m,n)(\alpha_2))]$ . Therefore, we have the following conclusions.  $\Box$ 

**Corollary 4.1.** Let v and u be positive integers. If  $n = 2^v$ , then  $L(D^i(m, n)(2^u)) = 2^{u-v-1}$  for  $u+2 \ge v$ .

**Corollary 4.2.** Let *n* be a positive integer and *u* a positive integer such that  $u \ge 2$ . Then  $L(D^i(m,n)(2^u)) = 2^{u-1}$ .

## **5 CONCLUDING COMMENTS**

Lavers' Lemma 5 [15] suggests a way to generalize (3.1) to produce corresponding pyramids, and Horadam [13] and Subba Rao [26,27,28] contain further ideas on the study of intersections of sequences.

#### REFERENCES

- K. Alladi and V.E. Hoggatt, "Tribonacci numbers and Related Functions", *Fibonacci Quarterly*, 15(1), 42-45 (1977).
- [2] C. Banderier and S.Sylviane, "Why the Delannoy numbers?", *Journal of Statistical Planning and Inference*, **135**(1), 40-54 (2005).
- [3] A.K. Bera and A. Ghosh, "Neyman's smooth test and its use in econometrics", *Singapore Management University Research Collection School of Economics*, 6-2001, p.17 (2001).
- [4] P.Y. Blinov and Y. B.Y. Lemeshko, "A Review of the Properties of Tests for Uniformity", *Proceedings of the 12<sup>th</sup> International Conference on Actual Problems of Electronics Instrument Engineering (APEIE)*, Novosibirsk: NSTU/IEEE, pp.540-547 (2014).
- [5] S. Chowla, J. Cowles, and M. Cowles, "Congruence properties of Apéry numbers", *Journal of Number Theory*, **12**(2), 188-190 (1980).
- [6] K.S. Davis and W.A. Webb, "Pascal's triangle modulo 4", *The Fibonacci Quarterly*, **29**(1), 79-83 (1991).
- [7] O. Deveci and Y. Akuzum, "The cyclic groups and the semigroups via MacWilliams and Chebyshev matrices", *Journal of Mathematics Research*, 6(2), 55 (2014).

- [8] O. Deveci and E. Karaduman, "The cyclic groups via the Pascal matrices and the generalized Pascal matrices", *Linear algebra and its applications*, **437**(10), 2538-2545 (2012).
- [9] O. Deveci and A.G. Shannon "The complex-type *k*-Fibonacci sequences and their applications", *Communications in Algebra*, 1-16 (2020).
- [10] S.P. Eu, S.C. Liu, and Y.N. Yeh, "On the congruences of some combinatorial numbers", *Studies in applied mathematics*, **116**(2), 135-144 (2006).
- [11] J.M. Freeman, "A Strategy for Determining Polynomial Orthogonality", In Bruce E. Sagan and Richard P. Stanley (eds). *Mathematical Essays in honor of Gian-Carlo Rota*, Boston/Basel/Berlin: Birkhäuser, 239-244 (1998).
- [12] A. Granville, Arithmetic properties of binomial coefficients, I: Binomial coefficients modulo prime powers, In Organic mathematics, Proceedings of the workshop, Simon Fraser University, Burnaby, Canada, December. 12-14. American Mathematical Society (1997).
- [13] A.F. Horadam, "Generalizations of two theorems of K. Subba Rao", *Bulletin of the Calcutta Mathematical Society*, **58**(1), 23-29 (1966).
- [14] P.Y. Huang, S.C. Liu, and Y.N. Yeh, "Congruences of Finite Summations of the Coefficients in certain Generating Functions", *The Electronic Journal of Combinatorics*, **21**(2), P2-45 (2014).
- [15] T.G. Lavers, "The Fibonacci Pyramid", In G.E. Bergum, A.F. Horadam and A.N. Philippou (eds). *Applications of Fibonacci Numbers, Volume 7*. Dordrecht: Kluwer, pp. 255-263 (1998).
- [16] E. Lucas, "Sur les congruences des nombres eulériens et des coefficients différentiels des fonctions trigonométriques suivant un module premier", *Bulletin de la Société mathématique de France*, 6, 49-54 (1878).
- [17] K. Lü and J. Wang, "*k*-step Fibonacci Sequences Modulo *m*", *Utilitas Mathematica*, **71**, 169-178 (2007).
- [18] Y. Mimura, "Congruence properties of Apéry numbers", Journal of Number Theory, 16(1), 138-146 (1983).
- [19] J. Neyman, "Smooth' test for goodness of fit", *Scandinavian Actuarial Journal*, **3-4**, 149-199 (1937).
- [20] R.L. Plackett, "Karl Pearson and the Chi-Squared Test", *International Statistical Review*, **51**(1), 59-72 (1983).
- [21] J.W.C. Rayner, *The goodness of fit publications of J.W.C. Rayner. Volume 1.* Thesis for the degree of *Doctor of Philosophy*, the University of Wollongong, p.3 (1994).
- [22] J.W.C. Rayner and D.J. Best, "Neyman-type Smooth Tests for Location-Scale Families", *Biometrika*, **73**(2), 437-446 (1986).
- [23] N.J.A. Sloane, *The On-Line Encyclopedia of Integer Sequences*, (*OEIS*). *oeis.org*. San Diego CA: Academic Press (1964).
- [24] S.K. Stein, "The intersection of Fibonacci sequences," *Michigan Mathematics Journal*, **9**, 399-402 (1962).
- [25] S.K. Stein, "Finite models of identities", *Proceedings of the American Mathematical Society*, **14**, 216-222 (1963).
- [26] K. Subba Rao, "Some properties of Fibonacci numbers", American Mathematical Monthly, **60**, 680-684 (1953).
- [27] K. Subba Rao, "Some properties of Fibonacci numbers-I", *Bulletin of the Calcutta Mathematical Society*, **46**, 253-257 (1954).
- [28] K. Subba Rao, "Some properties of Fibonacci numbers-II", *Mathematics Student*, 27, 19-23 (1959).
- [29] Z.W. Sun, "On Delannoy numbers and Schröder numbers", *Journal of Number Theory*, **131**(12), 2387-2397(2011).
- [30] D.D. Wall, "Fibonacci series modulo *m*", *The American Mathematical Monthly*, **67**(6), 525-532 (1960).

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# NOTE ON A THEOREM OF ZEHNXIAG ZHANG

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**Summary.** A sequence of strictly positive integers is said to be primitive if none of its terms divides the others. In this paper, we give a new proof of a result, conjectured by P. Erdős and Z. Zhang in 1993, on a primitive sequence whose the number of the prime factors of the termes counted with multiplicity is at most 4. The objective of this proof is to improve the complexity, which helps to prove this conjecture.

## 1. INTRODUCTION

A sequence A of strictly positive integers is said to be primitive if none of its terms divides the others. We define the degree of A by  $deg(A) = max\{\Omega(a) \ a \in A\}$  where  $\Omega(a)$  is the number of prime factors of *a* counted with multiplicity, we take deg(A) = 0 if  $A = \{1\}$  or  $\emptyset$ . Erdős [2] showed that for a primitive set *A*,  $\sum_{a \in A} \frac{1}{a \log a} < \infty$ . Later in [3], Erdős asked if is true that for any primitive sequence *A*,

$$\sum_{a \in A, \ a \le n} \frac{1}{a \log a} \le \sum_{p \in P, \ p \le n} \frac{1}{p \log p} \text{ for } n > 1,$$

where P denotes the set of prime numbers. After a few years, Zhang [5], proved the following:

**Theorem**. For any primitive sequence A whose the number of the prime factors of the termes counted with multiplicity is at most 4, we have

$$\sum_{a \in A, \ a \leq n} \frac{1}{a \log a} \leq \sum_{p \in P, \ p \leq n} \frac{1}{p \log p} \text{ for } n > 1.$$

In our work, by using the new estimations of the n-th prime number, we simplify the complexity (the number N = 20000 decreased to 95). Throughout the paper we denotes by  $p_m$  the m-th prime number and we put  $f(A) = \sum_{a \in A} \frac{1}{a \log a}$  where, f(A) = 0 if deg(A) = 0.

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Key words and Phrases: Primitive Sequence, Prime Number, Erdős Conjecture.

For a primitive sequence A and  $m \ge 1$ , we pose

$$A_m = \{a \in A, \text{ the prime factors of } a \text{ are } \ge p_m\},\$$
  

$$A'_m = \{a \in A_m, p_m \mid a \},\$$
  

$$A''_m = \left\{\frac{a}{p_m} : a \in A'_m\right\}.$$

Clearly, the union  $A = \bigcup_{m \ge 1} A'_m$  is disjoint and  $deg(A''_m) < deg(A)$  when A is finit. Our method based on the fact that a primitive sequence A does not contain simultaneously  $p_1$  and  $p_1^4$ .

## 2. MAIN RESULTS

We need the following lemmas.

**Lemma 2.1** Let n > 1 be an integer, put  $F(n) = \log n + \log \log n - 1$  then

$$p_n \ge nF(n), \text{ for } n \ge 2 [1] \tag{1}$$

$$p_n > n(\log(nF(n)) - \alpha), \quad for n \ge 3$$
 (2)

$$p_n \le n(F(n) + \beta), \qquad for \ n \ge 95$$
 (3)

where  $\alpha = 1.127$  and  $\beta = 0.305$ .

**Proof.** Consider the function *g* defined on N by

$$n \mapsto g(n) = \frac{p_n}{n} - \log(nF(n))$$
 for  $n \ge 3$ ,

then according to (1), we have  $g(n) \ge h(n)$  where

$$h(n) = -1 - \log\left(1 + \frac{\log \log n - 1}{\log n}\right),$$

the study of the real function  $x \mapsto h(x)$  ( $x \ge 3$ ) gives us  $h(x) \ge h(e^{e^2}) > -\alpha$ , then  $g(n) > -\alpha$ , which is equivalent to

$$p_n > n(\log(nF(n)) - \alpha)$$
, for  $n \ge 3$ .

A computer calculation shows that for  $95 \le n < 7022$ , we have

$$p_n \le n(F(n) + \beta),$$

and on the other hand we have  $p_n \le n(\log n + \log \log n - 0.9385)$  where  $n \ge 7022$  [4], therefore the inequality (3) is verified for  $n \ge 95$ . This completes the proof.

**Lemma 2.2** For  $m \ge 1$  and  $j \in \{1, 2, 3\}$ , we have

$$\sum_{i \ge \max(m, j-1)} \frac{1}{p_i(k_j + \log p_i)} < \frac{1}{k_{j-1} + \log p_m},$$

where  $k_0 = 0.023$ ,  $k_1 = 0.3157$ ,  $k_2 = 0.901$  and  $k_3 = 2.079$ .

**Proof.** Put N = 95, C = 0.0713,

$$u_1 = 0.09435,$$
  $u_2 = 0.387,$   $u_3 = 0.9723$   
 $v_1 = 0,$   $v_2 = 0,$   $v_3 = -0.0074.$ 

It is clear that for  $m \ge N$  and  $j \in \{1, 2, 3\}$  we have  $\max(m, j - 1) = m$  and

$$C \ge -\log(F(m)) + \log(1 + \frac{1}{m}) + \log(F(m+1) + \beta)$$
  

$$C \le u_j - k_{j-1},$$
  

$$v_j = \alpha - k_j + 2u_j - 1.$$
(4)

Now Put

$$h_j(m) = \sum_{i \ge \max(m, j-1)} \frac{1}{p_i(k_j + \log p_i)}.$$

By (1) and (2) we have, for  $m \ge N$  and  $j \in \{1, 2, 3\}$ ,

$$p_i(k_j + \log p_i) > i(\log(iF(i)) - \alpha)(k_j + \log(iF(i))),$$

Since x7!  $\log(xF(x))$  increases for x > N, we have

$$h_j(m+1) < \int_m^\infty \frac{dt}{t \left( \log(tF(t)) - \alpha\right) \left( \log(tF(t)) + k_j \right)^2}$$

use the change of variable  $x = \log t$ , we obtain

$$h_j(m+1) < \int_{\log m}^{\infty} \frac{dt}{(L(x) - \alpha)(L(x) + k_j)}, where L(x) = \log(e^x F(e^x)).$$

Since, for  $x > \log N$ ,

$$\frac{1}{L'(x)} < \left(1 - \frac{1}{L(x) - 1}\right),$$

then

$$h_j(m+1) < \int_{\log m}^{\infty} \frac{\left(1 - \frac{1}{L(x) - 1}\right) L'(x) dx}{(L(x) - \alpha) \left(L(x) + k_j\right)}$$

by setting y = L(x) and  $y_m = L(\log m)$  we get

$$h_j(m+1) < \int_{y_m}^{\infty} \frac{(y-2)dy}{(y-1)(y-\alpha)(y+k_j)}.$$

For  $m \ge N$  and  $j \in \{1, 2, 3\}$  we put

$$g_j(m) = \frac{1}{k_{j-1} + \log p_m}$$

then according to (3) and (4) we have

$$g_{j}(m+1) \geq \frac{1}{k_{j-1} + \log((m+1)(F(m+1) + \beta))}$$
  
>  $\frac{1}{\log(mF(m)) + u_{j}} = \int_{y_{m}}^{\infty} \frac{dy}{(y+u_{j})^{2}}.$ 

We have for  $m \ge N$  and  $j \in \{1, 2, 3\}$ ,

$$(y-2)(y+u_j)^2 - (y-1)(y-\alpha)(y+k_j) \le 0.$$

So, for  $m \ge N$  and  $j \in \{1, 2, 3\}$ , we have  $h_j(m + 1) < g_j(m + 1)$  i.e.

$$h_j(m+1) < g_j(m+1) \text{ for } m \ge N.$$

A computer calculation gives for  $1 \le m \le N$  and  $j \in \{1, 2, 3\}$ ,

$$h_{j}(m) = \sum_{i \ge \max(m, j-1)}^{N} \frac{1}{p_{i}(k_{j} + \log p_{i})} + h_{j}(N+1)$$
  
$$< \sum_{i \ge \max(m, j-1)}^{N} \frac{1}{p_{i}(k_{j} + \log p_{i})} + \frac{1}{\log(NF(N)) + u_{j}} < g_{j}(m).$$

This completes the proof.

**Lemma 2.3** Let  $m \ge 1$  be fixed and let  $B = B_m$  be primitive with deg  $(B) \le 3$ . For  $1 \le t \le 4 - \deg(B)$ , we have

$$\sum_{b \in B} \frac{1}{b(t \log p_m + \log b)} < \frac{1}{k_{t-1} + \log p_m} \text{ where } p_1^{4-t} \notin B_1,$$
(5)

$$\sum_{b \in B} \frac{1}{b(t\log p_m + \log b)} < \frac{1}{k_0 + \log p_m} \text{ where } p_1^{-3} \notin B_1.$$
(6)

**Proof.** For  $m \ge 1$  and  $1 \le t \le 4 - \deg(B)$  put

$$g_t(B) = \sum_{b \in B} \frac{1}{b(t \log p_m + \log b)} \text{ where } (g_t(\emptyset) = 0).$$

By induction on deg(B). If deg(B) = 1 and  $1 \le t \le 3$  we have  $t \log p_m \ge t \log 2 > k_t$  and  $p_1 \ne B_1$  when t = 3, then by lemma 2 we get

$$g_t(B) = \sum_{b \in B} \frac{1}{b(t \log p_m + \log b)} < \sum_{i \ge \max(m, t-1)} \frac{1}{p_i(k_t + \log p_i)} < \frac{1}{k_{t-1} + \log p_m}.$$

If deg(B) = s > 1 and  $1 \le t \le 4 - s$ , we know that  $B = \bigcup_{i \ge m} B_i'$  is disjoint, so,

$$g_t(B) = \sum_{i \ge m} g_t(B_i') \text{ where } p_1^{4-t} \notin B_1'.$$

We have two cases: if  $\deg(B_i) \le 1$  then

$$g_t(B_i') < \frac{1}{p_i(k_t + \log p_i)},$$
 (7)

if  $\deg(B_i') > 1$  then

$$g_t(B_i') = \sum_{b \in B_{i''}} \frac{1}{p_i b((t+1)\log p_i + \log b)}$$
  
=  $\frac{1}{p_i} g_{t+1}(B_{i''})$  where  $p_i^{3-t} \notin B_1''$ ,

since  $\deg(B_i'') < s$  and  $t + 1 \le 4 - \deg(B_i'')$  we have

$$g_{t+1}(B_i'') < \frac{1}{k_t + \log p_i} \text{ where } p_1^{4-(t+1)} \notin B_1'',$$

thus

$$g_t(B_i') < \frac{1}{p_i(k_t + \log p_i)}.$$
 (8)

So, from (7), (8) and lemma 2 we obtain

$$g_t(B) < \frac{1}{k_{t-1} + \log p_m}$$
 where  $p_1^{4-t} \notin B_1$ .

For t = 1 we get the inequality (6), which ends the proof.

**Proof of theorem 2.4** Let *n* be fixed and let  $A = \{a: a \in A, a \le n\}$  be subsequence of *A* where deg  $A \le 4$ . Put  $\pi(n) = m$ , the number of primes  $\le n$ ; then  $A = \bigcup_{1 \le i \le m} A_i'$  is disjoint and  $f(A) = \sum_{1 \le i \le m} f(A_i')$ . Let  $1 \le i \le m$ , we distinguish the two following cases:

case 1: we suppose that  $p_1^4 \notin A$ , i.e.,  $p_1^3 \notin A_1''$ . If deg  $A_i' \leq 1$  then  $f(A_i') \leq \frac{1}{p_i \log p_i}$  and if deg  $A_i' > 1$  then

$$f(A'_{i}) = \frac{1}{p_{i}} \sum_{b \in A''_{i}} \frac{1}{b(\log p_{i} + \log b)}$$

where  $p_1^3 \notin A_1''$  and deg  $A_i'' \le \deg A_i' - 1 \le 3$ , so, according to (6), we get

$$\sum_{b \in A_{i''}} \frac{1}{b(\log p_i + \log b)} < \frac{1}{k_0 + \log p_i} < \frac{1}{\log p_i} \text{ where } p_1^3 \notin A_1'',$$

therefore

$$f(A'_i) \le \frac{1}{p_i \log p_i} \text{ for } 1 \le i \le m.$$
(9)

Case 2: if  $p_1^4 \in A$ , since A is a primitive sequence then  $p_1 \notin A'_1$ , so,  $\deg(A'_1 - \{p_1^4\}) \neq 1$ , i.e.,

$$f(A'_1 - \{p_1^4\}) < \frac{1}{p_1(k_0 + \log p_1)},$$

Thus

$$f(A'_{1}) = f(\{p_{1}^{4}\}) + f(A'_{1} - \{p_{1}^{4}\})$$
  
=  $\frac{1}{p_{1}^{4} \log p_{1}^{4}} + \frac{1}{p_{1}(k_{0} + \log p_{1})} < \frac{1}{p_{1} \log p_{1}}$ 

And from (9) we have  $f(A'_1) \le \frac{1}{p_i \log p_i}$  for  $2 \le i \le m$ , Then

$$f(A'_1) \le \frac{1}{p_i \log p_i} \text{ for } 1 \le i \le m,$$

$$(10)$$

thus, by (9) and (10) we get

$$f(A) = \sum_{1 \le i \le m} \frac{1}{p_i \log p_i}.$$

This completes the proof.

# **3. CONCLUSION**

Using a new estimate of n-th prime with appropriate division of primitive sequence lead us to simplify the complexity. It would of interest to apply the obtained result to study the Erdős conjecture for primitive sequences of higher degree.

# REFERENCES

[1] P. Dusart, "The k-th prime is greater than  $k(\ln k + \ln \ln k - 1)$  for  $k \ge 2$ ", *Math. Comp.* 68, 411-415 (1999).

[2] P. Erdős, "Note on sequences of integers no one of which is divisible by any other", *J. Lond. Math. Soc*, **10**, 126-128 (1935).

[3] P. Erdős, Seminar at the University of Limoges, (1988).

[4] G. Robin, "Estimation de la Fonction de Tchebychef  $\theta$  sur le k-ème Nombre Premier et Grandes Valeurs de la Function  $\omega(n)$  Nombre de Diviseurs Premiers de n", *Acta Arith.*, **52**, 367-389 (1983).

[5] Z. Zhang, "On a conjecture of Erdős on the sum  $\sum 1/a_i \log a_i$ ", J. Number Theory, **39**, 14-17 (1991).

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# FACTOR GENERALIZED BE-SEMIGROUPS THROUGH HOMOMORPHISMS

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**Summary.** In this paper, we generalize the concept of homomorphism from BE-semigroups to generalized BE-semigroups. In order to show the existence, we construct some examples. Furthermore, we characterize generalized BE-semigroups by using homomorphism. In particular, we show that through every homomorphism, we may get factor generalized BE-semigroup.

## **1 INTRODUCTION**

Two classes of abstract algebras had been defined by Tanaka and Iseki. These are called BCK-algebras [1] and BCI-algebras [2]. It is well known that every BCK-algebra is a BCIalgebra, i.e. in other words, BCI-algebra is a generalization of a BCK-algebra. Moreover, Neggers and Kim [3] introduced the idea of a d-algebra which is a generalized structure for a BCK-algebra. Furthermore, Jun et al. [4] defined a new class of an abstract algebra, named as a BH-algebra. It is known that a BH-algebra is a generalized structure of BCK and BCIalgebras. Later on, H.S. Kim and Y. H. Kim [5] introduced another generalized structure of a BCK-algebra known as a BE-algebra. The authors of [5] provided equivalent conditions for the filters in a BE-algebra and for this they used the concept of upper sets. Again in [6], Ahn and So defined ideals in BE-algebras and explored a number of associated properties of such ideals. The authors of [6, 7] also discussed upper sets and generalized upper sets and characterized them by different properties. In [8], Ahn and Kim combined two structures, i.e. BE-algebra and semigroup and defined the structure of a BE-semigroup. In the research article [9], the author introduced the idea of BE-homomorphisms of BE-semigroups and characterized BE-semigroups by the properties of BE-homomorphisms. Moreover, he introduced the concept of factor self-distributive BE-semigroups and investigated some of their properties. Recently the authors of [10] have given a new generalization of a BE-algebra known as PSRU-algebra. They have discussed left (resp. right) ideal as well as filter in the same structure and investigated a relationship between left ideal and filter.

# **2 PRELIMINARIES**

In this portion, we discuss generalized BE-semigroup which is a generalization of a BEsemigroup. We give some examples and discuss some of their properties. Furthermore, we discuss different classes of generalized BE-semigroups. Firstly, we are going to define generalized BE-algebra and for the definition, we refer the readers to [11].

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Keywords and Phrases: GBE-semigroup, Congruence relation, Homomorphism.

## **Definition 2.1**

Let  $\emptyset \neq \underline{R}$  be a set together with a binary operation "\*" and a constant "1<sub>R</sub>", then it is said to be a generalized BE-algebra (shortly denoted by GBE-algebra) if the following conditions are satisfied:

- (i)  $\forall v \in \mathbf{R}, v * v = 1_{\mathbf{R}},$
- (ii)  $\forall v \in \mathbf{R}, v * 1_{\mathbf{R}} = 1_{\mathbf{R}},$
- (iii)  $\forall v, \hat{e}, w \in \mathbf{R}, v * (\hat{e} * w) = \hat{e} * (v * w).$

The example which is given below shows the existence of the above structure.

# Example 2.2 [11]

Let  $\mathbf{\hat{W}} = \{1_{\mathbf{\hat{W}}}, 2, 3\}$  be a set and "\*" is defined in  $\mathbf{\hat{W}}$  in the following table.

	1 <i>ŵ</i>	2	3
1 <i>ŵ</i>	1 <i>ŵ</i>	1 <i>ŵ</i>	1 <i>ŵ</i>
2	1 <i>ŵ</i>	1 <i>ŵ</i>	3
3	1 <i>ŵ</i>	2	1 <i>ŵ</i>

Then  $(\mathbf{W}; *, 1_{\mathbf{W}})$  is a GBE-algebra.

Note that in GBE-algebra ( $\underline{R}$ ; \*, 1<sub><u>R</u></sub>), we define a relation " $\leq$ " by  $\underline{u} \leq \underline{s} \Leftrightarrow \underline{u} * \underline{s} = 1_{\underline{R}}$ . Throughout this paper, we shall always assume that  $\underline{u} \leq \underline{s}$  and  $\underline{s} \leq \underline{u}$  implies that  $\underline{u} = \underline{s}$ . Now one can easily see that the following identities are true in a GBE-algebra.

- (i)  $\boldsymbol{u} * (\boldsymbol{s} * \boldsymbol{u}) = 1_{\boldsymbol{R}}$ ,
- (ii)  $\boldsymbol{\mu} * ((\boldsymbol{\mu} * \boldsymbol{\beta}) * \boldsymbol{\beta}) = 1_{\underline{R}}.$

We now have the following definition which is taken from [11].

#### **Definition 2.3**

A GBE-algebra  $(\vec{U}; *, 1_{\vec{U}})$  is said to be self-distributive if  $\forall u, \hat{e}, t \in \vec{U}$ ,

$$u * (\hat{e} * t) = (u * \hat{e}) * (u * t).$$

Let us give an example in order to show the existence of a self-distributive GBE-algebra.

## Example 2.4 [11]

Assume that  $\mathbf{\hat{W}} = \{1_{\mathbf{\hat{W}}}, 2, 3\}$  be a set and "\*" is defined in  $\mathbf{\hat{W}}$  in the following table:

*	1 <i>ŵ</i>	2	3
1 <i>ŵ</i>	1 <i>ŵ</i>	1 <i>ŵ</i>	1 <i>ŵ</i>
2	1 <i>ŵ</i>	1 <i>ŵ</i>	3
3	1 <i>ŵ</i>	2	1 <i>ŵ</i>

Then  $\mathbf{W}$  is a self-distributive GBE-algebra.

Further, we have the following definitions which are taken from [11].

## **Definition 2.5**

A GBE-algebra  $(L; *, 1_L)$  is said to be transitive if for any  $\psi, \tilde{n}, v \in L$ 

$$\tilde{n} * v \leq (\boldsymbol{\mu} * \tilde{n}) * (\boldsymbol{\mu} * v).$$

Note that if  $(L; *, 1_L)$  is a GBE-algebra which is self-distributive, then  $(L; *, 1_L)$  must be transitive.

# **Definition 2.6**

Let us suppose that (W, \*) and (M, \*) are two GBE-algebras. A mapping  $\varphi : W \to M$  is said to be a homomorphism from W into M if

$$\varphi(\hat{e} * t) = \varphi(\hat{e}) * \varphi(t) \forall \hat{e}, t \in W.$$

#### **Definition 2.7**

Let we have a non-empty set K along with two binary operations " $\odot$ " and "\*" and a constant " $1_K$ ", then K is known to be a GBE-semigroup if it satisfies the conditions given below:

- (i)  $(\mathbf{K}; \mathbf{O})$  is a semigroup,
- (ii)  $(\mathbf{K}; *, 1_{\mathbf{K}})$  is a GBE-algebra,
- (iii) "O" is distributive (left and right) over "\*", that is,

$$\hat{e} \odot (\underline{t} * W) = (\hat{e} \odot \underline{t}) * (\hat{e} \odot W) \text{ and } (\hat{e} * \underline{t}) \odot W = (\hat{e} \odot W) * (\underline{t} \odot W) \forall \hat{e}, \underline{t}, W \in \mathbf{K}.$$

Let us give some examples.

#### Example 2.8 [11]

Let  $W = \{1_W, 2, 3, 4\}$  and define " $\odot$ " and "\*" in W in the following tables:

$\odot$	1 <sub>W</sub>	2	3	4
1 <i>w</i>	1 <i>w</i>	1 <i>w</i>	1 <i>w</i>	1 <i>w</i>
2	1 <i>w</i>	1 <i>w</i>	1 <i>w</i>	1 <i>w</i>
3	1 <i>w</i>	1 <i>w</i>	1 <i>w</i>	2
4	1 <i>w</i>	1 <i>w</i>	1 <i>w</i>	1 <i>w</i>

*	1 <i>w</i>	2	3	4
1 <i>w</i>				
2	1 <i>w</i>	1 <i>w</i>	1 <i>w</i>	1 <i>w</i>
3	1 <i>w</i>	2	1 <i>w</i>	2
4	1 <i>w</i>	1 <i>w</i>	1 <i>w</i>	1 <i>w</i>

Then  $(W; \bigcirc, *, 1_W)$  is a GBE-semigroup.

# Example 2.9

Let  $\vec{U} = \{1_{\vec{U}}, 2, 3, 4, 5\}$  and define "O" and "\*" in  $\vec{U}$  in the following tables:

$\odot$	1 <i>ů</i>	2	3	4	5
$1_{\vec{U}}$	1 <sub><i>Ů</i></sub>	$1_{\vec{U}}$	$1_{\vec{U}}$	$1_{\vec{U}}$	$1_{\vec{U}}$
2	1 <i>ů</i>	1 <sub><i>Ů</i></sub>	1 <sub><i>Ů</i></sub>	1 <sub><i>Ů</i></sub>	1 <i>ů</i>
3	1 <i>ů</i>	1 <sub>Ů</sub>	1 <sub><i>Ů</i></sub>	1 <sub>Ů</sub>	1 <sub><i>Ů</i></sub>
4	1 <i>ů</i>	1 <sub>Ů</sub>	1 <sub>Ů</sub>	1 <sub>Ů</sub>	1 <i>ů</i>
5	1 <i>ů</i>	1 <sub><i>Ů</i></sub>	1 <sub><i>Ů</i></sub>	1 <sub><i>Ů</i></sub>	5

*	1 <sub><i>Ů</i></sub>	2	3	4	5
1 <sub><i>Ů</i></sub>	1 <sub><i>Ů</i></sub>	3	3	4	1 <sub><i>Ů</i></sub>
2	1 <i>ů</i>	1 <sub>Ů</sub>	1 <sub>Ů</sub>	4	1 <i>ů</i>
3	1 <i>ů</i>	1 <sub>Ů</sub>	1 <sub>Ů</sub>	1 <sub>Ů</sub>	5
4	1 <i>ů</i>	2	3	1 <sub>Ů</sub>	1 <i>ů</i>
5	1 <i>ů</i>	1 <sub><i>Ů</i></sub>	1 <sub><i>Ů</i></sub>	1 <sub><i>Ů</i></sub>	1 <sub><i>Ů</i></sub>

Then  $(\vec{U}; \odot, *, 1_{\vec{U}})$  is a GBE-semigroup.

Let us give some properties.

# **Proposition 2.10** [11]

The following are true for a GBE-semigroup  $(\mathbf{W}; \odot, *, 1_{\mathbf{W}})$ .

(i) 
$$1_{\vec{W}} \odot \hat{e} = \hat{e} \odot 1_{\vec{W}} = 1_{\vec{W}} \forall \hat{e} \in \vec{W}$$
,

(ii)  $\hat{e} \leq s \Longrightarrow \hat{e} \odot v \leq s \odot v, v \odot \hat{e} \leq v \odot s \quad \forall \hat{e}, s, v \in \mathbf{M}.$ 

We are now going to define unit divisor. For the following definition we refer the readers to [11].

## **Definition 2.11**

In a GBE-semigroup  $(Y; \bigcirc, *, 1_Y)$ ,  $1_Y \neq v \in Y$  is a left unit divisor if  $\exists 1_Y \neq g \in Y$  such that  $v \odot g = 1_Y$ . Similarly we may define a right unit divisor.

Let  $1_Y \neq v \in Y$ , which is right as well as left unit divisor of *Y*, then it is called a unit divisor of *Y*.

#### **3 MAIN RESULTS THROUGH HOMOMORPHISMS**

In this section, we discuss factor GBE-semigroups through homomorphism. We show that every homomorphism defines a congruence relation on every GBE-semigroup. Once we get the said congruence relation, we shall get factor GBE-semigroup.

#### **Definition 3.1**

Let us suppose that  $(\mathbf{K}; \odot, *, 1_{\mathbf{K}})$  and  $(\mathbf{M}; \odot, *, 1_{\mathbf{M}})$  are two GBE-semigroups. A mapping  $\varphi : \mathbf{K} \to \mathbf{M}$  is said to be a homomorphism if

$$\varphi(v * s) = \varphi(v) * \varphi(s)$$
 and  $\varphi(v \odot s) = \varphi(v) \odot \varphi(s)$  for all  $v, s \in K$ .

A homomorphism  $\varphi$  is called a monomorphism (resp. epimorphism) if it is one-one (resp. onto). A homomorphism which is both one-one and onto is called an isomorphism. For any homomorphism  $\varphi: \mathbf{K} \to \mathbf{M}$ , the set  $\{ n \in \mathbf{K} : \varphi(n) = 1_M \}$  is called the kernel of  $\varphi$  and is represented by the symbol *Ker* ( $\varphi$ ) while the set  $\{ \varphi(n) : n \in \mathbf{K} \}$  is known as the image of  $\varphi$  and is represented by  $Im(\varphi)$ . The set of all homomorphisms from a GBE-semigroup  $\mathbf{K}$  to a GBE-semigroup  $\mathbf{M}$  is denoted by  $Hom(\mathbf{K}, \mathbf{M})$ .

Let us give some examples in order to show the existence of homomorphisms.

## Example 3.2

- 1) The identity function on any GBE-semigroup is always a homomorphism. Moreover, as the identity function is always a bijective function so it follows that the identity function on any GBE-semigroup is an isomorphism.
- 2) Let  $T = \{1_T, 2, 3, 4\}$  and  $\dot{N} = \{1_{\dot{N}}, 2, 3, 4, 5\}$  be the sets with the following Cayley tables:

$\odot$	$1_T$	2	3	4
1 <sub><i>T</i></sub>	1 <sub>T</sub>	1 <sub><i>T</i></sub>	$1_T$	1 <sub><i>T</i></sub>
2	1 <sub><i>T</i></sub>	1 <sub><i>T</i></sub>	$1_T$	1 <sub><i>T</i></sub>
3	1 <sub><i>T</i></sub>	1 <sub><i>T</i></sub>	$1_T$	2
4	1 <sub><i>T</i></sub>	1 <sub><i>T</i></sub>	$1_T$	1 <sub><i>T</i></sub>

*	$1_T$	2	3	4
1 <sub><i>T</i></sub>	$1_T$	$1_T$	$1_T$	1 <sub><i>T</i></sub>
2	$1_T$	$1_T$	$1_T$	1 <sub><i>T</i></sub>
3	$1_T$	2	$1_T$	2
4	$1_T$	$1_T$	$1_T$	1 <sub><i>T</i></sub>

0	$1_{\dot{N}}$	2	3	4	5
$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$
2	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$
3	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$
4	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$
5	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	5

$\begin{array}{c c c c c c c c c c c c c c c c c c c $						
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	*	$1_{\dot{N}}$	2	3	4	5
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$1_{\dot{N}}$	$1_{\dot{N}}$	3	3	$1_{\dot{N}}$	$1_{\dot{N}}$
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	4	$1_{\dot{N}}$
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$	5
$5 \qquad 1_{\dot{N}} \qquad 1_{\dot{N}} \qquad 1_{\dot{N}} \qquad 1_{\dot{N}} \qquad 1_{\dot{N}} \qquad 1_{\dot{N}}$	4	$1_{\dot{N}}$	2	3	$1_{\dot{N}}$	$1_{\dot{N}}$
	5	1 <sub>Ň</sub>	1 <sub>Ň</sub>	$1_{\dot{N}}$	$1_{\dot{N}}$	$1_{\dot{N}}$

Then  $(\mathbf{T}; \odot, *, 1_{\mathbf{T}})$  and  $(\dot{\mathbf{N}}; \odot, *, 1_{\dot{\mathbf{N}}})$  are GBE-semigroups.

Define  $\varphi: T \to \dot{N}$  by

$$\varphi(1_T) = 1_{\dot{N}}, \, \varphi(2) = 1_{\dot{N}}, \, \varphi(3) = 1_{\dot{N}} \text{ and } \varphi(4) = 4.$$

Then we can easily check that  $\varphi$  is a homomorphism from  $(T; \bigcirc, *, 1_T)$  into  $(\dot{N}; \bigcirc, *, 1_N)$ .

Let us state and prove some properties. The properties are true in case of BE-semigroups. We convert them into GBE-semigroups.

# **Proposition 3.3**

Let  $\psi : L \to K$  be a homomorphism of GBE-semigroups  $(L; \odot, *, 1_L)$  and  $(K; \odot, *, 1_K)$ . Then

- (i)  $\psi$  (1<sub>L</sub>) = 1<sub>K</sub>,
- (ii) Let  $t * w = 1_L$  for all  $t, w \in L$ , then  $\psi(t) * \psi(w) = 1_K$ .

## Proof.

Here  $\psi(1_L) = \psi(1_L * 1_L) = \psi(1_L) * \psi(1_L) = 1_K$ . Therefore (i) is satisfied. Let  $\underline{t}, w \in L$  and  $\underline{t} * w = 1_L$ . By using (i), we have  $\psi(\underline{t}) * \psi(w) = \psi(\underline{t} * w) = \psi(1_L) = 1_K$ .

# **Proposition 3.4**

Assume that  $(\underline{T}; \bigcirc, *, 1_{\underline{T}})$  and  $(\underline{M}; \bigcirc, *, 1_{\underline{M}})$  are GBE-semigroups. Let  $\psi : \underline{T} \to \underline{M}$  be a homomorphism. Then  $\psi$  is 1-1  $\Leftrightarrow$  *Ker*  $(\psi) = \{1_{\underline{T}}\}$ .

#### Proof.

Let  $\psi : \underline{T} \to M$  is a monomorphism. Let  $\tilde{e} \in Ker(\psi) \Rightarrow \psi(\tilde{e}) = 1_M \Rightarrow \psi(\tilde{e}) = \psi(1_T)$ , by Proposition 3.3. As  $\psi$  is 1-1, so it follows that  $\tilde{e} = 1_T$ . Thus  $Ker(\psi) = \{1_T\}$ .

Conversely, suppose that  $Ker(\psi) = \{1_I\}$ . We need to show that  $\psi$  is 1-1. For this let  $\tilde{e}, v \in I$  be such that  $\psi(\tilde{e}) = \psi(v) \Rightarrow \psi(\tilde{e}) * \psi(v) = \psi(v) * \psi(v) \Rightarrow \psi(\tilde{e} * v) = 1_M \Rightarrow \tilde{e} * v \in Ker(\psi) = \{1_I\} \Rightarrow \tilde{e} * v = 1_I \Rightarrow \tilde{e} \leq v$ . Similarly, again taking  $\psi(\tilde{e}) = \psi(v) \Rightarrow \psi(\tilde{e}) * \psi(\tilde{e}) = \psi(v) * \psi(\tilde{e}) \Rightarrow 1_M = \psi(v * \tilde{e}) \Rightarrow v * \tilde{e} \in Ker(\psi) = \{1_I\} \Rightarrow v * \tilde{e} = 1_I \Rightarrow v \leq \tilde{e}$ . It follows that  $\tilde{e} = v \Rightarrow \psi$  is a monomorphism.

#### **Proposition 3.5**

Let us suppose that  $\psi : W \to M$  is a monomorphism of two GBE-semigroups  $(W; \odot, *, 1_W)$  and  $(M; \odot, *, 1_M)$ . Let  $v \in W$  be a unit divisor of W. Then  $\psi(v)$  is a unit divisor of M.

#### Proof.

Suppose  $1_W \neq v \in W$  is a left unit divisor of W, then  $\exists 1_W \neq t \in W$  such that  $v \odot t = 1_W \Rightarrow \psi$   $(v \odot t) = \psi(1_W) \Rightarrow \psi(v) \odot \psi(t) = 1_M$ , as  $\psi(1_W) = 1_M$  and  $\psi$  is a homomorphism. It implies that  $\psi(v)$  is a left unit divisor of M. Similarly let  $1_W \neq v \in W$  be a right unit divisor of W, then  $\exists 1_W \neq t \in W \ni t \odot v = 1_W \Rightarrow \psi(t \odot v) = \psi(1_W) \Rightarrow \psi(t) \odot \psi(v) = 1_M$ , as  $\psi(1_W) = 1_M$  and  $\psi$  is a homomorphism. It implies that  $\psi(v)$  is a right unit divisor of M. This proves what we wanted.

#### **Proposition 3.6**

Suppose that  $(L; \bigcirc_1, *_1, 1_L)$ ,  $(\dot{M}; \bigcirc_2, *_2, 1_{\dot{M}})$  and  $(\dot{N}; \bigcirc_3, *_3, 1_{\dot{N}})$  are GBE-semigroups. Let  $\psi \in Hom(L, \dot{M})$  and suppose that  $\beta \in Hom(\dot{M}, \dot{N})$ , then  $\beta \circ \psi \in Hom(L, \dot{N})$ .

## Proof.

Let  $\psi: L \to \dot{M}$  and  $\beta: \dot{M} \to \dot{N}$  be homomorphisms, then we show  $\beta \circ \psi: L \to \dot{N}$  is a homomorphism. Let  $v, \hat{e} \in L$ , then

$$\beta \circ \psi (v *_1 \hat{e}) = \beta (\psi (v *_1 \hat{e}))$$
$$= \beta (\psi (v) *_2 \psi (\hat{e})) \qquad (\because \psi \text{ is a homomorphism})$$

 $= \beta (\psi(v)) *_{3} \beta (\psi(\hat{e})) \quad (\because \beta \text{ is a homomorphism})$  $= \beta \circ \psi(v) *_{3} \beta \circ \psi(\hat{e}).$ 

Similarly,

$$\beta \circ \psi (v \odot_1 \hat{e}) = \beta (\psi (v \odot_1 \hat{e}))$$
$$= \beta (\psi (v) \odot_2 \psi(\hat{e})) \quad (\because \psi \text{ is a homomorphism})$$
$$= \beta (\psi(v)) \odot_3 \beta (\psi (\hat{e})) (\because \beta \text{ is a homomorphism})$$
$$= \beta \circ \psi (v) \odot_3 \beta \circ \psi (\hat{e}).$$

It follows that  $\beta \circ \psi : L \longrightarrow \dot{N}$  is a homomorphism or in other words,  $\beta \circ \psi \in Hom(L, \dot{N})$ .

## Theorem 3.7

Let us assume that  $(W; \odot, *, 1_W)$  and  $(M; \odot, *, 1_M)$  are two GBE-semigroups and  $\varphi \in Hom(W, M)$  and furthermore suppose that W is transitive, then  $\varphi(W)$  is transitive.

#### Proof.

Let  $\varphi(\hat{e}), \varphi(\hat{r}), \varphi(w) \in \varphi(W)$ . Then  $(\varphi(\hat{e}) * \varphi(w)) * ((\varphi(\hat{e}) * \varphi(\hat{r})) * (\varphi(\hat{e}) * \varphi(w))) = \varphi(\hat{r} * w) * (\varphi(\hat{e} * \hat{r}) * \varphi(\hat{e} * w))$   $= \varphi(\hat{r} * w) * \varphi((\hat{e} * \hat{r}) * (\hat{e} * w))$   $= \varphi((\hat{r} * w) * ((\hat{e} * \hat{r}) * (\hat{e} * w)))$   $= \varphi(1w)$  $= 1_M.$ 

Hence,  $(\varphi(\hat{e}) * \varphi(w)) \leq ((\varphi(\hat{e}) * \varphi(\dot{r})) * (\varphi(\hat{e}) * \varphi(w)))$ . Therefore,  $\varphi(W)$  is transitive.

## Theorem 3.8

Let  $(\mathbf{K}; \odot, *, 1_{\mathbf{K}})$  and  $(\mathbf{M}; \odot, *, 1_{\mathbf{M}})$  be two GBE-semigroups. Assume that  $\varphi : \mathbf{K} \to \mathbf{M}$  is a monomorphism and  $\varphi(\mathbf{K})$  is transitive, then  $\mathbf{K}$  is transitive.

#### Proof.

Let us suppose that  $\dot{r}$ ,  $\hat{e}$ ,  $v \in \mathbf{K}$ . Then  $(\varphi(\hat{e}) * \varphi(v)) * ((\varphi(\dot{r}) * \varphi(\hat{e})) * (\varphi(\dot{r}) * \varphi(v))) = 1_M$ , and thus  $\varphi((\hat{e} * v) * ((\dot{r} * \hat{e}) * (\dot{r} * v))) = 1_M$  implies that  $\varphi((\hat{e} * v) * ((\dot{r} * \hat{e}) * (\dot{r} * v))) = \varphi(1_K)$ . As  $\varphi$  is a monomorphism, so by Proposition 3.4,  $(\hat{e} * v) * ((\dot{r} * \hat{e}) * (\dot{r} * v)) = 1_K$ . Thus,  $\mathbf{K}$  is transitive.

## Theorem 3.9

Suppose  $(L; \bigcirc_1, *_1, 1_L)$ ,  $(M; \bigcirc_2, *_2, 1_M)$  and  $(N; \bigcirc_3, *_3, 1_N)$  are GBE-semigroups. Let  $p: L \to M$  be an epimorphism and  $\overline{g}: L \to N$  a homomorphism. Further suppose that *Ker*  $(p) \subseteq Ker(\overline{g})$ , then  $\exists$  one and only one homomorphism  $v: M \to N \ni v$  o  $p = \overline{g}$ , i.e. in other words the diagram



commutes.

## Proof.

Let  $g \in M$ . As p is surjective so  $\exists n \in L \ni p(n) = g$ . Let us define a mapping

$$v: \mathbf{M} \longrightarrow \mathbf{N}$$
 by  $v(s) = v(p(\dot{n})) = \bar{g}(\dot{n}).$ 

Well-defined: Let  $w, y \in L$ . If g = p(w) = p(y) then,  $1_M = p(w) *_2 p(y)$ . Now as p is a homomorphism, so it follows that  $1_M = p(w *_1 y)$ . Hence,  $w *_1 y \in Ker(p)$ . As  $Ker(p) \subseteq Ker(\bar{g})$ , we have  $1_N = \bar{g}(w) *_3 \bar{g}(y) = \bar{g}(w *_1 y)$ . Similarly, we get  $\bar{g}(y) *_3 \bar{g}(w) = 1_N$ . Thus, it follows that  $\bar{g}(w) = \bar{g}(y) \implies v$  is well-defined. Furthermore, we prove that v is a homomorphism. Now assume  $\hat{e}, t \in M$ , then  $\exists w, y \in L$  such that  $\hat{e} = p(w)$  and t = p(y), as p is onto. Now we have,

$$v(\hat{\varrho} \odot_2 \underline{t}) = v(p(w) \odot_2 p(u))$$
  
=  $v(p(w \odot_1 \underline{u}))$  (:  $p$  is a homomorphism)  
=  $\overline{g}(w \odot_1 \underline{u})$  (:  $v(p(\dot{n})) = \overline{g}(\dot{n}))$   
=  $\overline{g}(w) \odot_3 \overline{g}(\underline{u})$  (:  $\overline{g}$  is a homomorphism)  
=  $v(p(w)) \odot_3 v(p(\underline{u}))$   
=  $v(\hat{\varrho}) \odot_3 v(\underline{t})$ 

and

$$v(\hat{\varrho} *_{2} \underline{\ell}) = v(p(w) *_{2} p(\underline{u}))$$

$$= v(p(w *_{1} \underline{u})) \qquad (\because p \text{ is a homomorphism})$$

$$= \overline{g}(w *_{1} \underline{u}) \qquad (\because v(p(\underline{n})) = \overline{g}(\underline{n}))$$

$$= \overline{g}(w) *_{3} \overline{g}(\underline{u}) \qquad (\because \overline{g} \text{ is a homomorphism})$$

$$= v(p(w)) *_{3} v(p(w))$$
$$= v(\hat{e}) *_{3} v(t).$$

Hence v is a homomorphism.

Now

$$v \circ p(\dot{n}) = v(p(\dot{n})) = \bar{g}(\dot{n}) \Longrightarrow v \circ p = \bar{g}.$$

#### **Uniqueness:**

Let  $v_1: \mathbf{M} \to \mathbf{N}$  be homomorphism such that  $v_1 \circ p = \overline{g}$ .

Now

$$v_1 \circ p(\dot{n}) = \bar{g}(\dot{n}) = v \circ p(\dot{n}) \Longrightarrow v_1(p(\dot{n})) = v(p(\dot{n})) \Longrightarrow v_1(s) = v(s) \Longrightarrow v_1 = v.$$

Hence v is unique.

#### Theorem 3.10

Let us suppose that  $(L; \bigcirc_1, *_1, 1_L)$ ,  $(M; \bigcirc_2, *_2, 1_M)$  and  $(N; \bigcirc_3, *_3, 1_N)$  are GBEsemigroups. Let  $\psi: L \to N$  be a homomorphism and  $\gamma: M \to N$  be a monomorphism. Further, suppose that  $Im(\psi) \subseteq Im(\gamma)$  then there is one and only one homomorphism  $\varphi: L \to M$  such that  $\gamma \circ \varphi = \psi$ , i.e. the diagram



commutes.

#### Proof.

For  $z \in L$ , then  $\psi(z) \in Im(\psi) \subseteq Im(\gamma) \Longrightarrow \psi(z) \in Im(\gamma)$ . Since  $\gamma$  is a monomorphism so  $\exists$  one and only one element  $m \in M \ni \gamma(m) = \psi(z)$ . Let us define a mapping  $\varphi: L \to M$  by  $\varphi(z) = m$ , then  $\gamma \circ \varphi(z) = \gamma(\varphi(z)) = \gamma(m) = \psi(z)$ . It follows that  $\gamma \circ \varphi = \psi$ . Now in order to prove that  $\varphi$  is a homomorphism, assume  $w, s \in L$ , then

$$\gamma (\varphi (w *_1 \xi)) = \psi (w *_1 \xi)) \qquad (since \gamma \circ \varphi (z) = \psi (z))$$
$$= \psi (w) *_3 \psi (\xi) \qquad (since \psi is a homomorphism)$$
$$= \gamma (\varphi (w)) *_3 \gamma (\varphi (\xi)) \qquad (since \gamma (\varphi (z)) = \psi (z))$$

 $= \gamma \left( \varphi \left( w \right) *_2 \varphi \left( s \right) \right)$  (since  $\gamma$  is a homomorphism)

As  $\gamma$  is a one-one so we have  $\varphi(w *_1 s) = \varphi(w) *_2 \varphi(s)$ . Similarly,

$$\gamma (\varphi (w \odot_1 \varsigma)) = \psi (w \odot_1 \varsigma)$$

$$= \psi (w) \odot_3 \psi (\varsigma) \qquad (since \psi is a homomorphism)$$

$$= \gamma (\varphi (w)) \odot_3 \gamma (\varphi (\varsigma))$$

$$= \gamma (\varphi (w) \odot_2 \varphi (\varsigma)) \qquad (since \gamma is a homomorphism)$$

As  $\gamma$  is a monomorphism so we obtain  $\varphi(w \odot_1 \varsigma) = \varphi(w) \odot_2 \varphi(\varsigma)$ . Now let  $\varphi_1: L \to M$  be a homomorphism such that  $\gamma \circ \varphi_1 = \psi$ . Now,

$$\gamma \circ \varphi_{1}(z) = \psi(z)$$

$$\Rightarrow \gamma \circ \varphi_{1}(z) = \gamma \circ \varphi(z)$$

$$\Rightarrow \gamma(\varphi_{1}(z)) = \gamma(\varphi(z))$$

$$\Rightarrow \varphi_{1}(z) = \varphi(z) \qquad (since \gamma is a monomorphism)$$

$$\Rightarrow \varphi_{1} = \varphi.$$

Thus,  $\varphi$  is unique.

We are now going to define left (resp. right) congruence relations in a GBE-semigroup.

#### **Definition 3.11**

Let  $(W; \odot, *, 1_W)$  be a GBE-semigroup and let  $\rho$  be a relation on W, then  $\rho$  is known to be a left compatible relation if for all  $\hat{\varrho}$ ,  $\dot{n}$ ,  $w \in W \ni (\hat{\varrho}, \dot{n}) \in \rho \Longrightarrow (w \odot \hat{\varrho}, w \odot \dot{n}) \in \rho$  and  $(w * \hat{\varrho}, w * \dot{n}) \in \rho$ . In the same way, let  $\rho$  be a relation on a GBE-semigroup  $(W; \odot, *, 1_W)$ , then  $\rho$  is known to be a right compatible relation if for all  $\hat{\varrho}$ ,  $\dot{n}$ ,  $w \in W \ni (\hat{\varrho}, \dot{n}) \in \rho \Longrightarrow$  $(\hat{\varrho} \odot w, \dot{n} \odot w) \in \rho$  and  $(\hat{\varrho} * w, \dot{n} * w) \in \rho$ .

#### **Definition 3.12**

Let  $\rho$  be a relation on a GBE-semigroup ( $\mathbf{K}$ ;  $\odot$ , \*,  $1_{\mathbf{K}}$ ), then  $\rho$  is called compatible if for all  $\hat{e}, \dot{n}, v, \varsigma \in \mathbf{K} \ni (\hat{e}, \dot{n}), (v, \varsigma) \in \rho \Longrightarrow (\hat{e} \odot v, \dot{n} \odot \varsigma), (\hat{e} * v, \dot{n} * \varsigma) \in \rho$ .

It should be noted that if a relation is left compatible as well as equivalence relation, then it is known to be a left congruence relation. Also note that if a relation is right compatible as well as equivalence relation, then it is known to be a right congruence relation. Furthermore, note that if a relation is compatible as well as equivalence relation, then it known to be a congruence relation.

Let us give some examples in order to understand the above concepts.

## Example 3.13

- (i) It is obvious that  $\nabla = W \times W$  and  $\Delta = \{(\varsigma, \varsigma) : \varsigma \in W\}$  are congruence relations on a GBE-semigroup  $(W; \odot, *, 1_W)$ .
- (ii) Let  $U = \{1_U, 2, 3, 4\}$  and the operations "\*" and " $\odot$ " be defined as follows:

Ο	1 <sub>U</sub>	2	3	4
1 <sub>U</sub>	1 <sub>U</sub>	$1_{U}$	$1_{U}$	1 <sub>U</sub>
2	1 <sub>U</sub>	$1_{U}$	1 <sub>U</sub>	1 <sub>U</sub>
3	1 <sub>U</sub>	1 <sub>U</sub>	1 <sub>U</sub>	2
4	1 <sub>U</sub>	$1_{U}$	1 <sub>U</sub>	1 <sub>U</sub>

*	$1_{U}$	2	3	4
1 <sub>U</sub>	$1_{U}$	$1_{U}$	$1_{U}$	1 <sub>U</sub>
2	$1_{U}$	$1_{U}$	$1_{U}$	1 <sub>U</sub>
3	$1_{U}$	2	1 <sub>U</sub>	2
4	1 <sub>U</sub>	1 <sub>U</sub>	1 <sub>U</sub>	1 <sub>U</sub>

Then  $(\underline{U}; \odot, *, 1_{\underline{U}})$  is a GBE-semigroup. Let  $\theta = \Delta \cup \{(2, 1_{\underline{U}}), (1_{\underline{U}}, 2)\}$ . Here  $\theta$  is a congruence relation on  $\underline{U}$ .

Let us state and prove some results. The results are true in case of semigroups and we convert them into GBE-semigroups. The following result gives us equivalent conditions for congruence relations in GBE-semigroups.

#### **Proposition 3.14**

Let  $\rho$  be an equivalence relation on a GBE-semigroup (K;  $\odot$ , \*,  $1_K$ ). Then the following are equivalent:

- (i)  $\rho$  is a congruence relation on the GBE-semigroup **K**.
- (ii)  $\rho$  is left and right congruence relation on the GBE-semigroup **K**.

## Proof.

(i)  $\Rightarrow$  (ii) In order to prove that  $\rho$  is left as well as right congruence relation, assume that  $\hat{\rho}$ ,  $\tilde{n}, v \in \mathbf{K}$  such that  $(\hat{\rho}, \tilde{n}) \in \rho$ . Now  $(v, v) \in \rho$ , because  $\rho$  is reflexive. As  $\rho$  is compatible, so it follows that  $(v \odot \hat{\rho}, v \odot \tilde{n}), (v * \hat{\rho}, v * \tilde{n}) \in \rho$ . It follows that  $\rho$  is a left congruence relation. Similarly, we can also prove that  $(\hat{\rho} \odot v, \tilde{n} \odot v), (\hat{\rho} * v, \tilde{n} * v) \in \rho$ . It follows that  $\rho$  is a right congruence relation.

(ii)  $\Rightarrow$  (i) In order to prove that  $\rho$  is a congruence relation suppose  $\hat{e}$ ,  $\tilde{n}$ ,  $v, \varsigma \in \mathbf{K} \ni (\hat{e}, \tilde{n})$ ,  $(v, \varsigma) \in \rho$ . Now  $(\hat{e} \odot v, \tilde{n} \odot v)$ ,  $(\hat{e} * v, \tilde{n} * v) \in \rho$ , because  $\rho$  is right compatible and  $(\tilde{n} \odot v, \tilde{n} \odot \varsigma)$ ,  $(\tilde{n} * v, \tilde{n} * \varsigma) \in \rho$ , because  $\rho$  is left compatible. By transitivity, it follows that  $(\hat{e} \odot v, \tilde{n} \odot \varsigma)$ ,  $(\hat{e} * v, \tilde{n} * \varsigma) \in \rho$ . It proves what we wanted.

The below theorem confirms that every homomorphism gives us a congruence relation.

#### Theorem 3.15

Suppose  $(W; \odot, *, 1_W)$  and  $(T; \odot, *, 1_T)$  are two GBE-semigroups. Let  $\check{h}: W \to T$  be a homomorphism. Then  $\check{h}$  defines a congruence relation  $\delta$  on W as follows:

$$\delta = \{(\varsigma, v) \in W \times W: h(\varsigma) = h(v)\}.$$

#### Proof.

In order to prove that h defines the above congruence relation  $\delta$  on W, we need to prove that  $\delta$  is a compatible equivalence relation on W. First, we prove that  $\delta$  is an equivalence relation on W.

## **Reflexive:**

As  $\check{h}(s) = \check{h}(s) \forall s \in W$ , so it follows that  $(s, s) \in \delta \forall s \in W$ . Thus  $\delta$  is reflexive.

### Symmetric:

Assume  $\xi, v \in W \ni (\xi, v) \in \delta \implies \check{h}(\xi) = \check{h}(v) \implies \check{h}(\xi) \implies (v, \xi) \in \delta$ . Thus  $\delta$  is symmetric.

#### **Transitive:**

Let  $\xi, v, \psi \in W$  such that  $(\xi, v), (v, \psi) \in \delta \implies \check{h}(\xi) = \check{h}(v)$  and  $\check{h}(v) = \check{h}(\psi)$ . By transitive property of equality, it follows that  $\check{h}(\xi) = \check{h}(\psi) \implies (\xi, \psi) \in \delta$ . Thus  $\delta$  is transitive.

We now show that  $\delta$  is a compatible relation on W. Assume that  $\varsigma$ , v, u,  $\hat{e} \in W \ni (\varsigma, v)$ ,  $(u, \hat{e}) \in \delta \Longrightarrow \check{h}(\varsigma) = \check{h}(v)$  and  $\check{h}(u) = \check{h}(\hat{e})$ .

Now,

$$\check{h}(\varsigma) \odot \check{h}(\psi) = \check{h}(v) \odot \check{h}(\hat{\varphi}) \text{ and } \check{h}(\varsigma) * \check{h}(\psi) = \check{h}(v) * \check{h}(\hat{\varphi})$$
$$\implies \check{h}(\varsigma \odot \psi) = \check{h}(v \odot \hat{\varphi}) \text{ and } \check{h}(\varsigma * \psi) = \check{h}(v * \hat{\varphi})$$
$$\implies (\varsigma \odot \psi, v \odot \hat{\varphi}) \text{ and } (\varsigma * \psi, v * \hat{\varphi}) \in \delta.$$

Hence, it follows that  $\delta$  is a compatible relation on W. This completes the proof.

We are now going to define congruence class and then discuss factor GBE-semigroup.

#### **Definition 3.16**

Let  $(W; \bigcirc, *, 1_W)$  be a GBE-semigroup. If  $\delta$  is a congruence relation on W then we define for  $\psi \in W$ 

$$y \delta = \{s \in W: (s, y) \in \delta\}$$

which is called a congruence class corresponding to an element u. Let  $W / \delta = \{u \delta : u \in W\}$ , that is  $W / \delta$  consists of all congruence classes corresponding to the elements of

W. Our aim is to show that  $W / \delta$  is a GBE-semigroup. For this, we define " $\Theta$ " and "\*" on  $W / \delta$  as follows:

$$u \delta \odot s \delta = (u \odot s) \delta$$

and

$$\mathfrak{u}\,\delta \,\ast\,\mathfrak{s}\,\delta = (\mathfrak{u}\,\ast\,\mathfrak{s})\,\delta \,\,\forall\,\mathfrak{u}\,\delta,\mathfrak{s}\,\delta \in W/\delta.$$

# Well-defined:

Assume  $v_1 \delta$ ,  $v_2 \delta$ ,  $\dot{s}_1 \delta$ ,  $\dot{s}_2 \delta \in W/\delta$  such that

$$v_{1} \delta = v_{2} \delta \text{ and } \dot{s}_{1} \delta = \dot{s}_{2} \delta$$

$$\Rightarrow (v_{1}, v_{2}) \in \delta \text{ and } (\dot{s}_{1}, \dot{s}_{2}) \in \delta$$

$$\Rightarrow (v_{1} \odot \dot{s}_{1}, v_{2} \odot \dot{s}_{2}) \text{ and } (v_{1} * \dot{s}_{1}, v_{2} * \dot{s}_{2}) \in \delta \quad (\because \delta \text{ is a congruence relation})$$

$$\Rightarrow (v_{1} \odot \dot{s}_{1}) \delta = (v_{2} \odot \dot{s}_{2}) \delta \text{ and } (v_{1} * \dot{s}_{1}) \delta = (v_{2} * \dot{s}_{2}) \delta$$

$$\Rightarrow v_{1} \delta \odot \dot{s}_{1} \delta = v_{2} \delta \odot \dot{s}_{2} \delta \text{ and } v_{1} \delta * \dot{s}_{1} \delta = v_{2} \delta * \dot{s}_{2} \delta.$$

We now prove that  $(W / \delta, \Theta)$  is a semigroup.

## **Closure property:**

It is clear from the definition.

## Associative property:

Let  $\dot{r} \delta$ ,  $v \delta$ ,  $\xi \delta \in W/\delta$ , then

$$(\dot{r}\,\delta\,\Theta\,v\,\delta)\,\Theta\,\underline{t}\,\delta = (\dot{r}\,\odot\,v)\,\delta\,\Theta\,\underline{t}\,\delta$$
$$= ((\dot{r}\,\odot\,v)\,\odot\,\underline{t})\,\delta$$
$$= (\dot{r}\,\odot\,(v\,\odot\,\underline{t}))\,\delta \quad (\because\,W\,\text{is a GBE-semigroup})$$
$$= \dot{r}\,\delta\,\Theta\,(v\,\odot\,\underline{t})\,\delta$$
$$= \dot{r}\,\delta\,\Theta\,(v\,\delta\,\odot\,\underline{t}\,\delta).$$

Thus associative property holds under " $\Theta$ ". Thus,  $(W / \delta, \Theta)$  is a semigroup.

We now show that  $(W/\delta; *, 1_W \delta)$  is a GBE-algebra. For this we have

(i) 
$$v \delta * v \delta = (v * v) \delta = 1_W \delta$$
 for all  $v \delta \in W / \delta$ .

(ii)  $v \delta * 1_W \delta = (v * 1_W) \delta = 1_W \delta$  for all  $v \delta \in W / \delta$ .

(iii)  $v \delta * (\mu \delta * \hat{e} \delta) = v \delta * (\mu * \hat{e}) \delta$ 

$$= (v * (\psi * \hat{\varphi})) \delta$$
  
=  $(\psi * (v * \hat{\varphi})) \delta$  (: W is a GBE-semigroup)  
=  $\psi \delta * (v * \hat{\varphi}) \delta$   
=  $\psi \delta * (v \delta * \hat{\varphi} \delta)$  for all  $v \delta$ ,  $\psi \delta$ ,  $\hat{\varphi} \delta \in W/\delta$ .

We now show that distributive laws hold in  $W/\delta$ . For this, let  $\tilde{e} \delta$ ,  $w \delta$ ,  $\dot{n} \delta \in W/\delta$ , then

$$\tilde{e} \,\delta \,\Theta \,(w \,\delta \,*\, \dot{n} \,\delta) = \tilde{e} \,\delta \,\Theta \,(w \,*\, \dot{n}) \,\delta$$
$$= (\tilde{e} \,\Theta \,(w \,*\, \dot{n})) \,\delta$$
$$= ((\tilde{e} \,\Theta \,w) \,*\, (\tilde{e} \,\odot\, \dot{n})) \,\delta \qquad (\because \mathbf{W} \text{ is a GBE-semigroup})$$
$$= (\tilde{e} \,\Theta \,w) \,\delta \,*\, (\tilde{e} \,\odot\, \dot{n}) \,\delta$$
$$= (\tilde{e} \,\delta \,\Theta \,w \,\delta) \,*\, (\tilde{e} \,\delta \,\Theta\, \dot{n} \,\delta).$$

Also

$$(\tilde{e} \ \delta \ * \ w \ \delta) \ \Theta \ \dot{n} \ \delta = (\tilde{e} \ * \ w) \ \delta \ \Theta \ \dot{n} \ \delta$$
$$= ((\tilde{e} \ * \ w) \ \odot \ \dot{n}) \ \delta$$
$$= ((\tilde{e} \ \odot \ \dot{n}) \ * (w \ \odot \ \dot{n})) \ \delta \qquad (\because W \ is \ a \ GBE-semigroup)$$
$$= (\tilde{e} \ \odot \ \dot{n}) \ \delta \ * (w \ \odot \ \dot{n}) \ \delta$$
$$= (\tilde{e} \ \delta \ \odot \ \dot{n} \ \delta) \ * (w \ \delta \ \odot \ \dot{n} \ \delta).$$

The above calculation shows  $(W / \delta, \Theta, *, 1_W \delta)$  is a GBE-semigroup and is called quotient or factor GBE-semigroup.

The following results give us some properties of quotient GBE-semigroups.

# Theorem 3.17

Let  $\delta$  be a congruence relation on a GBE-semigroup ( $\hat{W}$ ;  $\mathfrak{O}_1, *_1, 1_{\hat{W}}$ ). Then  $\hat{W}/\delta$  is a GBE-

semigroup with respect to the following binary operations.

- (i)  $\acute{w} \delta \Theta_1 \varsigma \delta = (\acute{w} \Theta_1 \varsigma) \delta$ ,
- (ii)  $\dot{w} \delta *_1 \varsigma \delta = (\dot{w} *_1 \varsigma) \delta \forall \dot{w} \delta, \varsigma \delta \in \mathbf{W} / \delta.$

Let us define  $\delta^{\#}: \hat{W} \to \hat{W}/\delta$  by  $\delta^{\#}(\hat{w}) = \hat{w} \delta \forall \hat{w} \in \hat{W}$ , then  $\delta^{\#}$  is an epimorphism. Let  $\psi: \dot{W} \to T$  be a homomorphism, where  $(\dot{W}; \odot_1, *_1, 1_{\dot{W}})$  and  $(T; \odot_2, *_2, 1_T)$  are GBEsemigroups, then the relation

Ker 
$$\psi = \{(\dot{w}, \varsigma) \in \acute{W} \times \acute{W}: \psi(\dot{w}) = \psi(\varsigma)\}$$

,

is a congruence relation on  $\hat{W}$ . Moreover, there is a monomorphism  $\beta: \hat{W} / Ker \psi \to T \ni Im(\beta) = Im(\psi)$  and  $\beta(Ker \psi)^{\#} = \psi$ .

#### Proof.

 $\hat{W}/\delta$  is a GBE-semigroup with respect to the binary operation "O" and "\*" and it is clear from the above discussion. We now prove that  $\delta^{\#}: \hat{W} \to \hat{W}/\delta$  is an epimorphism.

## Well-defined:

Let  $\hat{e}, v \in \mathbf{W}$  be  $\exists \hat{e} = v \Longrightarrow \hat{e} \delta = v \delta \Longrightarrow \delta^{\#}(\hat{e}) = \delta^{\#}(v) \Longrightarrow \delta^{\#}$  is well-defined.

#### Homomorphism:

Let  $w_1, w_2 \in \mathbf{W}$ , then

$$\delta^{\#}(w_1 \bigodot_1 w_2) = (w_1 \oslash_1 w_2) \delta$$
$$= w_1 \delta \oslash_1 w_2 \delta$$
$$= \delta^{\#}(w_1) \oslash_1 \delta^{\#}(w_2)$$

and

$$\delta^{\#}(w_1 *_1 w_2) = (w_1 *_1 w_2) \delta$$
  
=  $w_1 \delta *_1 w_2 \delta$   
=  $\delta^{\#}(w_1) *_1 \delta^{\#}(w_2).$ 

It follows that,  $\delta^{\#}$  is a homomorphism.

#### **Onto:**

Clearly  $\delta^{\#}$  is onto, because for each  $\dot{w} \, \delta \in \dot{W} / \delta$  there exists  $\dot{w} \in \dot{W}$  such that  $\delta^{\#}(\dot{w}) = \dot{w} \, \delta$ . Thus,  $\delta^{\#}$  is an epimorphism.

The relation Ker  $\psi = \{(\psi, \varsigma) \in \mathbf{W} \times \mathbf{W}: \psi(\psi) = \psi(\varsigma)\}\$  is a congruence relation because of Theorem 3.15.

Now define,  $\beta: \hat{W} / Ker \psi \to T$  by  $\beta(w Ker \psi) = \psi(w) \forall w Ker \psi \in \hat{W} / Ker \psi$ . First we show that the defined map is a monomorphism. For this,

## Well-defined:

Let  $w_1 Ker \psi$ ,  $w_2 Ker \psi \in \acute{W} / Ker \psi$  be such that

$$w_1 \mathbf{Ker} \ \psi = w_2 \mathbf{Ker} \ \psi$$
$$\implies (w_1, w_2) \in \mathbf{Ker} \ \psi$$

$$\Rightarrow \psi(w_1) = \psi(w_2)$$
$$\Rightarrow \beta(w_1 \operatorname{Ker} \psi) = \beta(w_2 \operatorname{Ker} \psi).$$

Thus,  $\beta$  is well-defined.

## Homomorphism:

Let  $v Ker \psi$ ,  $\hat{e} Ker \psi \in \hat{W} / Ker \psi$ , then

$$\beta(v \operatorname{Ker} \psi *_2 \hat{e} \operatorname{Ker} \psi) = \beta((v *_1 \hat{e}) \operatorname{Ker} \psi)$$
  
=  $\psi(v *_1 \hat{e})$   
=  $\psi(v) *_2 \psi(\hat{e})$  (::  $\psi$  is a homomorphism)  
=  $\beta(v \operatorname{Ker} \psi) *_2 \beta(\hat{e} \operatorname{Ker} \psi)$ 

and

$$\beta(v \operatorname{Ker} \psi \odot_2 \hat{e} \operatorname{Ker} \psi) = \beta((v \odot_1 \hat{e}) \operatorname{Ker} \psi)$$
$$= \psi(v \odot_1 \hat{e})$$
$$= \psi(v) \odot_2 \psi(\hat{e}) \quad (\because \psi \text{ is a homomorphism})$$
$$= \beta(v \operatorname{Ker} \psi) \odot_2 \beta(\hat{e} \operatorname{Ker} \psi)$$

Thus,  $\beta$  is a homomorphism.

# **One-One:**

Let  $\psi_1 \operatorname{Ker} \psi$ ,  $\psi_2 \operatorname{Ker} \psi \in \acute{W} / \operatorname{Ker} \psi$  be such that

$$\beta(\psi_1 \operatorname{Ker} \psi) = \beta(\psi_2 \operatorname{Ker} \psi)$$
$$\Rightarrow \psi(\psi_1) = \psi(\psi_2)$$
$$\Rightarrow (\psi_1, \psi_2) \in \operatorname{Ker} \psi$$
$$\Rightarrow \psi_1 \operatorname{Ker} \psi = \psi_2 \operatorname{Ker} \psi.$$

Thus,  $\beta$  is one-one. It follows that  $\beta$  is a monomorphism. We now prove  $Im(\beta) = Im(\psi)$ . Here,

$$Im(\psi) = \{\psi(w) : w \in \mathbf{\acute{W}}\} = \{\beta(w \operatorname{Ker} \psi) : w \operatorname{Ker} \psi \in \mathbf{\acute{W}} / \operatorname{Ker} \psi\} = Im(\beta).$$

At the end, we show that  $\beta(\operatorname{Ker} \psi)^{\#} = \psi$ . In other words,  $(\beta(\operatorname{Ker} \psi)^{\#})(\psi) = \psi(\psi) \forall \psi \in W$ . Here,

$$(\beta(\operatorname{Ker} \psi)^{\#})(u) = \beta((\operatorname{Ker} \psi)^{\#}(u)) = \beta(u \operatorname{Ker} \psi) = \psi(u).$$

## Theorem 3.18

Let  $\rho$  be a congruence relation on a GBE-semigroup  $(V; \bigcirc_1, *_1, 1_V)$  and let  $\varphi: V \to T$  be a monomorphism from  $(V; \bigcirc_1, *_1, 1_V)$  to  $(T; \bigcirc_2, *_2, 1_T)$  such that  $\rho \subseteq Ker \varphi$ . Then there is a unique homomorphism  $\beta: V/\rho \to T \ni Im(\beta) = Im(\varphi)$  and  $\beta \circ \rho^{\#} = \varphi$ .

## Proof.

Define  $\beta: V/\rho \rightarrow T$  as follows:

$$\beta(v \rho) = \varphi(v) \ \forall v \rho \in V/\rho.$$

# Well-defined:

Assume that  $\psi \rho, \varsigma \rho \in V/\rho$  are such that

$$\dot{w} \rho = \varsigma \rho$$
$$\Rightarrow (\dot{w}, \varsigma) \in \rho \subseteq Ker \varphi$$
$$\Rightarrow (\dot{w}, \varsigma) \in Ker \varphi$$
$$\Rightarrow \varphi(\dot{w}) = \varphi(\varsigma)$$
$$\Rightarrow \beta(\dot{w} \rho) = \beta(\varsigma \rho).$$

Thus,  $\beta$  is well-defined.

## Homomorphism:

Let  $\underline{w} \rho$ ,  $\underline{\hat{e}} \rho \in V / \rho$  then,

$$\beta(\psi \rho * \hat{\psi} \rho) = \beta((\psi *_1 \hat{\psi}) \rho)$$
  
=  $\varphi(\psi *_1 \hat{\psi})$   
=  $\varphi(\psi) *_2 \varphi(\hat{\psi})$  (:  $\varphi$  is a homomorphism)  
=  $\beta(\psi \rho) *_2 \beta(\hat{\psi} \rho)$ 

and

$$\beta(\boldsymbol{u} \ \rho \ \odot \ \hat{\boldsymbol{\varrho}} \ \rho) = \beta((\boldsymbol{u} \ \odot_1 \ \hat{\boldsymbol{\varrho}}) \ \rho)$$
  
=  $\varphi(\boldsymbol{u} \ \odot_1 \ \hat{\boldsymbol{\varrho}})$   
=  $\varphi(\boldsymbol{u}) \ \odot_2 \varphi(\hat{\boldsymbol{\varrho}})$  (::  $\varphi$  is a homomorphism)  
=  $\beta(\boldsymbol{u} \ \rho) \ \odot_2 \beta(\hat{\boldsymbol{\varrho}} \ \rho).$ 

Thus,  $\beta$  is a homomorphism. We now prove  $Im(\beta) = Im(\varphi)$ .

Here,

$$Im(\varphi) = \{\varphi(v) : v \in V\} = \{\beta(v \rho) : v \rho \in V/\rho\} = Im(\beta).$$

We now show that  $\beta \circ \rho^{\#} = \varphi$ . In other words,  $(\beta \rho^{\#})(v) = \varphi(v) \forall v \in V$ . Here

$$(\beta \rho^{\#})(v) = \beta(\rho^{\#}(v)) = \beta(v \rho) = \varphi(v),$$

#### Uniqueness:

Let  $\beta_1: V/\rho \to T$  be a homomorphism such that  $\beta_1 \rho^{\#} = \varphi$ .

Now,

$$\beta_1 \rho^{\#}(v) = \beta_1(\rho^{\#}(v)) = \beta_1(v \rho) = \varphi(v) = \beta \rho^{\#}(v) = \beta(v \rho).$$

It follows that  $\beta_1(v \rho) = \beta(v \rho)$  and so  $\beta_1 = \beta$ .

# Theorem 3.19

Let  $\rho$ ,  $\sigma$  be congruence relations on a GBE-semigroup (W;  $\odot$ , \*,  $1_W$ ) such that  $\rho \subseteq \sigma$ . Then

$$\sigma/\rho = \{(\underline{u}\,\rho, \hat{e}\,\rho) \in W/\rho \times W/\rho : (\underline{u}, \hat{e}) \in \sigma\}$$

is a congruence relation on  $W/\rho$  and  $(W/\rho)/(\sigma/\rho) \cong W/\sigma$ .

#### Proof.

First we show that  $\sigma/\rho$  is a congruence relation on  $W/\rho$ .

#### **Reflexive:**

As  $(\underline{u}, \underline{u}) \in \sigma \forall \underline{u} \in W$ , because  $\sigma$  is reflexive, so it follows that  $(\underline{u} \rho, \underline{u} \rho) \in \sigma / \rho$ . Thus,  $\sigma / \rho$  is reflexive.

## Symmetric:

Take  $\psi \rho$ ,  $\hat{\varrho} \rho \in W/\rho \ni (\psi \rho, \hat{\varrho} \rho) \in \sigma / \rho \Longrightarrow (\psi, \hat{\varrho}) \in \sigma \Longrightarrow (\hat{\varrho}, \psi) \in \sigma$ , because  $\sigma$  is symmetric. Thus,  $(\hat{\varrho} \rho, \psi \rho) \in \sigma / \rho$ . This implies that  $\sigma / \rho$  is symmetric.

## **Transitive:**

Let  $\mu \rho$ ,  $\hat{e} \rho$ ,  $\nu \rho \in W/\rho$  be such that  $(\mu \rho, \hat{e} \rho)$ ,  $(\hat{e} \rho, \nu \rho) \in \sigma/\rho \Longrightarrow (\mu, \hat{e})$ ,  $(\hat{e}, \nu) \in \sigma \Longrightarrow$  $(\mu, \nu) \in \sigma$ , because  $\sigma$  is transitive. Thus,  $(\mu \rho, \nu \rho) \in \sigma/\rho$  and so  $\sigma/\rho$  is transitive.

It follows that  $\sigma/\rho$  is an equivalence relation.

## For compatibility:

Let  $\psi \rho$ ,  $\hat{e} \rho$ ,  $v \rho$ ,  $\tilde{n} \rho \in W/\rho$  be such that  $(\psi \rho, \hat{e} \rho)$ ,  $(v \rho, \tilde{n} \rho) \in \sigma/\rho \Longrightarrow (\psi, \hat{e})$ ,  $(v, \tilde{n}) \in \sigma \Longrightarrow (\psi \odot v, \hat{e} \odot \tilde{n})$ ,  $(\psi * v, \hat{e} * \tilde{n}) \in \sigma$ , because  $\sigma$  is compatible. Thus, it follows that

$$((\underline{u} \odot \underline{v}) \rho, (\underline{\hat{e}} \odot \tilde{n}) \rho), ((\underline{u} * \underline{v}) \rho, (\underline{\hat{e}} * \tilde{n}) \rho) \in \sigma / \rho.$$

In other words,

$$(\underline{u}\,\rho\,\bigcirc_1\,v\,\rho,\,\hat{e}\,\rho\,\bigcirc_1\,\tilde{n}\,\rho),\,(\underline{u}\,\rho*_1\,v\,\rho,\,\hat{e}\,\rho*_1\,\tilde{n}\,\rho)\in\sigma/\rho.$$

It follows that  $\sigma/\rho$  is a compatible relation. Hence,  $\sigma/\rho$  is a congruence relation.

Define  $\varphi: W/\rho \longrightarrow W/\sigma$  by  $\varphi(w\rho) = w\sigma \forall w\rho \in W/\rho$ .

#### Well-defined:

Suppose  $w_1 \rho, w_2 \rho \in W/\rho \ni$ 

$$w_1 \rho = w_2 \rho$$
  

$$\Rightarrow (w_1, w_2) \in \rho$$
  

$$\Rightarrow (w_1, w_2) \in \rho \subseteq \sigma$$
  

$$\Rightarrow (w_1, w_2) \in \sigma$$
  

$$\Rightarrow w_1 \sigma = w_2 \sigma$$
  

$$\Rightarrow \varphi(w_1 \rho) = \varphi(w_2 \rho).$$

Thus,  $\varphi$  is well-defined.

## Homomorphism:

Let  $\hat{w} \rho$ ,  $s \rho \in W/\rho$  then,

$$\varphi(\psi \ \rho \ *_1 \ g \ \rho) = \varphi((\psi \ * \ g) \rho)$$
$$= (\psi \ * \ g) \ \sigma$$
$$= \psi \ \sigma \ *_2 \ g \ \sigma$$
$$= \varphi(\psi \ \rho) \ *_2 \ \varphi(g \ \rho).$$

Also,

$$\varphi(\acute{w} \rho \odot_1 \varsigma \rho) = \varphi((\acute{w} \odot \varsigma)\rho)$$
$$= (\acute{w} \odot \varsigma) \sigma$$
$$= \acute{w} \sigma \odot_2 \varsigma \sigma$$

$$= \varphi(\psi \rho) \odot_2 \varphi(\wp \rho).$$

Thus,  $\varphi$  is a homomorphism. Now by Theorem 3.17, there is a monomorphism  $: (W/\rho)/Ker \varphi \to W/\sigma$  which may be defined by

$$(\mu \rho(\operatorname{Ker} \varphi)) = \mu \sigma \forall \mu \rho(\operatorname{Ker} \varphi) \in (W/\rho) / \operatorname{Ker} \varphi.$$

## **Onto:**

As for each  $\psi \sigma \in W/\sigma \exists \psi \rho(Ker \varphi) \in (W/\rho)/Ker \varphi$  such that  $\beta(\psi \rho(Ker \varphi)) = \psi \sigma$ , so it follows that  $\beta$  is onto. Thus,  $(W/\rho)/Ker \varphi \cong W/\sigma$ . We now show that  $Ker \varphi = \sigma/\rho$ .

Here,

$$Ker \ \varphi = \{(\psi \ \rho, \hat{e} \ \rho) \in W/\rho \times W/\rho; \ \varphi(\psi \ \rho) = \varphi(\hat{e} \ \rho)\}$$
$$= \{(\psi \ \rho, \hat{e} \ \rho) \in W/\rho \times W/\rho; \ \psi \ \sigma = \hat{e} \ \sigma)\}$$
$$= \{(\psi \ \rho, \hat{e} \ \rho) \in W/\rho \times W/\rho; \ (\psi, \hat{e}) \in \sigma\}$$
$$= \sigma/\rho.$$

Thus,  $(W/\rho)/(\sigma/\rho) \cong W/\sigma$ .

## **4** CONCLUSION

In this paper, a homomorphism between two generalized BE-semigroups has been defined with some non-trivial examples. Further, it has been shown that each such homomorphism defines a congruence relation. The congruence relation has been utilized to obtain quotient generalized BE-semigroups. Properties analogous to first, second and third isomorphism theorems have been explored. Results discussed in this paper have applications in different fields of mathematics and computer science for defining and developing various algebraic structures.

## REFERENCES

[1] K. Is'eki and S. Tanaka, "An introduction to the theory of BCK-algebras", *Mathematica Japonica*, **23**, 1-26 (1978).

[2] K. Is'eki, "On BCI-algebras", Mathematics Seminar Notes, 8 (1), 125-130 (1980).

[3] J. Neggers and H.S. Kim, "On d-algebras", Mathematica Slovaca, 49, 19-26 (1999).

[4] Y.B. Jun, E.H. Roh and H.S. Kim, "On BH-algebras", *Scientiae Mathematicae Japonicae Online*, 1, 347-354 (1998).

[5] H.S. Kim and Y. H. Kim, "On BE-algebras", *Scientiae Mathematicae Japonicae Online*, **2006** (e), 1299-1302 (2006).

[6] S.S. Ahn and K.S. So, "On ideals and upper sets in BE-algebras", *Scientiae Mathematicae Japonicae*, **68** (2), 279-285 (2008).

[7] S.S. Ahn and K.S. So, "On generalized upper sets in BE-algebras", *Bulletin of the Korean Mathematical Society*, **46** (2), 281-287 (2009).

[8] S.S. Ahn and Y.H. Kim, "On BE-semigroups", *International Journal of Mathematics and Mathematical Sciences*, **2011**, Article ID 676020, 8 pages (2011).

[9] A.H. Handam, "On BE-homomorphisms of BE-semigroups", *International Journal of Pure and Applied Mathematics*, **78** (8), 1211-1220 (2012).

[10] P. Yiarayong and P. Wachirawongsakorn, "A new generalization of BE-algebras", *Heliyon*, 4, Article ID e00863, 17 pages (2018).

[11] Javeria, *Generalized BE-semigroups*, M.Phil. Thesis, Abbottabad University of Science and Technology, Abbottabad, Pakistan, (2019).

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# SOME PROPERTIES OF k-GENERALIZED FIBONACCI NUMBERS

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**Summary.** In the present paper, we propose some properties of the new family k-generalized Fibonacci numbers which related to generalized Fibonacci numbers. Moreover, we give some identities involving binomial coefficients for k-generalized Fibonacci numbers.

## **1 INTRODUCTION**

Fibonacci numbers have a great importance in mathematics. It is one of the most popular sequences that have a lot of applications in many branch of mathematics as in diverse sciences [1, 2, 6, 7, 10-13, 16-20]. The Fibonacci numbers  $F_n$  are given by the recurrence relation

$$F_{n+1} = F_n + F_{n-1}, \qquad n \ge 1$$

with the initial conditions  $F_0 = 0$  and  $F_1 = 1$ . Koshy [9] written one of the most popular books of Fibonacci and Lucas numbers, and gave numerous recurrence relations, generalizations and applications of Fibonacci and Lucas numbers. For  $a, b \in \mathbb{R}$  and  $n \ge 1$ , the well-known generalized Fibonacci numbers are defined

$$G_{n+1} = G_n + G_{n-1}$$

where  $G_0 = a$  and  $G_1 = b$ .

Falcon and Plaza [4] introduced general k-Fibonacci numbers and gave some properties of these numbers. Guleç et al. [5] presented some properties of generalized Fibonacci numbers with binomial coefficients.

El-Mikkawy and Sogabe [3] proposed a new family of *k*-Fibonacci numbers and gave the relationship between the *k*-Fibonacci numbers and Fibonacci numbers as follow:

$$F_n^{(k)} = (F_m)^{k-r} (F_{m+1})^r$$
,  $n = mk + r$ .

In [14], Özkan et al. defined a new family of k-Lucas numbers and gave some identities of the new family of k-Fibonacci and k-Lucas numbers. Özkan et al. [15] introduced some identities of the new family of k-Fibonacci numbers. In this study, we present some identities of the new family of k-generalized Fibonacci numbers. We give relationships between the new family of k-Fibonacci numbers and kgeneralized Fibonacci numbers. Also, we introduce Cassini formulas of k-generalized Fibonacci numbers and some properties involving binomial coefficients. The rest of the paper is organized as follows: In Section 2 (Preliminaries), the fundamental definitions and theorems are given. Then main theorems and proofs are introduced in Section 3.

#### 2010 Mathematics Subject Classification: 11B39.

Key words and Phrases: Fibonacci numbers; generalized Fibonacci numbers; generalized k-Fibonacci numbers.

## **2 PRELIMINIARIES**

**Definition 2.1.** [21] For  $n, k \ (k \neq 0) \in \mathbb{N}$ , the new family of *k*-generalized Fibonacci numbers are defined by

$$G_n^{(k)} = \frac{1}{(\sqrt{5})^k} ([a+b\alpha]\alpha^{m+1} - [a+b\beta]\beta^{m+1})^r ([a+b\alpha]\alpha^m - [a+b\beta]\beta^m)^{k-r}$$

where n = mk + r,  $0 \le r < k$  and  $m \in \mathbb{N}$ .

It is clear that for a = 0 and b = 1,  $G_n^{(k)} = F_n^{(k)}$  and for k = 1, r = 0 and n = m,  $G_n^{(1)} = G_n$ . Then they gave the relationship of between the new family of k-generalized Fibonacci numbers and generalized Fibonacci numbers as follow:

$$G_n^{(k)} = (G_m)^{k-r} (G_{m+1})^r, \qquad n = mk + r.$$
 (2.1)

## **Theorem 2.2.** [9]

i.  $G_{n+1}^3 - G_n^3 - G_{n-1}^3 = 3G_{n+1}G_nG_{n-1}$ 

ii. 
$$\sum_{i=1}^{n} F_i G_{3i} = F_n F_{n+1} G_{2n+1}$$

iii. 
$$G_n^2 + G_{n-1}^2 = (3a - b)G_{2n-1} - (a^2 + ab - b^2)F_{2n-1}$$

iv. 
$$F_{2n+1} = F_{n+1}^2 + F_n^2$$

v. 
$$G_{n-1}^6 + G_n^6 + G_{n+1}^6 = 2[2G_n^2 + (a^2 + ab - b^2)(-1)^n]^3 + 3G_{n-1}^2G_n^2G_{n+1}^2$$

vi. 
$$G_{n+t}G_{n+t-2} - G_{n+t-1}^2 = (a^2 + ab - b^2)(-1)^{n+t-1}F_k^2$$

Theorem 2.3. [15]

$$\sum_{i=1}^{n} F_i F_{3i} = F_{2n+1}^{(2)} \Big( F_{2n+3}^{(2)} - F_{2n-1}^{(2)} \Big)$$

**Theorem 2.4.** [3]

i. 
$$\sum_{i=0}^{k-1} (-1)^i {\binom{k-1}{i}} F_{mk+i}^{(k)} = (-1)^{k-1} F_m F_{(m-1)(k-1)}^{(k-1)}$$

ii. 
$$\sum_{i=0}^{k-1} {\binom{k-1}{i}} F_{mk+i}^{(k)} = F_m F_{(m+2)(k-1)}^{(k-1)}$$

## **3 MAIN RESULTS**

In this section, we present some properties of the new famil*x*-*g***£**neralized Fibonacci numbers.

**Theorem 3.1.** For  $n \ge 1$ , we have

$$G_{2n+2}^{(2)} + G_{2n}^{(2)} = 2 G_{2n+1}^{(2)} + G_{2n-2}^{(2)}$$

**Proof.** Using Theorem 2.2 (i), we have
$$\begin{split} G_{n+1}^3 - G_n^3 &= G_{n-1}^3 + 3G_{n+1}G_nG_{n-1} \\ (G_{n+1} - G_n)(G_{n+1}^2 + G_{n+1}G_n + G_n^2) &= G_{n-1}(G_{n-1}^2 + 3G_{n+1}G_n) \\ G_{n-1}\Big(G_{2n+2}^{(2)} + G_{2n+1}^{(2)} + G_{2n}^{(2)}\Big) &= G_{n-1}\Big(G_{2n-2}^{(2)} + 3G_{2n+1}^{(2)}\Big) \\ G_{2n+2}^{(2)} + G_{2n+1}^{(2)} + G_{2n}^{(2)} &= G_{2n-2}^{(2)} + 3G_{2n+1}^{(2)} \\ G_{2n+2}^{(2)} + G_{2n}^{(2)} &= 2 G_{2n+1}^{(2)} + G_{2n-2}^{(2)} \,. \end{split}$$

**Theorem 3.2.** For  $n \ge 1$ , we have

$$(3a-b)\sum_{i=1}^{n}F_{i}G_{3i} = F_{2n+1}^{(2)}\left(G_{2n+3}^{(2)} - G_{2n-1}^{(2)}\right) + (a^{2} + ab - b^{2})\sum_{i=1}^{n}F_{i}F_{3i}.$$

**Proof.** Using Theorem 2.2 (ii), (iii), (iv) and Theorem 2.3, we have

$$(3a - b) \sum_{i=1}^{n} F_i G_{3i} = (3a - b) F_n F_{n+1} G_{2n+1}$$

$$= F_n F_{n+1} (G_n^2 + G_{n+1}^2 + (a^2 + ab - b^2) F_{2n+1})$$

$$= F_n F_{n+1} (G_n (G_{n+1} - G_{n-1}) + G_{n+1} (G_{n+2} - G_n))$$

$$+ (a^2 + ab - b^2) (F_{n+1}^2 + F_n^2))$$

$$= F_n F_{n+1} (-G_n G_{n-1} + G_{n+1} G_{n+2})$$

$$+ (a^2 + ab - b^2) (F_{n+2} F_{n+1} - F_n F_{n-1}))$$

$$= F_{2n+1}^{(2)} \left( G_{2n+3}^{(2)} - G_{2n-1}^{(2)} + (a^2 + ab - b^2) (F_{2n+3}^{(2)} - F_{2n-1}^{(2)} \right) \right)$$

$$= F_{2n+1}^{(2)} \left( G_{2n+3}^{(2)} - G_{2n-1}^{(2)} \right) + (a^2 + ab - b^2) F_{2n+1}^{(2)} (F_{2n+3}^{(2)} - F_{2n-1}^{(2)})$$

$$= F_{2n+1}^{(2)} \left( G_{2n+3}^{(2)} - G_{2n-1}^{(2)} \right) + (a^2 + ab - b^2) F_{2n+1}^{(2)} (F_{2n+3}^{(2)} - F_{2n-1}^{(2)})$$

**Theorem 3.3.** For  $n \ge 1$ , we have

 $\left(G_{2n-2}^{(2)}\right)^3 + \left(G_{2n}^{(2)}\right)^3 + \left(G_{2n+2}^{(2)}\right)^3 = 2\left[2G_{2n}^{(2)} + (a^2 + ab - b^2)(-1)^n\right]^3 + 3G_{2n-2}^{(2)}G_{2n}^{(2)}G_{2n+2}^{(2)}.$  **Proof.** Using Theorem 2.2 (v), we get

$$\left(G_{2n-2}^{(2)}\right)^3 + \left(G_{2n}^{(2)}\right)^3 + \left(G_{2n+2}^{(2)}\right)^3 = (G_{n-1}^2)^3 + (G_n^2)^3 + (G_{n+1}^2)^3$$
  
=  $G_{n-1}^6 + G_n^6 + G_{n+1}^6$   
=  $2[2G_n^2 + (a^2 + ab - b^2)(-1)^n]^3 + 3G_{n-1}^2G_n^2G_{n+1}^2$ 

$$= 2 \left[ 2G_{2n}^{(2)} + (a^2 + ab - b^2)(-1)^n \right]^3 + 3G_{2n-2}^{(2)}G_{2n}^{(2)}G_{2n+2}^{(2)}$$

**Theorem 3.4.** For  $n \ge 1$ , we have

$$G_{2n+2}^{(2)} - G_{2n}^{(2)} = G_{2n-2}^{(2)} + 2 G_{2n-1}^{(2)}$$

**Proof.** From equation (2.1) and recurrence relation of generalized Fibonacci numbers, we get

$$G_{2n+2}^{(2)} - G_{2n}^{(2)} = G_{n+1}^2 - G_n^2$$
  
=  $(G_{n+1} - G_n)(G_{n+1} + G_n)$   
=  $G_{n-1}(G_{n+1} + G_n)$   
=  $G_{n-1}G_{n+1} + G_{n-1}G_n$   
=  $G_{n-1}(G_n + G_{n-1}) + G_{n-1}G_n$   
=  $G_{n-1}^2 + 2G_{n-1}G_n$   
=  $G_{2n-2}^{(2)} + 2G_{2n-1}^{(2)}$ .

**Theorem 3.5.** For  $n \ge 1$ , we have

$$G_{2n-2}^{(2)} + G_{2n-1}^{(2)} = G_{2n}^{(2)} + (a^2 + ab - b^2)(-1)^n$$

**Proof.** Using Theorem 2.2 (vi), we have

$$G_{2n-2}^{(2)} + G_{2n-1}^{(2)} = G_{n-1}^2 + G_n G_{n-1}$$
  
=  $G_{n-1}(G_{n-1} + G_n)$   
=  $G_{n-1}G_{n+1}$   
=  $G_n^2 + (a^2 + ab - b^2)(-1)^n$   
=  $G_{2n}^{(2)} + (a^2 + ab - b^2)(-1)^n$ .

**Theorem 3.6.** For  $n \ge 1$ , we have

$$G_{4n+5}^{(4)} = \left(G_{2n}^{(2)}\right)^2 + G_{4n+1}^{(4)} + 2G_{4n-3}^{(4)} + \left(G_{2n-2}^{(2)}\right)^2 + 3G_{2n+3}^{(2)}G_{2n-1}^{(2)}.$$

**Proof.** Using Theorem 2.2 (i), we have

$$\begin{aligned} G_{4n+5}^{(4)} &= (G_{n+1})^3 G_{n+2} \\ &= (G_n^3 + G_{n-1}^3 + 3G_{n+1}G_n G_{n-1})G_{n+2} \\ &= G_n^3 G_{n+2} + G_{n-1}^3 G_{n+2} + 3G_{n+2}G_{n+1}G_n G_{n-1} \\ &= G_n^3 (G_n + G_{n+1})G_{n-1}^3 (2G_n + G_{n-1}) + 3G_{2n+3}^{(2)}G_{2n-1}^{(2)} \\ &= \left(G_{2n}^{(2)}\right)^2 + G_{4n+1}^{(4)} + 2G_{4n-3}^{(4)} + \left(G_{2n-2}^{(2)}\right)^2 + 3G_{2n+3}^{(2)}G_{2n-1}^{(2)}. \end{aligned}$$

**Theorem 3.7.** For  $k, n, t \ge 1$ , we have

$$G_{kn+t}^{(k)}G_{kn+t-2}^{(k)} - \left(G_{kn+t-1}^{(k)}\right)^2 = \begin{cases} G_n^{2k-2}(-1)^n(a^2 + ab - b^2), & t = 1\\ 0, & t \neq 1 \end{cases}$$

**Proof.** For t = 1, we get

$$\begin{aligned} G_{kn+1}^{(k)} G_{kn-1}^{(k)} - \left( G_{kn}^{(k)} \right)^2 &= (G_n^{k-1} G_{n+1}) (G_{n-1} G_n^{k-1}) - (G_n^k)^2 \\ &= G_{n-1} G_n^{2k-2} G_{n+1} - G_n^{2k} \\ &= G_n^{2k-2} [G_{n-1} G_{n+1} - G_n^2] \\ &= G_n^{2k-2} (-1)^n (a^2 + ab - b^2) \,. \end{aligned}$$

For  $t \neq 1$ , we get

$$\begin{aligned} G_{kn+t}^{(k)}G_{kn+t-2}^{(k)} &- \left(G_{kn+t-1}^{(k)}\right)^2 = (G_n^{k-t}G_{n+1}^t)(G_n^{k-t+2}G_{n+1}^{t-2}) - (G_n^{k-t+1}G_{n+1}^{t-1})^2 \\ &= G_n^{2k-2t+2}G_{n+1}^{2t-2} - G_n^{2k-2t-2}G_{n+1}^{2t-2} \\ &= 0 \,. \end{aligned}$$

**Theorem 3.8.** For  $n \ge 1$ , we have

$$G_{2(n+s-1)}^{(2)} - G_{n+s}G_{n+s-2} = (-1)^{n+s}(a^2 + ab - b^2).$$

**Proof.** From the equation (2.1) and Theorem 2.2. (vi), we acquire

$$G_{2(n+s-1)}^{(2)} - G_{n+s}G_{n+s-2} = G_{n+s-1}^2 - G_{n+s}G_{n+s-2}$$
  
=  $-(G_{n+s}G_{n+s-2} - G_{n+s-1}^2)$   
=  $-((-1)^{n+s-1}(a^2 + ab - b^2))$   
=  $(-1)^{n+s}(a^2 + ab - b^2).$ 

**Theorem 3.9.** For  $n \ge 1$ , we have

$$\sum_{i=1}^{k-1} (-1)^i \binom{k-1}{i} G_{mk+i}^{(k)} = (-1)^{k-1} G_m G_{(m-1)(k-1)}^{(k-1)}.$$

**Proof.** By using the equation (2.1) and the well known binomial property, we obtain

$$\sum_{i=1}^{k-1} (-1)^i \binom{k-1}{i} G_{mk+i}^{(k)} = (-1)^{k-1} \sum_{i=1}^{k-1} (-1)^{k-1-i} \binom{k-1}{i} G_m^{k-i} G_{m+1}^i$$
$$= (-1)^{k-1} G_m \sum_{i=1}^{k-1} \binom{k-1}{i} (-G_m)^{k-i-1} G_{m+1}^i$$

$$= (-1)^{k-1} G_m (G_{m+1} - G_m)^{k-1}$$
  
=  $(-1)^{k-1} G_m G_{m-1}^{k-1}$   
=  $(-1)^{k-1} G_m G_{(m-1)(k-1)}^{(k-1)}$ .

**Theorem 3.10.** For  $n \ge 1$ , we have

1. 1

$$\sum_{i=1}^{k-1} \binom{k-1}{i} G_{mk+i}^{(k)} = G_m G_{(m+2)(k-1)}^{(k-1)}.$$

**Proof.** By taking account the equation (2.1) and the well known binomial property, we get

$$\sum_{i=1}^{k-1} \binom{k-1}{i} G_{mk+i}^{(k)} = \sum_{i=1}^{k-1} \binom{k-1}{i} G_m^{k-i} G_{m+1}^i$$
$$= G_m \sum_{i=1}^{k-1} \binom{k-1}{i} G_{m+1}^i (G_m)^{k-i-1}$$
$$= G_m (G_{m+1} + G_m)^{k-1}$$
$$= G_m G_{m+2}^{k-1}$$
$$= G_m G_{(m+2)(k-1)}^{(k-1)}.$$

#### **4** CONCLUSIONS

In this study, we prove that some identities of the new family of k-generalized Fibonacci numbers. Then, we show that some properties of the new family of k-generalized Fibonacci numbers related to generalized Fibonacci numbers. Furthermore, we extend Cassini's formula to the new family of k-generalized Fibonacci numbers and present identities comprising binomial coefficients for the new family of k-generalized Fibonacci numbers.

#### REFERENCES

- [1] C.M. Campbell and P.P. Campbell, "The Fibonacci length of certain centro-polyhedral groups", *Journal of Applied Mathematics and Computing*, **19**(1-2), 231-240 (2005).
- [2] Ö. Deveci, E. Karaduman, C.M. Campbell, "On the k-Nacci sequences in finite binary polyhedral groups", *Algebra Colloquium*(AC), **18**, Special Issue, 945–954 (2011).
- [3] M. El-Mikkawy and T. Sogabe, "A new family of k-Fibonacci numbers", *Applied Mathematics and Computation*, **215**(12), 4456-4461 (2010).
- [4] S. Falcon and A. Plaza, "On the Fibonacci k-numbers", *Chaos, Solitons & Fractals*, **32** (5), 1615-1624 (2007).
- [5] H.H. Gulec, N. Taskara, K. Uslu, "A new approach to generalized Fibonacci and Lucas numbers with binomial coefficients", *Applied Mathematics and Computation*, **220**, 482-486 (2013).
- [6] I. Kaddoura and B. Mourad, "On a new improved unifying closed formula for all Fibonacci-type sequences and some applications", *Journal of Number Theory*, **182**, 271-283 (2018).
- [7] E. Kilic and D. Taşci, "On the generalized order-k Fibonacci and Lucas numbers", The Rocky

Mountain Journal of Mathematics, 1915-1926 (2006).

- [8] S. Koparal and N. Ömür, "Some Congruences Involving Catalan, Pell and Fibonacci Numbers", *Mathematica Montisnigri*, **48**, 10-18 (2020).
- [9] T. Koshy, *Fibonacci and Lucas Numbers with Applications*, Wiley–Interscience, New York, (2001).
- [10] G. Lee and M. Asci, "Some Properties of the (*p*, *q*)-Fibonacci and (*p*, *q*)-Lucas Polynomials", *Journal of Applied Mathematics*, **2012** (2012).
- [11] E. Özkan, "3-Step Fibonacci Sequences in Nilpotent Groups", *Applied Mathematics and Computation*, **144**, 517-527 (2003).
- [12] E. Özkan, "On General Fibonacci Sequences in Groups", *Turkish Journal of Mathematics*, 27 (4), 525-537 (2003).
- [13] E. Özkan, "On truncated Fibonacci sequences", Indian Journal of Pure and Applied Mathematics, **38**(4), 241-251 (2007).
- [14] E. Özkan, İ. Altun, A.A. Göçer, "On relationship among a new family of k-Fibonacci, k-Lucas numbers, Fibonacci and Lucas numbers", *Chiang Mai J. Sci.*, **44**(4), 1744-1750 (2017).
- [15] E. Özkan, A. Aydoğdu, İ. Altun, "Some Identities for A Family of Fibonacci And Lucas Numbers", *Journal of Mathematics and Statistical Science*, **3**(10), 295-303 (2017).
- [16] J.L. Ramírez, "On convolved generalized Fibonacci and Lucas polynomials", *Applied Mathematics and Computation*, **229**, 208-213 (2014).
- [17] M.P. Saikia and A. Laugier, "Some Properties of Fibonacci Numbers, Generalized Fibonacci Numbers and Generalized Fibonacci Polynomial Sequences", *Kyungpook Mathematical Journal*, 57(1), 1-84 (2017).
- [18] P. Stanimirović, J. Nikolov, I. Stanimirović, "A generalization of Fibonacci and Lucas matrices", *Discrete applied mathematics*, **156**(14), 2606-2619 (2008).
- [19] D. Tasci and E. Kilic, "On the order-k generalized Lucas numbers", *Applied mathematics and computation*, **155**(3), 637-641 (2004).
- [20] R.B. Taher and M. Rachidi, "On the matrix powers and exponential by the r-generalized fibonacci sequences methods: the companion matrix case", *Linear Algebra and Its Applications*, 370, 341-353 (2003).
- [21] N. Yilmaz, Y. Yazlik, N. Taskara, "On the k-Generalized Fibonacci Numbers", *Selcuk Journal of Applied Mathematics*, **13**(1), 83-88 (2012).

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# SCENARIO OF ACCELERATED UNIVERSE EXPANSION UNDER EXPOSURE TO ENTROPIC FORCES RELATED TO WITH THE ENTROPIES OF BARROW AND TSALLIS-CIRTO

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**Summary.** In the work within the framework of "entropic cosmology", the scenario of the cosmological accelerated expansion of a flat, homogeneous and isotropic Universe under the influence of entropic forces is considered without the concept of dark energy– a hypothetical medium with negative pressure. Assuming that the horizon of the Universe has its own temperature and entropy, which arises during the holographic storage of information on the screen of the horizon surface, the entropy models of the Universe associated with the Bekenstein–Hawking entropy and the non-extensive Barrow and Tsallis–Cirto entropies are considered. The modified equations of acceleration and continuity of Friedman with governing power terms having an entropic nature are derived both within the framework of Einstein's general theory of relativity and on the basis of a thermodynamic approach that allows modeling the non-adiabatic evolution of the Universe. At the same time, models based on nonextensive entropies predict the existence of both a decelerating and accelerating Universe.

## **1. INTRODUCTION**

In the last years of the twentieth century (1998), an unexpected discovery was made in cosmology related to the accelerating expansion of the Universe. Currently, this fact has been confirmed by a huge number of observational data and numerous cosmological experiments concerning the microwave background, large-scale structure, and other dimensions of the Universe (see, for example, [1-2]). In this regard, modern cosmological concepts are fully consistent with the Friedman–Robertson–Walker model of a homogeneous, isotropic, and almost flat (infinite) and open Universe, continuously expanding with acceleration [3-5].

Despite the growing amount of observational evidence for the existence of an accelerated expansion of the Universe, its nature and fundamental origin are still an unresolved issue. As it is know, the ratio of ordinary (baryonic) matter, dark matter and dark energy is approximately. 1:10:25. Consequently, the evolution of the Universe is completely dominated by cold dark matter and dark energy – the so-called cosmic vacuum [6-7], the energy density of which is currently associated with the cosmological constant  $\Lambda = 1.1 \times 10^{-56} sm^{-2}$ .

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The constant  $\Lambda$  determines antigravity in the Einstein modified general theory of relativity (GR) by Einstein [4].

The cosmological vacuum has everywhere and always constant positive density  $\rho_v = \Lambda c^2/8\pi G$  and negative pressure  $P_v = -c^2 \rho_v$ . According to Friedman's cosmology of a homogeneous and isotropic universe, gravitation is created not only by the density of the material medium, but also by its pressure in combination  $\rho + 3P/c^2$ . The vacuum causes antigravity precisely because its effective gravitating energy  $\rho_G = \rho_v + 3P_v/c^2 = -2\rho_v$  is negative at positive density. Since the density of the vacuum (dark energy) exceeds the total density of all other types of cosmic energy, then antigravitation is stronger than gravitation. Under this condition, the cosmological expansion must occur with acceleration [8]. Thus, the cosmological accelerated expansion of the Universe is completely determined by the acting in parallel gravitational and antigravitational forces described by the modified general relativity approach.

It should be noted, however, that at present there are a number theories in support that of gravity are called. In contrast to the Standard Model, which combines three interactions in nature but gravity, the "Theory of Everything" (or M-theory), unifies all forces and particles in nature, but it not fully complies with General relativity [9].

Among the many scenarios for the accelerated expansion of the Universe, the so-called "entropic cosmology" has recently attracted much attention, according to which gravity is perceived as a kind of force associated with a change in entropy. The concept of the cosmological entropic force was proposed by the Dutch physicist ("string theorist") Eric Verlinde, who in his article [10] developed a rather "crazy" theory, according to which the phenomenon of gravity is explained through entropy, i.e. the force of gravity is inherently thermodynamic in origin [11], 2010). In this work, the author argues that the central concept necessary for the emergence of gravity is information (more precisely, the amount of information associated with matter and its distribution) in terms of entropy. The most important assumption of the theory is that information associated with a certain region of space obeys the holographic principle (see, for example, [12] and relies heavily on the physics of black holes [13-14].

In the cited article, it was shown that within the holographic principle of the formation of space<sup>i)</sup> gravity inevitably arises, which is identified with the entropy force caused by changes in information<sup>ii)</sup>, associated with the growth of the area occupied by material bodies. According to the holographic picture of the world, entropy is stored on holographic screens, and space appears between two similar screens. With this approach, the gravitational force in space is determined by the entropy gradient, or the so-called entropic force.

Nearly the same time, within the framework of the Verlinde hypothesis, Easson et al. [15] developed a heuristic theory of the accelerated expansion of the Universe, based on the entropic force. Authors of that work have demonstrated that accelerated expansion is an inevitable consequence of an increase in entropy associated with the storage of holographic information on a surface screen located on the event horizon (space-time region) of the Universe. As a result, with this approach, the progress in physical understanding of the process of accelerated expansion of

<sup>&</sup>lt;sup>i</sup>) Here, holography refers to information about the Universe encoded on a screen, which is interpreted as a twodimensional surface of the Universe.

<sup>&</sup>lt;sup>ii</sup>) According to the holographic principle, the growth of information associated with an increase in the surface of the Universe occupied by material bodies leads to an increase in entropy; hence the emergence of a gradient of entropy (entropy force) directed against the increase in the radius of the specified surface area. And this is gravity.

the Universe was achieved based on entropic forces, without the concept of dark energy – hypothetical medium with negative pressure.

In other words, contrary to the widespread explanation of the observed accelerated expansion of the Universe, which appears in the presence of a driving force (in the Friedman equations) due to dark energy, an alternative interpretation of such a force was proposed - an entropic force. The latter was associated with the entropy and temperature of the horizon of the Universe, which arise when storing information on the screen of the surface of the horizon.

Finally, in a number of subsequent works (see, for example, [16-29]) devoted to entropic cosmology, the scenario of the accelerated expansion of the Universe under the influence of entropic forces of various nature was discussed, proceeding from the idea that the horizon of the Universe (like the event horizon of a black hole) has its own entropy and temperature. In all these studies, along with the de Sitter temperature [30], various entropy entities were used (in particular, the Bekenstein–Hawking entropy [13], the non-extensive Tsallis–Cirto entropy [31], the modified (equally-distributed) entropy Renyi [32] and others). Instead of the cosmological constant in the equations of Einstein's general theory of relativity, an additional so-called governing term was added, associated with the entropy and temperature of the event horizon of the Universe. Using modified Friedman equations, it was shown that such models explain the current accelerating expansion of the Universe and they are in good agreement with the data on supernovae. Let us note that the cosmological acceleration found in this case (considered as a consequence of the entropic force) turns out to be relatively small (of the order of the Hubble constant), in contrast to the huge value of accelerated expansion, which is confusing to most cosmologists, predicted by quantum field theory in combination with general relativity<sup>iii</sup>.

Thus, the study of the influence of entropic forces on the accelerated expansion of the Universe is of interest, since due to the anti-gravitational action, it is these forces that can play the role of mysterious dark energy both in the form of a cosmological constant and in the form of scalar fields [33]. In entropic cosmology, it is assumed that the horizon of the Universe has associated temperature and entropy due to information stored on the surface of the event horizon holographically.

Here we concern some elementary considerations intended to show how the entropy force, which has a thermodynamic nature, is related to the entropy of a large body. For this, we use the second law of thermodynamics for a macroscopic body, in the form of the Gibbs relation dE = TdS - PdV. Since for a very large body with a change in its volume (due to the displacement of the boundary dr), the surface area A and internal energy E practically do not change, then one can write 0 = TdS - P(Adr). Hence, it follows that if the entropy changes due to increase of radius of the volume, then the force  $F_s = PA = TdS/dr$  arises. Since the space-time-dependent entropy (evolving in time and reaching a maximum in the final thermal state), expands in space, its gradient appears, which is interpreted as an entropic force.

<sup>&</sup>lt;sup>iii</sup>) The identification of the cosmological constant with the vacuum energy does not allow, unfortunately, to penetrate into the essence of dark energy and leads to a still unsolvable problem, which consists in the fact that the observed value of the dark energy density  $\rho_{\Lambda_{abs}} \approx (10^{-3} eV)^4$  and its theoretically predicted value  $\rho_{\Lambda_{ih}} \approx 10^{18} (GeV)^4$ differ by 120 orders of magnitude (here,  $V = V(\varphi)$  the potential of the scalar fields  $\varphi$  (inflaton) [4].

In the presented work, which is related to modeling the accelerated expansion of a flat, homogeneous and isotropic Universe, modified Friedman equations are obtained, in which instead of the cosmological constant there appears an additional control term (driving force) associated with changes in entropy and temperature on the Hubble horizon of the Universe. The surface area of the Universe is a key characteristic that determines its entropy and information content. Along with the traditional Bekenstein–Hawking entropy [15], which is proportional to the area of the Hubble horizon, we also incorporate the non-additive Tsallis–Cirto entropy [31], which is proportional to the horizon volume, and the non-additive entropy of Barrow [34-36], taking into account the fractal structure of the Hubble horizon. For these entropies, modified Friedman equations have been constructed to explain the cosmological expansion of the Universe without dark energy. In this case, the corresponding entropic forces predetermine both deceleration and/or accelerated expansion of the Universe. It is important to note that the construction of new models of the evolution of the Universe is carried out on the basis of the recently introduced nonadditive Barrow entropy, which is a new holographic model of entropy associated with the modification of the horizon of the Universe surface due to quantum gravitational effects.

#### 2. SOME ELEMENTS OF CLASSICAL COSMOLOGY

#### 2.1 Gravitational field equations

First, we will consider a flat evolutionary model of the Universe, which is infinite in space, homogeneous, isotropic and expanding. In this case, the Universe is modeled by some cosmological fluid, the particles of which are galaxies. At this level of large-scale averaging, the structure of the Universe is symmetric and has no singularities. In classical cosmology, models of the evolving Universe are constructed on the basis of Einstein's equations of general relativity (see, for example, [4, 33, 37].

The expansion of the Universe is governed by the equations of the gravitational field, which have the following general form [4, 8]:

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R - \Lambda(t)g_{\mu\nu} = \kappa T_{\mu\nu}.$$
<sup>(1)</sup>

Here  $ds^2 = g_{\mu\nu}dx^{\mu}dx^{\nu}$  – four-dimensional space-time interval in general relativity,  $g_{\mu\nu}$  – metric tensor,  $g_{\mu\nu}g^{\nu\beta} = \delta^{\beta}_{\mu}$ ;  $R_{\mu\nu} = g^{\alpha\beta}R_{\mu\nu\alpha\beta}$  – Ricci tensor;  $R_{\mu\nu\alpha\beta}$  – the Riemann–Christoffel tensor, composed of the products of the first derivatives  $(\partial g_{\rho\nu}/\partial x_{\alpha}) \cdot (\partial g_{\beta\mu}/\partial x_{\rho})$  and the second derivatives  $\partial^2 g_{\mu\nu}/\partial x_{\alpha}\partial x_{\beta}$  of the metric tensor;  $R = g^{\mu\nu}R_{\mu\nu}$  – scalar curvature of four-dimensional space;  $\kappa = 8\pi G/c^4$  – Einstein gravitational constant;  $T_{\mu\nu}$  – the energy-momentum tensor, which plays the role of the source of the gravitational field; c – speed of light in vacuum,  $\Lambda$  – the cosmological "constant" introduced by Einstein, which can often be omitted; G – gravitational constant.

In flat hyperspace, the space-time linear interval has the form  $ds^2 = c^2 dt^2 - a(t)^2 (dx^2 + dy^2 + dz^2)$ , which corresponds to the metric tensor with Galilean components<sup>iv</sup>

$$g_{00} = c^2; \ g_{11} = g_{22} = g_{33} = -a(t)^2; \ g_{\mu\nu} = 0 \text{ at } \mu \neq \nu; \ g_{\mu\nu} = g^{\mu\nu},$$
 (2)

where t – the space time coordinate; a(t) – expansion coefficient (Robertson–Walker scale factor [4]. For the case of an ideal cosmological fluid<sup>v)</sup> the energy-momentum tensor in a locally inertial Cartesian coordinate system has the form  $T_{\mu\nu} = (\rho c^2 + P)u_{\mu}u_{\nu} + Pg_{\mu\nu}$ , where  $\rho = \rho(t)$ ,  $P = P(\rho)$  are, respectively, the density and scalar pressure of the cosmological fluid (including matter and radiation) at the moment of time t. Here a four-dimensional velocity  $u_{\mu} = \partial x_{\mu}/\partial s$  is introduced, which is determined by the condition that in the accompanying locally inertial Cartesian coordinate system its components are equal  $u_0 = 1$  and  $u_{\mu\neq0} = 0$ . Thus, at rest, the tensor components  $T_{\mu\nu}$  have the following form [3]:

$$T_{00} = \rho c^2; \quad T_{11} = T_{22} = T_{33} = -P; \quad T_{\mu\nu} = 0 \quad npu \quad \mu \neq \nu.$$
(3)

Note that in a flat model of the Universe, the three-dimensional curvature is zero, but the fourdimensional space remains curved.

#### 2.2 Friedman's cosmological model

Let us consider Friedman's standard model for a flat open universe<sup>vi</sup>).

From Einstein's equations (1) under the above assumptions <sup>vii)</sup> two Friedman equations for the scale factor a(t) follow [3]

$$\left(\frac{a_{r_t}}{a}\right)^2 \equiv H(t)^2 = \frac{8\pi G}{3}\rho(t) + \frac{\Lambda/3}{_{omitted}},$$
(4)

<sup>&</sup>lt;sup>iv)</sup> Almost all modern cosmology is based on this Robertson-Walker metric.

<sup>&</sup>lt;sup>v)</sup> An ideal fluid is defined as a medium for which at each point there is a locally inertial Cartesian frame of reference moving with the fluid, in which the fluid itself looks the same in all directions.

<sup>&</sup>lt;sup>vi)</sup> Space is flat only if the ratio  $\Omega := \rho / \rho_{cr} \cong 1$ , where  $\rho_{cr} \cong 3H^2 / 8\pi G$  is the critical mass density (matter + radiation),  $\rho_{cr} = 10^{-29} g / sm^3$ . According to modern observational data, the value  $\Omega = 1.02 \pm 0.02$ .

<sup>&</sup>lt;sup>vii)</sup> Space is flat only if the ratio  $\Omega := \rho / \rho_{cr} \approx 1$ , where  $\rho_{cr} \approx 3H^2 / 8\pi G$  is the critical mass density (matter + radiation),  $\rho_{cr} = 10^{-29} g / sm^3$ . According to modern observational data, the value  $\Omega = 1.02 \pm 0.02$ .

$$\frac{1}{a(t)}a_{tt} = \left[\frac{dH(t)}{dt} + H(t)^2\right] = -\frac{4\pi G}{3}\left(\rho(t) + \frac{3P(t)}{c^2}\right) + \frac{\Lambda/3}{omitted},$$
(5)

which describe an expansion of the Universe. Here, the dot denotes the time derivatives;  $H(t) := a_{rt}/a$  – the Hubble parameter, or the Hubble expansion rate of the Universe (in the modern period  $H_0 = 2.2 \times 10^{-18} c^{-1}$ );  $\rho = \rho_m + \rho_\gamma$  – total density of matter and radiation. Equations (4) and (5) include an additional governing parameter  $\Lambda/3$  that, if properly defined, can explain the accelerated expansion of the late Universe [33].

From equations (4) and (5) it is easy to obtain the following continuity equation – "energy conservation law"

$$\rho_{t}(t) + 3\frac{a_{t}(t)}{a(t)} \left[ \rho(t) + \frac{P(t)}{c^{2}} \right] = 0.$$
(6)

To do this, it is necessary to differentiate (4) and combine the result with the ratio (5), which the pressure satisfies. Note that equation (6) can also be derived directly from the first law of thermodynamics, if we consider the Universe as a thermodynamic system bounded by the visible horizon and expanding adiabatically ([38], see also Section 5.1. of this work).

Equation (6) can be written as  $a d\rho / da = -3(\rho + P / c^2)$ , or, which is the same

$$d(\rho a^3) / da = -3Pc^{-2}a^2.$$
<sup>(7)</sup>

If the dependence of pressure P(t) on a(t) is known, it is possible, by solving equation (4) (at  $\Lambda = 0$ ), to determine a(t) for all times. Thus, the fundamental equations of dynamic cosmology are the Einstein equations (4), the energy conservation equation (6) and the equation of state.

Cosmological models based on the Robertson–Walker metric, in which a(t) it is determined from these equations, are called Friedman models [39]. Note that the solution a(t) obtained in this way automatically satisfies Eq. (5), since differentiating (4) with respect to time and using (7), we obtain

$$2a_{t}a_{t}a_{t} = \frac{8\pi G}{3a}a_{t}\left[-\rho a^{2} + \frac{d}{da}(\rho a^{3})\right] = \frac{8\pi G}{3a}a_{t}\left(-\rho a^{2} - 3\frac{P}{c^{2}}a^{2}\right)$$

which is equivalent to equation (5).

Equation (7) can be easily solved in the case of an equation of state in the form  $P = w \rho$  with a time-independent coefficient w. In this case, equation (6) leads to a solution  $P \sim a^{-3-3w}$ , which, in particular, is applicable in the following frequently encountered limiting cases:

- if the main contribution to the energy density of the Universe is made by nonrelativistic matter with negligible pressure, then it follows from (7) that

$$\rho(t) \sim a(t)^{-3} \text{ when } P \ll \rho; \qquad (8)$$

- if the contribution of relativistic particles, such as photons, prevails in the energy density, then  $P = \rho/3$ , and from (7) one obtains

$$\rho(t) \sim a(t)^{-4}$$
 when  $P = \rho / 3$ ; (9)

- in the case of a cosmological vacuum, when  $P = -c^2 \rho$ , equation (7) has a solution in the form of a constant  $\rho$ , known (up to generally accepted numerical factors) as the cosmological constant  $\Lambda$ , or vacuum density.

The currently known observations of the accelerating expansion of the Universe are consistent with the existence of a constant vacuum energy equal to  $\rho c^2$ . The very existence of an accelerating expansion, in accordance with equation (5), requires that a significant part of the energy density of the Universe should be in such a form for which  $\rho + 3P/c^2 < 0$ , in contrast to ordinary matter and radiation. This form is called dark energy in cosmology [4].

#### 3. ACCELERATED EXPANSION OF THE UNIVERSE

#### **3.1.** Entropy force associated with the Bekenstein–Hawking entropy

In this work, to explain the accelerated expansion of the Universe, we will use a different approach (without dark energy), in which the ideas of information, holography, entropy and temperature play a central role (see [10, 22, 40]). Consideration of the entropic force on the holographic horizon of an expanding flat Universe, which has associated entropy and temperature, leads to the so-called entropic cosmology, which assumes that it is the entropic force acting on the Hubble horizon and directed outward towards the horizon that is responsible for the phenomenon of accelerated expansion. For this reason, there is no ambiguous dark energy component in the cosmological equations.

With this approach, by analogy with the thermodynamic characteristics of the Hubble horizon of a black hole described by its temperature and entropy, entropy cosmology assumes that the region of the expanding flat Universe (coinciding with the Hubble horizon) has a temperature proportional to the de Sitter temperature [30] and the associated Bekenstein–Hawking entropy [15]. In this case, the problem of the relationship between the cosmological constant and the entropic force is solved in a natural way [10].

In entropic cosmology, the Hubble horizon (radius)  $R_H$  and the temperature of the cosmological horizon of the Universe  $T_H \simeq \gamma T_S$  are determined by the expressions [15]

$$R_H = c H^{-1}, (10)$$

$$T_H = \gamma \frac{\hbar}{2\pi k_B} H = \frac{\hbar}{2\pi k_B} \frac{c}{R_H},\tag{11}$$

where  $k_B$  and  $\hbar = h/2\pi$  are the Boltzmann constant and the reduced Dirac constant, respectively;  $\gamma$  – non-negative free order parameter O(1) (usually  $\gamma \sim 1/2$  or  $3/2\pi$ , which corresponds to the parameter for the screen temperature obtained in [15].

The temperature of the horizon of the Universe, closely related to the de Sitter temperature  $T_S = \hbar H / 2\pi k_B$ , can be estimated as

$$T_H \simeq \frac{\hbar H}{2\pi k_B} \times \mathcal{O}(1) \sim 3 \times 10^{-30} K \,, \tag{12}$$

which is much lower than the temperature of the cosmic microwave background, T = 2.73K. The entropy associated with the horizon of the Universe is given by the following Bekenstein–Hawking relation [13]

$$S_{BH} = k_B \left(\frac{A_H}{A_{Pl}}\right) = k_B \frac{c^3}{\hbar G} A_H, \qquad (13)$$

where  $A_H$  is the size of the area of the standard horizon (surface area of the Hubble radius area  $R_H$ );  $A_{Pl} = \hbar G / c^3 \approx 2.612 \times 10^{-70} m^2$  – Planck area. Substituting the quantity  $A_H = \pi R_H^2 = \pi c^2 H^{-2}$  into relation (13), we obtain

$$S_{BH} = k_B \left(\frac{c^3}{\hbar G}\right) \pi R_H^2 = \left(\frac{k_B \pi c^5}{\hbar G}\right) \frac{1}{H^2} = \frac{K}{H^2} \sim (2.6 \pm 0.3) \times 10^{122} k_B.$$
(14)

A positive constant is introduced here

$$K := \frac{\pi k_B c^5}{\hbar G} = \frac{\pi k_B c^2}{L_{Pl}^2} = \frac{\pi k_B c^2}{A_{Pl}} > 0 , \qquad (15)$$

where  $L_{Pl} = \sqrt{\hbar G / c^3}$  is the Planck length.

Increasing the radius  $R_H$  by  $dR_H$  increases the entropy  $S_{BH}$  by  $dS_{BH}$  in accordance with the formula

$$dS_{BH} = \left(\frac{k_B c^3}{\hbar G}\right) 2\pi R_H dR_H =$$
$$= \left(\frac{k_B c^3}{\hbar G}\right) 2\pi \left(\frac{c}{H}\right) dR_H \sim (2.6 \pm 0.3) \times 10^{122} k_B \frac{dR_H}{R_H}.$$

The entropy force  $F_{BH}$  corresponding to the growth of the Bekenstein–Hawking entropy can be defined as

$$F_{BH} = -T_H \frac{dS_{BH}}{dr_H}.$$
 (16)

Here, the minus sign indicates the direction of increasing entropy or screen, which in this case is the event horizon [15].

Substituting now relations (11) and (13) into (16) and using the formula for the area  $A_H$  of the standard horizon, we obtain the following expression for the entropic force

$$F_{BH} = -T_H \frac{dS_{BH}}{dR_H} = -\gamma \frac{\hbar H}{2\pi k_B} \times \frac{d}{dr_H} \left[ \frac{K}{H^2} \right] = \frac{2\hbar H}{2\pi k_B} \frac{K}{H^3} \frac{dH}{dr_H} =$$
$$= \gamma \frac{1}{H^2} \frac{c^5}{G} \frac{dH}{dR_H} = -\gamma \frac{1}{H^2} \frac{c^6}{G} \frac{1}{R_H^2} = -\gamma \frac{c^4}{G}.$$
(17)

The pressure  $P_{BH}$  of this force on the cosmological horizon of the Universe is determined by the formula

$$P_{BH} = \frac{F_{BH}}{4A_H} = -\gamma \frac{c^4}{G} \frac{1}{4\pi R_H^2} = -\gamma \frac{c^2}{4\pi G} H^2 = -\gamma \frac{2\rho_{cr}}{3} c^2$$
(18)

(where  $\rho_{cr} := 3H^2/8\pi G$  is the critical mass density of matter and radiation). This value is close to the measured negative pressure (tension) of dark energy in the form of a cosmological constant [4]. Thus, in the holographic approach, pressure arises not due to the negative pressure of dark energy, but due to the entropic tension due to the entropic content on the horizon of the Universe. The presence of such tension is equivalent to outward cosmic acceleration <sup>viii</sup>). In other words, the acceleration of the universe arises as a natural consequence of the entropy change at the horizon of the Universe.

# **3.2.** Accelerated expansion of the Universe under the influence of the Bekenstein–Hawking entropy force

We will now assume that in entropy cosmology the effective pressure  $P'_{BH}$  based on the Bekenstein–Hawking entropy is determined by the relation

$$P'_{BH} = P + P_{BH} = P - \gamma \frac{c^2}{4\pi G} H^2 .$$
 (19)

When using  $P'_{BH}$ , equations (5) and (6) take the following form:

viii) Note that from the possibility of describing the cosmic acceleration of the Universe by an entropic force, it does not follow that gravity itself is an entropic force [10].

$$\frac{a_{tt}}{a} = -\frac{4\pi G}{3} \left( \rho(t) + \frac{3P(t)}{c^2} \right) + \gamma H(t)^2,$$
(20)

$$\rho_{t} + 3H(t) \left[ \rho(t) + \frac{P}{c^2} \right] = \gamma \frac{3}{4\pi G} H(t)^3.$$
 (21)

These equations can be considered as modified equations of acceleration (5) and continuity (6) for entropy cosmology, obtained using the Bekenstein–Hawking entropy. The quantity  $H^2$  in these equations is related to the entropic force, which can explain the accelerated expansion of the Universe without introducing the concept of dark energy – the cosmic vacuum (associated with the cosmological constant), the energy density of which is negative. Note that the Beken-stein –Hawking entropy is proportional to the area of the cosmological horizon of the Universe, due to which the model based on this entropy predicts only the Universe expanding with uniform acceleration. This model of the accelerated expansion of the Universe is capable to provide a good fit with supernova data [15, 22].

# 4. ENTROPIC FORCE ASSOCIATED WITH NON-ADDITIVE ENTROPY OF BARROW AND TSALLIS-CIRTO

Recently [35] proposed a model of the quantum gravitational foam of space-time was proposed to estimate the entropy of black holes and the Universe, the surface of which can have a complex fractal structure of the cosmological horizon down to arbitrarily small scales (up to a scale of the order of the Planck length) due to quantum gravitational effects. The introduction of the fractal structure of the horizon (space-time region) of the Universe leads to an increase in its surface area. As you know, the surface area of the Universe is a key characteristic that determines its entropy and information content.

The complex fractal structure of the horizon of the Universe results in a finite volume, but with an infinite (or finite) area [35]. According to the thermodynamics of black holes, the possible effects of the quantum-gravitational foam of space-time in the region of the cosmological horizon lead to a new definition of the entropy of the Universe – to the non-additive entropy of Barrow  $S_B$  [35] related to the additive Bekenstein–Hawking entropy as follows:  $S_B / k_B = (S_{BH} / k_B)^{1+D/2}$ . Substituting the values  $S_{BH}$  and  $k_B$  into this ratio yields  $S_B \sim 10^{120(1+D/2)}$ . Here, the parameter  $D (0 \le D \le 1)$  is the fractal mass dimension of the quantum-gravitational foam, which quantitatively determines the deformation of the structure of the horizon of the Universe<sup>ix</sup>.

ix) It should be noted that when defining the Barrow entropy, the complex fractal structure of the cosmological horizon is modeled by an analogue of the spherical "Koch snowflake" using an infinite decreasing hierarchy of touching spheres around the Schwarzschild event horizon. Nevertheless, this simple model of possible manifestations of quantum-gravitational effects has important implications for estimates of the entropy of the Universe, which is usually slightly larger than in the baseline scenario.

It is easy to show that Barrow's entropy obeys the following pseudo-additive law for two independent systems N and M:

$$\frac{S_B(N+M)}{k_B} = \left( \left[ \frac{S_B(N)}{k_B} \right]^{\frac{2}{2+D}} + \left[ \frac{S_B(M)}{k_B} \right]^{\frac{2}{2+D}} \right)^{\frac{2+D}{2}}$$

Entropy  $S_B$  can be written as follows:

$$S_{B} = k_{B} \left(\frac{A_{H}}{A_{Pl}}\right)^{1+D/2} = k_{B} \left(\frac{\pi R_{H}^{2}}{A_{Pl}}\right)^{1+D/2} = \frac{k_{B}\pi c^{3}}{\hbar G} R_{H}^{2} \left(\frac{\pi R_{H}^{2}}{A_{Pl}}\right)^{D/2} = Kc^{-2} R_{H}^{2} \left(\frac{\kappa}{k_{B}} R_{H}^{2}\right)^{D/2} = \left(\frac{\kappa^{1+D/2}}{c^{2}k_{B}^{D/2}}\right) R_{H}^{2+D}.$$
(22)

Here  $A_{pl} = \hbar G / c^3 \approx 2.612 \times 10^{-70} m^2$  – Planck area;  $K := \pi k_B c^2 / A_{pl} > 0$ ;  $A_H$  – standard horizon area;. In the case D = 0 that corresponds to the simplest structure of the cosmological horizon of the Universe, the standard  $S_B \equiv S_{BH} = k_B (A_H / A_{Pl})$  Bekenstein–Hawking entropy considered above is restored.

When D=1, then there is a smooth space-time structure of the horizon of the Universe, at

which  $S_B \equiv S_{TC} = k_B \left(\frac{A_H}{A_{Pl}}\right)^{3/2}$ . In this case, formula (22) is similar to that for the non-additive

entropy of Tsallis and Cirto [31], introduced by these authors, when studying the evolution of a black hole on the basis of completely different physical principles, different from the fractal interpretation (see [41-44]). In order to obtain modified cosmological equations, we apply the procedure considered in the previous section to derive an expression for the entropy force, but now involving the Barrow entropy (22). It is evident that in the general case of a medium with fractal dimension ( $0 < D \le 1$ ), these equations, in contrast to the Friedman equations (20) and (21), will contain new additional terms that allow modeling the cosmological behavior of the Universe [34, 36, 45].

#### 4.1. Entropic Force Associated with Barrow's Entropy

At this point, we will consider the possibility of an accelerated cosmological expansion of the Universe, but using the Barrow entropy at its horizon. Barrow's entropy arises, in particular, due to the fact that the surface of the horizon of the Universe can deform due to quantumgravitational effects, and its deviation from the Bekenstein–Hawking entropy is quantitatively determined by the fractal dimension index D.

Increasing the radius  $R_H$  by  $dR_H$  increases the entropy  $S_B$  by  $dS_B$  in accordance with the expression

$$dS_B(D) = k_B(2+D) \left(\pi / A_{Pl}\right)^{1+D/2} R_H^{1+D} dR_H.$$
(23)

Then for the entropic force  $F_B$  arising from the modification of the horizon of the Universe, which is associated with quantum-gravitational effects, we will have:

$$F_{B} = -T_{H} \frac{dS_{B}}{dR_{H}} = -\gamma \left(\frac{\hbar c}{2\pi k_{B}R_{H}}\right) k_{B} \frac{\pi c^{3}}{\hbar G} \left(\frac{\pi}{A_{Pl}}\right)^{D/2} (2+D) R_{H}^{1+D} =$$
$$= -\gamma \frac{2+D}{2} \frac{c^{4}}{G} \left(\frac{\pi}{A_{Pl}}\right)^{D/2} R_{H}^{D} = -\gamma \frac{(2+D)}{2} \frac{c^{4+D}}{G} \left(\frac{K}{k_{B}}\right)^{D/2} H^{-D}.$$
(24)

Accordingly, the pressure  $P_B$  of this force on the cosmological horizon of the Universe is defined by the formula

$$P_B = \frac{F_B}{4A_H} = -\gamma \frac{c^4}{4\pi G} \left(\frac{K}{k_B}\right)^{D/2} \frac{(2+D)}{2} R_H^{D-2} = \gamma \frac{(2+D)}{2} \frac{c^{2+D}}{4\pi G} \left(\frac{K}{k_B}\right)^{D/2} H^{2-D}.$$
 (25)

In what follows, we will assume that in entropy cosmology the effective pressure  $P'_B$  based on the Barrow entropy is determined by the relation

$$P'_{B} = P + P_{B} = P - \gamma \frac{(2+D)}{2} \frac{c^{2+D}}{4\pi G} \left(\frac{K}{k_{B}}\right)^{D/2} H^{2-D}.$$
 (26)

When using  $P'_B$  the equations of acceleration (5) and continuity (6) take the form

$$\frac{1}{a(t)}a_{tt} = -\frac{4\pi G}{3} \left(\rho(t) + \frac{3}{c^2}P(t)\right) + \gamma \frac{(2+D)}{2}c^D \left(\frac{K}{k_B}\right)^{D/2} H(t)^{2-D} , \qquad (27)$$

$$\rho_{t}(t) + 3H(t) \left[ \rho(t) + \frac{P(t)}{c^2} \right] = \gamma \frac{3}{4\pi G} \frac{2+D}{2} c^D \left( \frac{K}{k_B} \right)^{D/2} H(t)^{3-D}.$$
(28)

-

It is important to note that in the case of fractal dimension D = 0 these equations will coincide with the modified Friedman equations (20) and (21), i.e., the deformation of the Bekenstein– Hawking holographic entropy is measured by a new index D, whereas the case of zero deformation (D = 0) corresponds to the entropy force Barrow, which fully complies with the stand-ard entropy force considered in [15].

At the same time, the authors of [34], based on observational data from a sample of the collection (SNIa) of supernovae and using direct measurements of the Hubble parameter by cosmic chronometers, showed that the value deformation parameter equal to D = 0.094, assuming that a small deviation from the standard holographic Bekenstein–Hawking entropy is preferable.

The case D=1 corresponds to the maximum deformation associated with the Tsallis–Cirto cosmological entropy [31]. The scenario for the manifestation of this entropy predicts both deceleration and/or accelerated expansion of the Universe [46].

In the general case, when 0 < D < 1 we have a new cosmological scenario for the manifestation of the entropic force, based on the Barrow entropy associated with the quantumgravitational effects of the horizon of the Universe. This scenario allows simulating the cosmological behavior of the Universe for the case of various modifications of Barrow's governing gravitational force [36].

## 4.2. Entropic force associated with the entropy of Tsallis-Cirto

Let us now consider entropic cosmology under the assumption that the cosmological horizon of the Universe has a temperature

$$T_{H} = \gamma \frac{\hbar}{2\pi k_{B}} \frac{c}{R_{H}} = \gamma \frac{\hbar}{2\pi k_{B}} H$$

and that the non-additive entropy of Tsallis-Cirto, is defined as follows [31]

$$S_{TC} = S_B(1) := k_B \left(\frac{A_H}{A_{Pl}}\right)^{3/2} = k_B \left(\frac{\pi R_H^2}{A_{Pl}}\right)^{3/2} = \frac{k_B \pi c^3}{\hbar G} R_H^2 \left(\frac{\pi R_H^2}{A_{Pl}}\right)^{1/2} = Kc^{-2} \left(\frac{\pi}{A_{Pl}}\right)^{1/2} R_H^3 = \left(\frac{K^3}{k_B c^4}\right)^{1/2} R_H^3 = cK \left(\frac{K}{k_B}\right)^{1/2} \frac{1}{H^3}.$$
(29)

It follows from formula (29) that the non-additive entropy  $S_{TC}$  is proportional to the volume of the horizon of the Universe, in contrast to the Bekenstein–Hawking entropy (14), which is proportional to its area.

Increasing the radius  $R_H$  by  $dR_H$  increases the Tsallis–Cirto entropy  $dS_{TC}$  in accordance with the ratio

$$dS_{TC} = 3\left(K^3 / k_B c^4\right)^{1/2} R_H^2 dR_H \,. \tag{30}$$

Using (30), we obtain the following expressions for the entropy force and pressure on the cosmic horizon of the Universe, corresponding to the Tsallis–Cirto entropy:

$$F_{TC} = -T_H \frac{dS_B}{dR_H} = -\gamma \frac{3}{2} \frac{c^4}{G} \left(\frac{\pi}{A_{Pl}}\right)^{1/2} R_H =$$
$$= -\gamma \frac{3}{2} \left(\frac{\hbar}{\pi k_B c}\right) \left(\frac{K^3}{k_B}\right)^{1/2} R_H = -\gamma \frac{3}{2} \left(\frac{c^4}{KG}\right) \left(\frac{K^3}{k_B}\right)^{1/2} R_H, \tag{31}$$

$$P_{TC} = \frac{F_{TC}}{4\pi R_H^2} = -\frac{3}{2} \gamma \frac{c^4}{4\pi G} \left(\frac{K}{k_B}\right)^{1/2} R_H^{-1} = -\gamma \frac{c^2}{4\pi G} \frac{3c}{2} \left(\frac{K}{k_B}\right)^{1/2} H.$$
 32)

Assuming, as it was made before, that in entropy cosmology the effective pressure  $P'_{TC}$  based on the Tsallis–Cirto entropy is determined by the relation  $P'_{TC} = P + P_{TC}$ , and substituting  $P'_{TC}$ in the equations of acceleration (5) and continuity (6); we will obtain:

$$\frac{a_{ttt}}{a} = -\frac{4\pi G}{3} \left( \rho(t) + \frac{3P(t)}{c^2} \right) + \frac{3c}{2} \left( \frac{K}{k_B} \right)^{1/2} \gamma H(t), \qquad (33)$$

$$\rho_{t} + 3H(t) \left[ \rho(t) + \frac{P(t)}{c^2} \right] = \frac{3}{4\pi G} \frac{3c}{2} \left( \frac{K}{k_B} \right)^{1/2} \gamma H(t)^2.$$
(34)

Equations (33) and (34) can be considered as modified equations of acceleration and continuity based on the generalized Tsallis–Cirto entropy. From equation (33) it follows that the governing force term in this model is proportional to the Hubble rate H expansion of the Universe, in contrast to the analogous entropy force term in the Bekenstein–Hawking model, which is proportional to  $H^2$ .

It should be noted that cosmological equations similar to equations (33) and (34) have been repeatedly discussed in the literature when modeling the evolution of the Universe based on different approximations of the variable cosmological term (see, for example, [46]). On the other hand, the entropy force (31) obtained from the generalized entropy Tsallis– Cirto behaves in the same way as the driving force of a viscous cosmological fluid with bulk viscosity  $\eta$ , which is used to explain the accelerated expansion of the Universe in models of viscous cosmology. In-

deed, the expression for the effective pressure  $P'_{TC}(t) = P(t) - \frac{3c^3}{8\pi G} \left(\frac{K}{k_B}\right)^{1/2} H(t)$  in equation

(34) is similar to the expression  $P'(t) = P(t) - 3\eta H(t)$  for pressure in viscous cosmology models designed to simulate dark matter. Models of this type assume that the Universe is filled with a cosmological fluid with bulk viscosity that can generate the entropy of a homogeneous and isotropic Universe (see [47-51). This similarity became possible due to the fact that the nonadditive entropy of Tsallis Cirto, introduced on the basis of the holographic principle, behaves as if it were the classical entropy of a homogeneous and isotropic Universe generated by the volumetric viscous stress of a cosmological fluid [48, 52-54].

Thus, using the holographic principle, which is associated with the existence of the Barrow entropy on the horizon of the Universe, in this work two models of the entropic force were considered: model (17) based on the Bekenstein–Hawking entropy, and model (31) based on non-additive Tsallis–Cirto entropy. These models describe the evolution of an accelerating Universe without using the concept of the cosmological constant or dark energy.

This implies that the Bekenstein–Hawking entropy force model predicts a uniformly accelerating Universe, while the Tsallis–Cirto model predicts both deceleration and accelerated expansion of the Universe [46, 55].

# 5. THERMODYNAMIC APPROACH TO THE DEVELOPMENT OF THE EQUATION OF ENERGY CONSERVATION

Let us now proceed to consideration of the non-adiabatic expansion of the Universe caused by Barrow's cosmological entropy on the Hubble horizon. For this purpose, we derive the generalized energy equation (6), modifying the thermodynamic approach developed in the monograph [38].

#### 5.1. Adiabatic expansion of the Universe

According to the first law of thermodynamics, the principle of conservation of total energy for non-additive systems can be written in the form dQ/dt = dE/dt + PdV/dt or in the form of the Gibbs relation [56, 57]

$$TdS / dt = dQ / dt = dE / dt + PdV / dt,$$
(35)

expressing the rate TdS/Dt of change in entropy S when an element of a non-additive medium moves along its trajectory. Here dQ is the heat transferred across the border from the environment to the element of the environment, dE and dV changes in the internal energy and volume of the area of matter and radiation, respectively. Relation (35) can be rewritten as

$$TdS = dQ = T\frac{dS}{dt}dt = \frac{dE + PdV}{dt}dt = (E_{,t} + PV_{,t})dt.$$
 (36)

Let us now consider a sphere of initial radius  $\hat{r}_s$ , expanding together with the universal expansion of the Universe, so that its own radius  $R_H(t)$  at the moment of time t is determined by the expression  $R_H = a(t)\hat{r}_s$ . Then the volume V(t) of the sphere is

$$V(t) = (4\pi/3)\hat{r}_s^3 a(t)^3 .$$
(37)

From this it follows

$$V_{t} = \frac{4\pi}{3} \hat{r}_s^3 (3a^2 a_{t}) = V\left(3\frac{a_{t}}{a}\right) = 3VH, \quad (a_{t}/a = H) .$$
(38)

For the internal energy of the sphere, we have  $E(t) = \varepsilon(t)V(t)$ , where  $\varepsilon(t)$  is the internal energy density, determined by the relation  $\varepsilon(t) = \rho(t)c^2$ . Hence, the rate of change in the internal energy of the sphere E(t) is determined as

$$E_{t} = \varepsilon_{t} V + \varepsilon V_{t} = (\varepsilon_{t} + 3H\varepsilon)V.$$
(39)

Substituting equations (38) and (39) into  $E_{t} + PV_{t}$ , we obtain

$$E_{t} + PV_{t} = (\varepsilon_{t} + 3H\varepsilon)V + 3PVH = [\varepsilon_{t} + 3H(\varepsilon + P)]V =$$
$$= [\rho_{t} + 3H(\rho + P/c^{2})]c^{2}V.$$
(40)

Finally, substituting relations (37) and (39) into equation (36), we obtain the first law of thermodynamics for an expanding or contracting Universe:

$$T\frac{dS}{dt} = (E_{\prime t} + PV_{\prime t}) = \left[\rho_{\prime t} + 3H\left(\rho + \frac{P}{c^{2}}\right)\right]c^{2}V =$$
$$= c^{2}\left[\rho_{\prime t} + 3H\left(\rho + P/c^{2}\right)\right](4/3)\pi R_{H}^{3}.$$
(41)

Let us now consider such motions of cosmic matter for which the entropy of each particle of the medium remains in the first approximation constant throughout the entire path of an element of the medium, i.e. dS / dt = 0. Such reversible and adiabatic motions are isentropic. For them, equation (41) is reduced to the previously obtained continuity equation (6) for the adiabatic expansion of the Universe

$$\rho_{t}(t) + 3 \frac{a_{t}(t)}{a(t)} \left[ \rho(t) + P(t) / c^{2} \right] = 0.$$

#### 5.2. Modified energy equation for modeling non-adiabatic expansion of the Universe

If the evolution of the Universe within the framework of non-adiabatic entropic cosmology is modeled, then  $dS/dt \neq 0$  (see [58-60]. To calculate TdS/dt in equation (41), we will use formula (24) related to the Barrow entropy [35], as the most general in the case under consideration. As a result, we will have

$$T_{H} \frac{dS_{B}}{dt} = \gamma \left(\frac{\hbar c}{2\pi k_{B}R_{H}}\right) k_{B} \frac{\pi c^{3}}{\hbar G} \left(\frac{\pi}{A_{Pl}}\right)^{D/2} (2+D) R_{H}^{1+D} \frac{dR_{H}}{dt} =$$
$$= \gamma \frac{2+D}{2} \frac{c^{4}}{G} \left(\frac{\pi}{A_{Pl}}\right)^{D/2} R_{H}^{D} \frac{dR_{H}}{dt} = -\gamma \frac{(2+D)}{2} \frac{c^{5+D}}{G} \left(\frac{K}{k_{B}}\right)^{D/2} H^{-D-2} H_{\prime t}.$$
(42)

Taking into account expression (42), the energy equation (41)

$$\left[\rho_{t}+3H\left(\rho+\frac{P}{c^{2}}\right)\right]=T_{H}\frac{dS_{B}}{dt}c^{-2}\left(\frac{3}{4\pi}R_{H}^{-3}\right)$$

in the case of non-adiabatic expansion of the Universe under the influence of the driving entropy force (associated with the Barrow entropy) takes the form

$$\rho_{t} + 3\frac{a_{t}}{a}\left(\rho + \frac{P}{c^{2}}\right) = -\frac{D+2}{2}c^{2D}\left(\frac{K}{k_{B}}\right)^{D/2}\left(\frac{3}{4\pi G}\right)\gamma H^{1-D}H_{t}.$$
(43)

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This is a modified equation of continuity obtained from the first law of thermodynamics under the assumption of non-adiabatic expansion of the Universe. The right-hand side of equation (43) is associated with a non-adiabatic process. If H = 0 or if H = const, then equation (43) is reduced to the continuity equation for the adiabatic expansion of the Universe. Note that a similar modification of the continuity equation for entropy cosmology has been studied for other cosmological models of the expansion of the Universe (see, for example, [18, 19].

Using equation (43), the following equations of continuity can be obtained in the case of nonadiabatic expansion of the Universe under the influence of the Bekestein–Hawking and Tsallis–Cirto entropic forces:

$$\rho_{\prime t} + 3 \frac{a_{\prime t}}{a} \left( \rho + \frac{P}{c^2} \right) = -\gamma \left( \frac{3}{4\pi G} \right) H H_{\prime t}, \quad (D = 0), \tag{44}$$

$$\rho_{t} + 3\frac{a_{t}}{a}\left(\rho + \frac{P}{c^{2}}\right) = -\gamma \frac{3c^{2}}{2}\left(\frac{K}{k_{B}}\right)^{1/2}\left(\frac{3}{4\pi G}\right)H_{t}, \quad (D=1).$$
(45)

4 10

#### 5.3. Simple models of non-adiabatic expansion of the Universe

In this subsection, using the modified continuity equation (43), we'll analyze two generalized Friedman equations (4) and (5) for the scale factor in the case of non-adiabatic expansion of the Universe under the influence of the Barrow entropy force.

For this purpose, we write equation (4) in the form

$$(a_{t})^{2} = \frac{8\pi G}{3}\rho a^{2} + f(t)a^{2}, \qquad (46)$$

where f(t) is a function depending on the type of entropy force, including high-order corrections. Differentiating this equation with respect to t, we obtain

$$2a_{t}a_{t}a_{t} = \frac{8\pi G}{3} \left( \rho_{t}a^{2} + 2\rho aa_{t} \right) + f_{t}a^{2} + 2faa_{t}$$

or, after dividing by  $2aa_{t}$ ,

$$\frac{a_{\prime tt}}{a} = \frac{4\pi G}{3} \left( \frac{1}{H} \rho_{\prime t} + 2\rho \right) + \frac{1}{2H} f_{\prime t} + f .$$
(47)

Now multiplying the energy equation (43) by  $a / a_{rt} = 1 / H$ , as a result we will have

$$\frac{\rho_{t}}{H} = -3(1+w)\rho - \frac{D+2}{2}c^{2D}\left(\frac{K}{k_B}\right)^{D/2}\left(\frac{3}{4\pi G}\right)\gamma H^{-D}H_{t}.$$
(48)

where the notation is introduced  $w = P / \rho c^2$ . Substituting relation (48) into equation (47), we finally obtain

$$\frac{a_{tt}}{a} = -\frac{4\pi G}{3} (1+3w) \rho - \frac{D+2}{2} c^{2D} \left(\frac{K}{k_B}\right)^{D/2} \gamma H^{-D} H_{tt} + \frac{1}{2H} f_{tt} + f \qquad (49)$$

Further, for the purpose of simulation, one should follow the work [15, 22] concept, where it was assumed that the term associated with the entropy force does not depend on the time derivative of the Hubble parameter. Following this assumption, we define the functions f(t) in such a way

that the term with  $H_{t}$  is absent in equation (49). If we put

$$f(t) = \gamma \frac{2+D}{2-D} c^{2D} \left(\frac{K}{k_B}\right)^{D/2} H(t)^{2-D},$$
(50)

we then obtain the following simple system of self-consistent equations, composed of the modified Friedman equations, acceleration and continuity:

$$\left(\frac{a_{t}}{a}\right)^{2} = \frac{8\pi G}{3}\rho a^{2} + \gamma \frac{2+D}{2-D}c^{2D} \left(\frac{K}{k_{B}}\right)^{D/2} H^{2-D},$$
(51)

$$\frac{a_{tt}}{a} = -\frac{4\pi G}{3} \left(1 + 3w\right) \rho + \gamma \frac{2 + D}{2 - D} c^{2D} \left(\frac{K}{k_B}\right)^{D/2} H^{2-D},$$
(52)

$$\rho_{t} + 3\frac{a_{t}}{a}\left(\rho + \frac{P}{c^{2}}\right) = -\frac{D+2}{2}c^{2D}\left(\frac{K}{k_{B}}\right)^{D/2}\left(\frac{3}{4\pi G}\right)\gamma H^{1-D}H_{t}.$$
(53)

This system of equations makes it possible to simulate a new scenario of the evolution of the Universe, if one considers it as a thermodynamic system bounded by the visible horizon, which expands nonadiabatically under the influence of the entropic force associated with the nonadditive entropy of Barrow.

Using the system of equations (51)-(53), it is possible to obtain a number of models that describe the non-adiabatic evolution of the Universe without using the concept of the cosmological constant, or dark energy. These models include, in particular, the non-adiabatic model based on the Bekenstein–Hawking entropy and the non-adiabatic model based on the Tsallis–Cirto nonadditive entropy. Assuming parameter D = 0 in formula (50), we will have  $f(t) = \gamma H(t)^2$  for the function f(t). In this case, a simple entropy model of the non-adiabatic expansion of the Universe based on the Bekenstein–Hawking entropy takes the form

$$(a_{t})^{2} = \frac{8\pi G}{3}\rho a^{2} + \gamma H^{2}, \qquad (54)$$

$$\frac{a_{\prime tt}}{a} = -\frac{4\pi G}{3} \left(1 + 3w\right) \rho + \gamma H^2,\tag{55}$$

$$\rho_{\prime t} + 3\frac{a_{\prime t}}{a} \left(\rho + \frac{P}{c^2}\right) = -\gamma \left(\frac{3}{4\pi G}\right) H H_{\prime t} \,. \tag{56}$$

Entropic force  $f = \gamma H^2$  in the equation. (54) coincides with the corresponding term in formula (55). The modified Friedman equations (54) and (55) correspond to equations (4) and (5) of the Friedman cosmological model. Using this system, it is possible to establish a number of properties of a non-adiabatically expanding Universe (see, for example, [23, 25].

If we put D=1 in formula (50), then for the function f(t) we obtain the following expression

$$f = 3\gamma c^2 \left( K / k_B \right)^{1/2} H \,, \tag{57}$$

and taking it into account the system (51)-(53) takes the form

$$\left(\frac{a_{t}}{a}\right)^2 = \frac{8\pi G}{3}\rho a^2 + \gamma 3c^2 \left(\frac{K}{k_B}\right)^{1/2} H, \qquad (58)$$

$$\frac{a_{\prime tt}}{a} = -\frac{4\pi G}{3} \left(1 + 3w\right) \rho + \gamma 3c^2 \left(\frac{K}{k_B}\right)^{1/2} H, \qquad (59)$$

$$\rho_{\prime t} + 3\frac{a_{\prime t}}{a} \left(\rho + \frac{P}{c^2}\right) = -\gamma \frac{3c^2}{2} \left(\frac{K}{k_B}\right)^{1/2} \left(\frac{3}{4\pi G}\right) H_{\prime t}.$$
 (60)

This system of equations underlies the simulation of the evolution of the non-adiabatically expanding Universe under the influence of the Tsallis–Cirto entropy force [31].

Thus, entropy cosmology using the procedure of "gravitational thermodynamics" using the Barrow entropy is quite effective for constructing a number of models describing the evolution of the Universe and allowing one to find quantitative estimates of the non-adiabatic accelerated expansion of the Universe in accordance with observational data.

#### CONCLUSION

Progress in astrophysics rooted in the ground-based and space astronomy greatly influenced the key concepts of our views about space environment, origin, evolution and fate of our Universe. For less than half a century since the beginning of space exploration [61] cosmology experienced dramatic changes and this process continuously escalates. New projects and break-throughs in theoretical approaches in the coming years open extremely challenging horizons in this intriguing branch of astrophysics and general science.

The modern cosmological data indicate that the Universe is expanding with acceleration. Unfortunately, a simple modified general relativity, which includes a key parameter – the cosmological constant  $\Lambda$ , characterizing an expansion cannot describe this phenomenon convincingly enough. Therefore, it becomes necessary to search for an approach that could be used to describe the accelerated expansion of the Universe more effectively.

One of the directions along this path consists in the construction of a modified theory of gravity, according to which the entropic force underlies the accelerated expansion of the Universe. The emergence of this force is an inevitable consequence of the growth of entropy at the post-inflationary stage of the quantum canvas of space-time, which can be associated with the storage of holographic information on the "surface screen of the Universe", similar in a certain sense to the event horizon of a black hole.

It should be noted that the holographic principle was put forward earlier in the study of physics of the black holes as an important property of quantum gravity, which states that the properties of space are encoded at its boundary (on the gravitational horizon of events). Based on this principle, Verlinde proposed an extended holographic picture in which Einstein's gravity arises from the statistical effect of a holographic screen. This approach proved to be effective for describing quantitatively the accelerated expansion of the Universe. A number of authors generalized the basic scenario of the evolution of the Universe, based on the use of entropic forces of various nature, with involvement of the assumption that the horizon of the Universe, like the event horizon of a black hole, has its own entropy and temperature.

Recently, Barrow proposed a model of the quantum gravitational canvas of space-time to estimate the entropy of black holes and the Universe, the surface of which can have a complex fractal structure of the cosmological horizon down to arbitrarily small scales (an order of the Planck length) due to quantum gravitational effects. As it is known, many solutions of the classical Einstein equations, in particular, the isotropic homogeneous cosmological model of Friedman–Robertson–Walker, contain singularities and cannot be analytically continued beyond them. In this regard, we face the fundamental problem of modern cosmology: what caused the growth of fluctuations and the emergence of a fragment of space-time on the infinite quantum canvas of the Universe, which concentrated within itself a huge energy ("vacuum energy") and why and how it was followed by inflation (de Sitter phase) and subsequently, the Big Bang left behind observed echo in the form of microwave background radiation (CMB). One way or another, the basis of such a scenario, which gave rise to the birth of the Universe, is addressed to quantum-gravitational effects [62].

In this work, an attempt is undertaken to better understand the physical mechanism of the accelerated expansion of a flat, homogeneous and isotropic Universe. Modified cosmological equations are obtained, containing new additional terms that coincide with the basic Friedman equations in the case when the Barrow deformation exponent corresponds to the fractal dimension D=0. However, in the general case  $0 < D \le 1$ , new governing terms appear associated with changes in the entropy of Barrow on the Hubble horizon of the Universe. It significantly exceeds its age, which affect the evolution of the main cosmological criteria, such as the scale factor, the deceleration parameter, the density of matter (involving visible and dark matter, radiation, neutrinos, etc.) and the growth of linear perturbations of matter. This should lead to a new phenomenological description of the thermal history of the Universe. The core for this conclusion is based on the results of this work, in which the validity of using the generalized second law of thermodynamics for the Barrow entropy was thoroughly investigated. On this basis, modified Friedman equations were obtained, which made it possible to explain the non-adiabatic expansion of the Universe in terms of entropy, without involving hypothetical dark energy as a texture (fabric) of the very expanding space. It seems reasonable to find out in this approximation a solution to the modified Einstein equations with quantum corrections and to establish whether there are physically interesting nonsingular solutions among them.

As one may see, entropy cosmology, based on the concepts of "gravitational thermodynamics" using the entropy of Barrow, is regarded as quite effective approach for quantitative assessment of the non-adiabatic accelerated expansion of the Universe and its possible change with time. The results of the analysis of possible solutions of the cosmological equations analyzed in this work will be presented in the following publications of the authors.

## REFERENCES

- [1] J.A.S. Lima, J. S. Alcaniz, "Constraining the cosmic equation of state from old galaxies at high redshift", *Mon. Not. R. Astron. Soc.* **317**, 893-896 (2000).
- [2] E. Komatsu, et al. "Seven-year Wilkinson Microwave Anisotropy Probe (WMAP) Observations: Cosmological Interpretation", *Astrophys. J. Suppl. Ser.* 192(2). article id. 18, 47 pp. (2011).
- [3] Ch.W. Mizner, K.S. Torn, J.A. Wheeler, *Gravitatsiya*. W.H. Freeman and Company. San Francisco. (1973).
- [4] S. Weinberg, *Cosmology*. Oxford University Press. (2008).
- [5] D.S. Gorbunov, V.A. Rubakov, "Introduction to the theory of the early universe: hot big bang theory", British Library Cataloguing-in-Publication Data. (2018).
- [6] E.J. Copeland, M. Sami, S. Tsujikawa, "Dynamics of dark energy", Int. J. Mod. Phys. D. 15(11), 1753-1935 (2006).
- [7] Y.-F. Cai, E.N. Saridakis, M.R. Setare, J-Q. Xia, "Quintom Cosmology: Theoretical implications and observations", *Phys. Rept.* **493**,1-60 (2010).
- [8] A.M. Cherepashchuk, A.D. Chernin, *Vselennaya, zhizn', chernyye dyry*. Fryazino: «Vek 2». (2004).
- [9] M.Ya. Marov, Kosmos: Ot Solnechnoy sistemy vglub' Vselennoy. M.: Fizmatlit. (2018).
- [10] E. Verlinde, "On the origin of gravity and the laws of Newton", *J. High Energy Phys.* **4**, 1-26 (2011).
- [11] T. Padmanabhan, "Thermodynamical Aspects of Gravity: New insights", *Rept. Prog. Phys.* **73**(4), 046901 (44pp) (2010).
- [12] L. Susskind, "The World as a hologram", J. Math. Phys. 36(11), 6377-6396 (1995).
- [13] J.D. Bekenstein, "Black Holes and Entropy", Phys. Rev. D. 7(8), 2333-2346. (1975).
- [14] S. W. Hawking, "Particle Creation By Black Holes", Commun Math. Phys. 43, 199-220 (1975).

- [15] D.A. Easson, P.H. Frampton, G.F. Smoot, "Entropic accelerating universe", *Physics Letters B*. **696**(3), 273-277 (2011).
- [16] T.S. Koivisto, D.F. Mota, M. Zumalacárregui, "Constraining entropic cosmology", J. Cosmol.Astropart. Phys. release 02. id.027 (2011).
- [17] Y.S. Myung, "Entropic force and its cosmological implications", *Astrophys. Space Sci.* 335 (2), 553-559 (2011).
- [18] Y.-F. Cai, J. Liu, H. Li, "Entropic cosmology: A unified model of inflation and late-time acceleration", *Physics Letters B*. **690**, 213-219 (2010).
- [19] Y.-F. Cai, E. Saridakis, "Inflation in entropic cosmology: Primordial perturbations and non-Gaussianities", *Physics Letters B*. 697, 280-287 (2011).
- [20] T. Qiu, E. N. Saridakis, "Entropic force scenarios and eternal inflation", *Phys. Rev. D.* 85. 043504 (2012).
- [21] S. Basilakos, D. Polarski, J. Sola, "Generalizing the running vacuum energy model and comparing with the entropic-force models", *Phys. Rev. D.* **86**(4), 043010 (2012).
- [22] D.A. Easson, P.H. Frampton, G.F. "Smoot, Entropic Inflation", International Journal of Modern Physics A, 27(12) id. 1250066 (2012).
- [23] N. Komatsu, S. Kimura, "Entropic cosmology for a generalized black-hole entropy", *Physical Review D.* 88, 083534 (2013).
- [24] N. Komatsu, S. Kimura, "Non-adiabatic-like accelerated expansion of the late universe in entropic cosmology", *Phys. Rev. D.* 87, 043531 (2013).
- [25] N. Komatsu, S. Kimura, "Evolution of the universe in entropic cosmologies via different formulations", *Physical Review D.* **89**(12), 123501 (2014).
- [26] N. Komatsu, "Thermodynamic constraints on a varying cosmological-constant-like term from the holographic equipartition law with a power-law corrected entropy", *Physical Review D.* 96, 103507 (2017)
- [27] A. Plastino, M.C. Rocca, "Entropic Forces and Newton's Gravitation". *Entropy.* 22(3), 273 (1-10) (2020).
- [28] A.D. Wissner-Gross, C.E. Freer, "Causal entropy forces", Phys. Rev. Lett. 110, 168702 (2013).
- [29] N.D. Keul, K. Oruganty, E.T.S. Bergman, N.R. Beattie, W.E. McDonald, R. Kadirvelraj, M.L. Gross, R.S. Phillips, S.C. Harvey, Z.A. Wood, "The entropic force generated by intrinsically disordered segments tunes protein function", *Nature*. 563, 584-588 (2018).
- [30] W. de Sitter, "On the relativity of inertia. Remarks concerning Einstein's latest hypothesis", *Proc. Roy. Acad. Sci. (Amsterdam).* **19**, 1217-1225 (1917).
- [31] C. Tsallis, L.J.L. Cirto, "Black hole thermodynamical entropy", *Eur. Phys. J. C.* **73**, id 2487 (2013).
- [32] V.G. Czinner, H. Iguchi, "Rényi entropy and the thermodynamic stability of black holes", *Phys. Lett. B.* **752**, 306-310 (2016).
- [33] S. Weinberg, "The cosmological constant problem", *Reviews of Modern Physics*. **61**(1), 1-23 (1989).
- [34] F.K. Anagnostopoulos, S. Basilakos, E.N. Saridakis, "Observational constraints on Barrow holographic dark energy", *Eur. Phys. J. C.* 80, 826 (1-9) (2020).
- [35] J. D. Barrow, "The area of a rough black hole", Physics Letters B. 808, 135643 (2020).
- [36] E.N. Saridakis, "Modified cosmology through spacetime thermodynamics and Barrow horizon entropy", *Journal of Cosmology and Astroparticle Physics*.

release 07, article id. 031 (2020).

- [37] R. Tolmen, *Otnositel'nost', termodinamika i kosmologiya*. M.: URSS: Knizhnyy dom «LIBROKOM». (2009).
- [38] B. Ryden, Introduction to Cosmology. Cambridge University Press. (2017).
- [39] A. Friedmann, "Über die Krümmung des Raumes", *Zeitschrift für Physik*. **10**, 377-386 (1922).
- [40] F.K. Anagnostopoulos, S. Basilakos, G. Kofinas, V. Zarikas, "Constraining the Asymptotically Safe Cosmology: cosmic acceleration without dark energy", // Journal of Cosmology and Astroparticle Physics, Issue 02, article id. 053 (2019).
- [41] D.F. Torres, H. Vucetich, A. Plastino, "Early Universe Test of Nonextensive Statistics", *Phys. Rev. Lett.* **79**(9), 1588-1590 (1997).
- [42] Y. Aditya, S. Mandal, P. Sahoo, D. Reddy, "Observational constraint on interacting Tsallis holographic dark energy in logarithmic Brans-Dicke theory", *The European Physical Journal C*, 79(12), id. (2019).
- [43] G. Wilk, Z. Wlodarczyk, "On the interpretation of nonextensive parameter q in Tsallis statistics and Levy distributions", *Phys. Rev. Lett.* **84**, 2770-2773 (2000).
- [44] S. Waheed, "Reconstruction paradigm in a class of extended teleparallel theories using Tsallis holographic dark energy", The European Physical Journal Plus, 135(1), article id.11 (2020).
- [45] E.N. Saridakis, S. Basilakos, "The generalized second law of thermodynamics with Barrow entropy", arXiv:2005. 08258 (2020).
- [46] S. Basilakos, M. Plionis, J. Sola, "Hubble expansion and structure formation in time varying vacuum models", *Phys. Rev. D.* **80**(8), 083511 (2009).
- [47] T. Padmanabhan, S.M. Chitre, "Viscous universes", *Physics Letters A*, 120(9), 433-436 (1987).
- [48] B. <u>Li</u>, J. Barrow, "Does bulk viscosity create a viable unified dark matter model?", *Physical Review D*, **79**(10), id. 103521 (2009).
- [49] A. Avelino, U. Nucamendi, "Exploring a matter-dominated model with bulk viscosity to drive the accelerated expansion of the Universe", *Journal of Cosmology and Astroparticle Physic.* **2010**(8), article no. 009 (2010).
- [50] X.-H Meng, X. Dou, "Friedmann cosmology with bulk viscosity: a concrete model for dark energy", *Communicationsin Theoretical Physics*. **52**(2), 377-38 (2009).
- [51] X. Dou, X.-H. Meng, "Bulk Viscous Cosmology: Unified Dark Matter", Advances in Astronomy, **2011**, id.829340 (2011).
- [52] O. Gron, "Viscous inflationary universe models", *Astrophysics and Space Science*. **173**, 191-225 (1990).
- [53] I. Brevik, O.G. Gorbunova, "Dark energy and viscous cosmology", *General Relativity* and Gravitation. **37**, 2039-2045 (2005).
- [54] L. Sebastian, "Dark viscous fluid coupled with dark matter and future singularity", *European Physical Journal C.* **69**, 547-553 (2010).
- [55] S. Basilakos, J. Sola, "Entropic-force dark energy reconsidered", *Phys. Rev. D.* **90**(2), 023008 (2014).
- [56] A.V. Kolesnichenko, "K postroyeniyu neadditivnoy termodinamiki slozhnykh sistem na osnove statistiki Kurado-Tsallisa", Preprinty IPM im. M.V. Keldysha. 25. 1-40 (2018).
- [57] A.V. Kolesnichenko, Statisticheskaya mekhanika i termodinamika Tsallisa neadditivnykh

system: Vvedenie v teoriyu i prilozheniya. Moskow: LENAND. (Sinergetika ot proshlogo k budushchemu. № 87), (2019).

- [58] A.V. Frolov, L. Kofman, "Inflation and de Sitter thermodynamics", *Journal of Cosmology and Astroparticle Physics*, Issue 05, article id. 009 (2003).
- [59] R.G. Cai, S.P. Kim, "First law of thermodynamics and Friedmann equations of Friedmann-Robertson-Walker universe", *Journal of High Energy Physics*, Issue 02, id. 050 (2005).
- [60] M. Akbar, R.G. Cai, "Thermodynamic Behavior of Friedmann Equations at Apparent Horizon of FRW Universe", *Phys. Rev. D.* **75**, 084003 (2007).
- [61] M.V.Keldysh., M.Ya. Marov. Space exploration. Moscow, Science (1981).
- [62] A.A. Starobinsky, "A new type of isotropic cosmological models without singularity", *Physics Letters B* . **91** (1), 99-103 (1980).

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# ON THE MATHEMATICAL MODEL OF COMBINED RAREFACTION AND COMPRESSION WAVES IN CONDENSED MATTER

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**Summary.**Two waves model where shock wave is combined with rarefaction wave appearing in laser ablation due to metal-nonmetal transition effect is investigated using conservation laws for mass and momentum fluxes for the steady-state regime of the process. This approach permits to obtain the relation between front velocities of the waves which shows that the rarefaction wave can be rather slow compared with the generated shock wave.

#### **1. INTRODUCTION**

Compression shock waves with supersound propagation speed are well known in mathematics and physics due to its practical importance and rather simple generation [1-3]. Rarefaction shock waves are not so widespread phenomena because, in particular, for its generation more special conditions are needed [3-6]. Laser ablation due to surface vaporization process can be considered as an example of slow speed rarefaction waves moving into the irradiated condensed matter. In [7] it was suggested that during laser metal ablation " induced transparency wave" arisen from metal- nonmetal transition (MNT) [8] can propagate into some metals which, in contrast to vaporization process, remain in liquid state with diminished density. The laser ablation with possible MNT effect is considered in many papers (see, e.g. [9-11] and references therein) without sufficient attention to hydrodynamic aspects of the problem.

In the present paper some properties of combined compression and rarefaction waves are investigated which, to our knowledge, have not been discussed before.

## 2. STATEMENT OF THE PROBLEM

In the considered condensed matter (liquid) which was initially at rest in the half-space  $z \ge 0$  with pressure  $P_0$ , density  $\rho_0$  and velocity  $V_0 = 0$  two combined compression and rarefaction waves are propagating with constant velocities, respectively, D > d > 0. The rarefaction wave movement is due to MNT effect mentioned above. Between compression and rarefaction wave fronts one has for velocity, pressure, and density the relations:  $V_1 > 0$ ,  $P_1 > P_0$ , and  $\rho_1 > \rho_0$  while after rarefaction wave front  $V_2 < 0$ ,  $P_2 > P_0$ , and  $\rho_c < \rho \le \rho_2$ , where  $\rho_c$  means critical density for liquid-vapor phase transition and P2 at the irradiated surface depends on the metal ablation regime conditions.

Conservation laws for mass and momentum fluxes at the two fronts are as follows:

$$\rho D = \rho_1 (D - V_1) \tag{1}$$

$$P + \rho D^2 = P_1 + \rho_1 (D - V_1)^2$$
(2)

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$$\rho_1(d - V_1) = \rho_2(d - V_2) \tag{3}$$

$$P_1 + \rho_1 (d - V_1)^2 = P_2 + \rho_2 (d - V_2)^2$$
(4)

From these equation it is possible to obtain useful relation between velocities of shock and rarefaction waves.

#### **3. RESULTS AND DISCUSSION**

To obtain the relation between d and D it is necessary to exclude from (1)-(4) velocities  $V_1$ ,  $V_2$  and pressure  $P_1$ , which can be done in a straightforward manner. From (1), (2) it follows:

$$D \cdot V_1 = D \cdot B_{01} \tag{5}$$

$$P = P_1 - \rho \ D^2 (1 - B_{01}) \tag{6}$$

where  $B_{01} = \rho_0 / \rho_1$ . Taking into account eqs. (1), (2) and notation  $B_{12} = \rho_1 / \rho_2$  one obtains for P<sub>1</sub>:

$$P_1 = P_2 + \rho_1 (d - V_1)^2 (B_{12} - 1) = P_2 + \rho_1 [d - D(1 - B_{01})]^2 (B_{12} - 1)$$
(7)

From (6), (7) then it follows:

$$P = P_2 + \rho_1 (B_{12} - 1) [d - D(1 - B_{01})]^2 - \rho \ D^2 (1 - B_{01})$$
(8)

After using the relation m = d/D one can rewrite (8) in the form:

$$\left\{ \frac{\left[\frac{P_2 - P_0}{\rho_1 D^2} - B_{01}(1 - B_{01})\right]}{1 - B_{12}} \right\} = \left[ (1 - B_{01}) - m \right]^2 \tag{9}$$

$$\left\{ \frac{\left[\frac{P_2 - P_0}{\rho_0 D^2} - (1 - B_{01})\right] B_{01}}{1 - B_{12}} \right\} = \left[ (1 - B_{01}) - m \right]^2 \tag{9a}$$

It is clear that in (9) the expression in brackets {} cannot be negative while its numerator cannot be positive because  $(1-B_{12}) < 0$ . At the threshold where the expression in brackets is zero one has for maximum value of  $B_{01M}$  and corresponding value of  $m_M$ :

$$(1 - B_{01M}) = \frac{P_2 - P_0}{\rho_0 D^2} \tag{10}$$

$$m_M = (1 - B_{01M}) \tag{11}$$

These equations permit to estimate approximately the threshold value of  $m_M$  and d for the experiment conditions [9,10] because in this case D differs from sound velocity but slightly. For example, at  $P_2 - P_0 \approx 300$  bar  $(3 \cdot 10^8 \text{ g/s}^2 \text{ cm})$  and  $\rho_0 D^2 \approx 3 \cdot 10^{11} \text{ g/s}^2 \text{ cm}$  this gives  $m_M \approx 10^{-3}$ . Above the threshold evolution of m is determined by the expression:

$$m = 1 - B_{01} \pm \left\{ \frac{B_{01} \left[ \frac{(P_2 - P_0)}{\rho_0 D^2} + B_{01} - 1 \right]}{1 - B_{12}} \right\}^{\frac{1}{2}}$$
(12)

where the solution with sign (+) is appropriate for  $B_{01} < B_{01M}$  due to the condition m > 0 while it is not so for the second solution with sign (-). Dependence of both solutions (12)

on  $B_{01}$  is shown in Fig.1 at different values of  $B_{12}$  and constant other parameters for simplicity. It should be mentioned that  $B_{01}$ ,  $B_{12}$ , D and  $P_2$  vary in accordance with equation of state and with MNT properties as well as with laser ablation regime which determines also value of d.



Fig.1 Dependencies of the value m on the ratio  $B_{01}$  for three fixed ratio  $B_{12}$  and one fixed ratio  $(P_2 - P_0)/\rho_0 D^2 = I - B_{01M} = 3.5 \cdot 10^{-3}$ 

#### **4. CONCLUSION**

Presented here investigation of mathematical properties pertinent to suggested model of combined compression and rarefaction waves permits to obtain the relation between the propagation velocities of the waves. The investigation is based on analysis of conservation laws for the steady-state mass and momentum fluxes. More detailed information on the considered regime can be obtained taking into account the energy flux conservation law as well as using time-dependent mathematical modeling of laser ablation with MNT effect.

#### REFERENCES

- [1] R. von Mises, *Mathematical theory of compressible fluid flow*, Academic Press Inc. Publishers, New York (1958).
- [2] L.D. Landau, E.M. Lifshicz, *Teoreticheskaya fizika*. *Gidrodinamika*, Moskva Nauka (1986).
- [3] Yu.P. Rajzer, Ya.B. Zel`dovich, *Fizika udarny`kh voln i vy`sokotemperaturny`kh gidrodinamicheskikh yavlenij*, Moskva, Fizmatlit (2008).
- [4] Ya.B. Zel`dovich, "O vozmozhnosti udarny`kh voln razrezheniya", *ZhE`TF (JETP)* **16** (4), 363-367 (1946).
- [5] A.G. Ivanov, S.A. Novikov, "Rarefaction Shock Waves in Iron and Steel", *JETP*, **13** (6), 1321-1323 (1961).
- [6] Ya.B. Zel`dovich, S.S. Kutateladze, V.E. Nakoryakov, A.A. Borisov, "Obnaruzhenie udarnoj volny` razrezheniya vblizi kriticheskoj tochki zhidkost` - par", *Vestnik AN SSSR*, 3, 3-21 (1983).
- [7] V.A. Batanov, F.V. Bunkin, A.M. Prokhorov, V.B. Fedorov, "Evaporation of Metallic Targets Caused by Intense Optical Radiation", *JETP*, 36 (2), 311-322 (1973).

- [8] L.D. Landau, Ya.B. Zel'dovich, "O sootnoshenii mezhdu zhidkim i gazoobrazny`m sostoyaniem u metallov", *ZhETF*, 14, 32-38 (1944).
- [9] S.N. Andreev, V.I. Mazhukin, N.M. Nikiforova, A.A. Samokhin, "On Possible Manifestations of the Induced Transparency During Laser Evaporation of Metals", *Quantum Electron.*, 33 (9), 771-776 (2003).
- [10] A.A. Samokhin, E.V. Shashkov, N.S. Vorobiev, A.E. Zubko, "On acoustical registration of irradiated surface displacement during nanosecond laser-metal interaction and metal-nonmetal transition effect", *Appl. Surf. Sci.*, 502, 144261 (2020).
- [11] A.A. Samokhin, P.A. Pivovarov, E.V. Shashkov, I.A. Stuchebrukhov, "On the evidence for metal-nonmetal transition in nanosecond laser ablation", *Phys.of Wave Phenom.* (in press 2021).

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# MODELING OF SHOCK-WAVE PROCESSES IN ALUMINUM UNDER THE ACTION OF A SHORT LASER PULSE

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**Summary.** A hydrodynamic model of shock-wave processes in a material under the action of a short high-intensity laser pulse is considered. The simulation is carried out for the case of an aluminum target 90  $\mu$ m thick, irradiated by a laser pulse with a duration of 70 ps and a maximum intensity of 14.7 TW/cm<sup>2</sup>. In the corresponding laboratory experiment, on the rear side of the target after irradiation, a spall of a part of the material is recorded at a depth of  $10 \pm 1 \mu$ m. Calculation of the time dependence of the pressure and density of aluminum in the spall plane makes it possible to determine the tensile strength of aluminum at a high strain rate.

## **1 INTRODUCTION**

The action of a short high-intensity laser pulse upon a target makes it possible to study the properties of the target material under shock-wave loading at a high strain rate [1–9]. Numerical modeling of such a process [2,3,6,10–16] provides additional possibilities for the interpretation of the obtained measurement results.

In this work, an example of a laboratory experiment on the action of a 70 ps laser pulse on an aluminum target is given. A description of the hydrodynamic model for the propagation of shock compression waves and adiabatic unloading along the target is presented. The results of modeling are presented and a conclusion is made about the magnitude of the spall strength of aluminum at the considered strain rate.

2010 Mathematics Subject Classification: 74J40, 76L05, 82D20, 82D35.

**Key words and phrases:** laser pulse action, aluminum, shock wave loading, adiabatic release, spall, tensile strength, high strain rate.

#### **2 EXPERIMENT**

The experiment was carried out on a Kamerton-T facility based on a neodymium glass laser (wavelength  $\lambda = 0.527 \ \mu$ m) [8, 10, 11]. A pulse with duration  $\tau = 70$  ps and energy  $E_1 = 3.57$  J was focused into a spot 0.63 mm in diameter on the surface of a 90- $\mu$ m-thick aluminum target. Taking into account the measured dependence of the laser radiation intensity on time, the maximum intensity of this pulse is estimated to be  $I_0 = 14.7 \text{ TW/cm}^2$ .

The result of the action of such a pulse is the formation of a spall of a part of the material on the rear side of the target. The spall occurred at a distance of  $10 \pm 1 \ \mu m$  from the rear surface; the diameter of the spalled plate is 0.66 mm.

#### **3 HYDRODYNAMIC MODEL**

The system of hydrodynamic equations for the one-dimensional case under consideration has the following form [17]:

$$\frac{\partial}{\partial t}\mathbf{U} + \frac{\partial}{\partial x}\mathbf{F} = 0, \tag{1}$$

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ e \end{pmatrix}, \qquad \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho u v \\ \rho u w \\ (e+P)u \end{pmatrix}, \qquad (2)$$

where t is the time coordinate; x is the spatial coordinate;  $\rho$  is the density of the material under consideration; P is the pressure; e is the full energy density,

$$e = \rho E + \frac{1}{2}\rho(u^2 + v^2 + w^2), \tag{3}$$

*E* is the specific internal energy; *u* is the particle velocity along the *x*-axis; v = 0 and w = 0 for the case.

In quasilinear non-conservative form, the system of equations (1) can be written as follows:

$$\frac{\partial}{\partial t}\mathbf{U} + \mathbf{A}\frac{\partial}{\partial x}\mathbf{U} = 0, \tag{4}$$

where

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ -u^2 + \theta b & 2u - ub & -vb & -wb & b \\ -uv & v & u & 0 & 0 \\ -uw & w & 0 & u & 0 \\ -uh + u\theta b & h - u^2 b & -uvb & -uwb & u + ub \end{pmatrix},$$
(5)  
$$h = \frac{e + P}{\rho}, \qquad \theta = q^2 - \frac{e}{\rho} + \frac{(\partial P / \partial \rho)_E}{b}, \qquad q^2 = u^2 + v^2 + w^2, \qquad b = \frac{(\partial P / \partial E)_{\rho}}{\rho}.$$
(6)

One can write matrix **A** in the form  $\mathbf{A} = \Omega \Lambda \Omega^{-1}$ , where

$$\Omega = \begin{pmatrix} 1 & 0 & 0 & 1 & 1 \\ u-c & 0 & 0 & u & u+c \\ v & 1 & 0 & v & v \\ w & 0 & 1 & w & w \\ h-uc & v & w & h-c^2b^{-1} & h+uc \end{pmatrix}, \quad \Lambda = \begin{pmatrix} u-c & 0 & 0 & 0 & 0 \\ 0 & u & 0 & 0 & 0 \\ 0 & 0 & u & 0 & 0 \\ 0 & 0 & 0 & u & 0 \\ 0 & 0 & 0 & 0 & u+c \end{pmatrix}, \quad (7)$$

$$\Omega^{-1} = \frac{b}{2c^2} \begin{pmatrix} \theta+ucb^{-1} & -u-cb^{-1} & -v & -w & 1 \\ -2vc^2b^{-1} & 0 & 2c^2b^{-1} & 0 & 0 \\ -2wc^2b^{-1} & 0 & 0 & 2c^2b^{-1} & 0 \\ 2h-2q^2 & 2u & 2v & 2w & -2 \\ \theta-ucb^{-1} & -u+cb^{-1} & -v & -w & 1 \end{pmatrix}, \quad (8)$$

$$\det \Omega = \frac{2c^3}{b}, \quad c = \sqrt{(\partial P/\partial \rho)_E + \frac{P}{\rho^2}(\partial P/\partial E)_\rho}. \quad (9)$$

Here, c is the adiabatic sound velocity. Using values c and h, one can obtain

$$\theta = q^2 - h + c^2 b^{-1}.$$
 (10)

The system of equations of motion (1) is closed by the equation of state of the target material in the form of a function

$$P = P(\rho, E), \tag{11}$$

which is taken according to the model [18–20].
## **4 SOLUTION METHOD**

With the use of the formulas for matrices from the previous section, the system of equations (1) and (11) can be solved by the Courant–Isaacson–Rees method [21]. The difference scheme of the method is as follows [17]:

$$\frac{\mathbf{U}_{j}^{k+1} - \mathbf{U}_{j}^{k}}{\Delta t} + \frac{\mathbf{F}_{j+1/2} - \mathbf{F}_{j-1/2}}{\Delta x} = 0,$$
(12)

$$\mathbf{F}_{m+1/2} = \frac{1}{2} \left( \mathbf{F}_{m}^{k} + \mathbf{F}_{m+1}^{k} \right) + \frac{1}{2} |\mathbf{A}|_{m+1/2}^{k} \left( \mathbf{U}_{m}^{k} - \mathbf{U}_{m+1}^{k} \right)$$
(13)

for m = j - 1 and j. Here, integer subscripts denote the values of the function at the centers of discrete grid cells in space, and half-integer ones—at the boundaries of the cells;  $\Delta x$  is the step of a uniform grid in space;  $\Delta t$  is the time step;

$$|\mathbf{A}| = \Omega |\Lambda| \Omega^{-1}, \tag{14}$$

$$|\Lambda| = \begin{pmatrix} |u-c| & 0 & 0 & 0 & 0\\ 0 & |u| & 0 & 0 & 0\\ 0 & 0 & |u| & 0 & 0\\ 0 & 0 & 0 & |u| & 0\\ 0 & 0 & 0 & 0 & |u+c| \end{pmatrix}.$$
 (15)

Matrix (15) can be represented as a sum of three matrices with multipliers:

where  $\alpha = |u - c| - |u|; \gamma = |u + c| - |u|.$ 

Denoting  $\Delta \mathbf{U} = \mathbf{U}_m - \mathbf{U}_{m+1}$  (with elements  $\Delta U = U_m - U_{m+1}$ ) and using (14) and (16), one can obtain

$$|\mathbf{A}|\Delta \mathbf{U} = |u| \begin{pmatrix} \Delta \rho \\ \Delta(\rho u) \\ \Delta(\rho v) \\ \Delta(\rho w) \\ \Delta e \end{pmatrix} + \alpha(f+g) \begin{pmatrix} 1 \\ u-c \\ v \\ w \\ h-uc \end{pmatrix} + \gamma(f-g) \begin{pmatrix} 1 \\ u+c \\ v \\ w \\ h+uc \end{pmatrix}, \quad (17)$$

where

$$f = \frac{b}{2c^2} [\theta \Delta \rho - u \Delta (\rho u) - v \Delta (\rho v) - w \Delta (\rho w) + \Delta e], \qquad g = \frac{1}{2c} [u \Delta \rho - \Delta (\rho u)].$$
(18)

Taking into account relations (6) as well as  $\Delta P \approx (\partial P/\partial \rho)_E \Delta \rho + (\partial P/\partial E)_\rho \Delta E$  and  $\Delta(\rho u) \approx \rho \Delta u + u \Delta \rho$ , it is possible to obtain approximate expressions for the factors *f* and *g*:

$$f \approx \frac{1}{2c^2} \Delta P, \qquad g \approx -\frac{\rho}{2c} \Delta u.$$
 (19)

So, in (13), one can use

$$|\mathbf{A}|_{m+1/2}^{k} (\mathbf{U}_{m}^{k} - \mathbf{U}_{m+1}^{k}) = \begin{pmatrix} |u|_{m+1/2}^{k} (\rho_{m}^{k} - \rho_{m+1}^{k}) + \beta_{m+1/2}^{k} \\ |u|_{m+1/2}^{k} ([\rho u]_{m}^{k} - [\rho u]_{m+1}^{k}) + [\beta u - \delta c]_{m+1/2}^{k} \\ |u|_{m+1/2}^{k} ([\rho v]_{m}^{k} - [\rho v]_{m+1}^{k}) + [\beta v]_{m+1/2}^{k} \\ |u|_{m+1/2}^{k} ([\rho w]_{m}^{k} - [\rho w]_{m+1}^{k}) + [\beta w]_{m+1/2}^{k} \\ |u|_{m+1/2}^{k} (e_{m}^{k} - e_{m+1}^{k}) + [\beta h - \delta uc]_{m+1/2}^{k} \end{pmatrix},$$
(20)

$$\beta_{m+1/2}^{k} = [\alpha(f+g) + \gamma(f-g)]_{m+1/2}^{k}, \qquad \delta_{m+1/2}^{k} = [\alpha(f+g) - \gamma(f-g)]_{m+1/2}^{k}, \qquad (21)$$

$$f_{m+1/2}^{k} = \left[\frac{1}{2c^{2}}\right]_{m+1/2}^{k} \left(P_{m}^{k} - P_{m+1}^{k}\right), \qquad g_{m+1/2}^{k} = -\left[\frac{\rho}{2c}\right]_{m+1/2}^{k} \left(u_{m}^{k} - u_{m+1}^{k}\right). \tag{22}$$

At the initial moment of time, the entire target was divided in thickness into cells of the same size, which were numbered from j = 1 to  $N_j = 1000$ . This gives the step of the grid in space  $\Delta x = 0.09 \ \mu$ m. The step in time was chosen from the condition  $\Delta t \leq \xi \Delta x / \max(|u| + c)$ , where  $\xi = 0.1$ .

At each time step, the boundaries of the cells shifted with a certain velocity D, which is the particle velocity u for the case under consideration:

$$x_{m+1/2}^{k+1} = x_{m+1/2}^{k} + D_{m+1/2}^{k} \Delta t.$$
(23)

The construction of a difference scheme for such a moving grid is based upon the system of hydrodynamic equations in integral form:

$$\oint_{L} (\mathbf{U} dx - \mathbf{F} dt) = 0, \tag{24}$$

where *L* is the contour that bounds the region of integration on the coordinate plane (x,t). As this contour *L*, it is suitable to take a difference cell with number *j* with height  $\Delta t$  and bases  $\Delta x_j^{k+1}$  and  $\Delta x_j^k$ , where  $\Delta x_m = x_{m+1/2} - x_{m-1/2}$ . Approximating integral equation (24), one can

obtain

$$(\mathbf{U}\Delta x)_{j}^{k+1} - (\mathbf{U}\Delta x)_{j}^{k} + \mathbf{F}_{j+1}\Delta t - \mathbf{F}_{j-1}\Delta t = 0,$$
(25)

or, instead of (12),

$$\frac{(\mathbf{U}\Delta x)_{j}^{k+1} - (\mathbf{U}\Delta x)_{j}^{k}}{\Delta t} + \mathbf{F}_{j+1} - \mathbf{F}_{j-1} = 0.$$
(26)

A local transition to a coordinate system that moves with constant velocity D relative to the original system (Galilean transformation) changes the original form of the system of equations (1):

$$\frac{\partial}{\partial t}\mathbf{U} + \frac{\partial}{\partial x}(\mathbf{F} - D\mathbf{U}) = 0.$$
(27)

In this regard, the flows (13) at the boundaries of the cells change:

$$\mathbf{F}_{m+1/2} = (\mathbf{F} - D\mathbf{U})_{m+1/2}$$
  
=  $\frac{1}{2} (\mathbf{F}_{m}^{k} + \mathbf{F}_{m+1}^{k}) - \frac{1}{2} (\mathbf{U}_{m}^{k} + \mathbf{U}_{m+1}^{k}) D_{m+1/2}^{k} + \frac{1}{2} |\mathbf{A}_{D}|_{m+1/2}^{k} (\mathbf{U}_{m}^{k} - \mathbf{U}_{m+1}^{k}), \qquad (28)$   
 $|\mathbf{A}_{D}| = \Omega |\Lambda_{D}| \Omega^{-1}, \qquad (29)$ 

$$\mathbf{A}_D| = \Omega |\Lambda_D| \Omega^{-1}, \tag{29}$$

$$|\Lambda_D| = \begin{pmatrix} |u-D-c| & 0 & 0 & 0 & 0\\ 0 & |u-D| & 0 & 0 & 0\\ 0 & 0 & |u-D| & 0 & 0\\ 0 & 0 & 0 & |u-D| & 0\\ 0 & 0 & 0 & 0 & |u-D+c| \end{pmatrix}.$$
 (30)

#### **5** INITIAL CONDITIONS

The initial values of pressure, density and particle velocity were set constant over the target: P = 0.1 MPa,  $\rho = \rho_0 = 2.712$  g/cm<sup>3</sup> and u = v = w = 0. The initial value of specific internal energy was taken according to the used equation of state for aluminum.

## **6 BOUNDARY CONDITIONS**

On the irradiated surface of the target, a pressure profile

$$P(t) = P_{a} 16^{-(t-t_{0})^{2} \tau^{-2}} \text{ (for } 0 < t < t_{l}\text{)}, \qquad P(t) = 0 \text{ (for } t \leq 0 \text{ or } t_{l} \leq t\text{)}$$
(31)

was set, calculated using approximated dependence of the laser radiation intensity

$$I_{\rm l}(t) = I_0 16^{-(t-t_0)^2 \tau^{-2}}$$
(32)

and the scaling relation, which is formulated for the range  $4.3 < I_0 \leq 1000 \text{ TW/cm}^2$  [22, 23]:

$$P_{\rm a} = P_{\rm a0} (\lambda_{I0} I_0 / \lambda)^{2/3} [A_{\rm u} / (2Z)]^{3/16}, \tag{33}$$

where  $P_{a0} = 1.2$  TPa;  $\lambda_{I0} = 10^{-2} \ \mu \text{m cm}^2/\text{TW}$ ;  $A_u$  and Z are the atomic mass (u) and the atomic number of the target material respectively,  $A_u = 26.98154$  and Z = 13 for aluminum. On the rear side of the target, pressure was set equal to zero.

## 7 SIMULATION RESULTS

The simulation was performed for the case of loading pressure pulse (31) with the magnitude  $P_a = 516$  GPa according to equation (33);  $t_0 = 123$  ps,  $t_l = 246$  ps.

Figure 1 illustrates the change in pressure during the propagation of compression and rarefaction waves through the aluminum target. In figure 1(a), one can see that the rarefaction wave follows the shock wave while both move towards the rear side of the target. After the shock wave has reached the rear side, one more rarefaction wave begins to move backward [see figure 1(b)]. When these two rarefaction waves meet, a spalling phenomenon occurs.

Figure 2 shows the calculated pressure and density histories in three planes, which correspond to the initial distances from the rear side of the target 9, 10 and 11  $\mu$ m.

The curves shown in figure 2(a) allow one to estimate the maximum possible tensile stress  $\sigma_{\text{max}}$  in the sample in the spall plane. The absolute value of the pressure at the minimum on the curve for the plane where the spallation occurred in the experiment is this maximum possible tensile stress. The difference in values in two adjacent planes (for which the initial position differs from the initial position of the spall plane by the value of the error in determining the spall depth), divided in half, gives the average error in determining the maximum possible tensile stress in the sample.

The calculated curves shown in figure 2(*b*) allow one to estimate the maximum strain rate  $\rho_0 dV/dt = -\rho_0 \rho^{-2} d\rho/dt$  in the spall plane at the stage of tension at negative pressures. Here,  $V = \rho^{-1}$  is the specific volume. Starting from the point of zero pressure, when the sample is stretched, the strain rate decreases monotonically to zero at the point of minimum pressure. Then, with time, the tensile stress decreases, and the strain rate becomes negative (i.e., the density increases with pressure).

In the case under consideration,  $\sigma_{\text{max}} \pm \Delta \sigma_{\text{max}} \approx 7.2 \pm 0.5$  GPa,  $\rho_0 dV/dt \pm \Delta (\rho_0 dV/dt) \approx 0.22 \pm 0.01$  ns<sup>-1</sup> for aluminum.



Figure 1: Pressure in the target at t = 3.6, 7.4, 11 (*a*), 12.7, 15.2 and 18 ns (*b*) along the coordinate axis *x*, which is perpendicular to the irradiated surface, with the origin at the point of the initial position of this surface before the experiment.



Figure 2: Pressure (a) and density (b) histories in three planes that correspond to the initial distances from the back of the target 9, 10 and 11  $\mu$ m. The thin vertical lines correspond to the moments of reaching the maximum tensile stress (negative pressure).

## 8 CONCLUSIONS

Thus, in a laboratory experiment on irradiating a 90- $\mu$ m-thick aluminum plate with a 70 ps laser pulse with a maximum intensity of 14.7 TW/cm<sup>2</sup>, a spall was obtained at a distance of 10 ± 1  $\mu$ m from the rear surface of the target. A hydrodynamic model has been developed for the propagation and interaction of shock and release waves in a target under such a pulsed action. As a result of the calculation using the developed model, the maximum possible tensile stress in the sample in the spall plane is determined as 7.2±0.5 GPa and the maximum strain rate at the stage of tension at negative pressures is determined as 0.22±0.01 ns<sup>-1</sup>.

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#### REFERENCES

- [1] S. I. Anisimov, A. M. Prokhorov, and V. E. Fortov, "The use of powerful lasers for the study of matter under superhigh pressures", *Usp. Fiz. Nauk*, **142**(3), 395–434 (1984).
- [2] V. E. Fortov, D. Batani, A. V. Kilpio, I. K. Krasyuk, I. V. Lomonosov, P. P. Pashinin, E. V. Shashkov, A. Yu. Semenov, and V. I. Vovchenko, "The spall strength limit of matter at ultrahigh strain rates induced by laser shock waves", *Laser Part. Beams*, **20**(2), 317–320 (2002).
- [4] M. A. Barrios, D. G. Hicks, T. R. Boehly, D. E. Fratanduono, J. H. Eggert, P. M. Celliers, G. Collins, and D. D. Meyerhofer, "High-precision measurements of the equation of state of hydrocarbons at 1–10 Mbar using laser-driven shock waves", *Phys. Plasmas*, **17**(5), 056307 (2010).
- [5] S. I. Ashitkov, M. B. Agranat, G. I. Kanel', P. S. Komarov, and V. E. Fortov, "Behavior of aluminum near an ultimate theoretical strength in experiments with femtosecond laser pulses", *JETP Lett.*, **92**(8), 516–520 (2010).
- [6] R. E. Rudd, T. C. Germann, B. A. Remington, and J. S. Wark, "Metal deformation and phase transitions at extremely high strain rates", *MRS Bull.*, **35**(12), 999–1006 (2010).
- [7] S. I. Ashitkov, P. S. Komarov, A. V. Ovchinnikov, E. V. Struleva, and M. B. Agranat, "Deformation dynamics and spallation strength of aluminium under a single-pulse action of a femtosecond laser", *Quantum Electron.*, 43(3), 242–245 (2013).
- [8] I. K. Krasyuk, P. P. Pashinin, A. Yu. Semenov, K. V. Khishchenko, and V. E. Fortov, "Study of extreme states of matter at high energy densities and high strain rates with powerful lasers", *Laser Phys.*, 26(9), 094001 (2016).
- [9] C. A. McCoy, S. X. Hu, M. C. Marshall, D. N. Polsin, D. E. Fratanduono, Y. H. Ding, P. M. Celliers, T. R. Boehly, and D. D. Meyerhofer, "Measurement of the sound velocity and Grüneisen parameter of polystyrene at inertial confinement fusion conditions", *Phys. Rev. B*, **102**(18), 184102 (2020).
- [10] S. A. Abrosimov, A. Bazhulin, V. Voronov, I. Krasyuk, P. Pashinin, A. Semenov, I. Stuchebryukhov, and K. V. Khishchenko, "Study of mechanical properties of aluminum, AMg6M alloy, and poly-

methyl methacrylate at high strain rates under the action of picosecond laser radiation", *Dokl. Phys.*, **57**(2), 64–66 (2012).

- [11] S. A. Abrosimov, A. P. Bazhulin, V. V. Voronov, A. Geras'kin, I. Krasyuk, P. Pashinin, A. Semenov, I. A. Stuchebryukhov, K. V. Khishchenko, and V. E. Fortov, "Specific features of the behaviour of targets under negative pressures created by a picosecond laser pulse", *Quantum Electron.*, 43(3), 246–251 (2013).
- [12] A. A. Samokhin, V. I. Mazhukin, M. M. Demin, A. V. Shapranov, and A. E. Zubko, "On critical parameters manifestations during nanosecond laser ablation of metals", *Math. Montis.*, 43, 38–48 (2018).
- [13] S. Yu. Gus'kov, I. K. Krasyuk, A. Yu. Semenov, I. A. Stuchebryukhov, and K. V. Khishchenko, "Extraction of the shock adiabat of metals from the decay characteristics of a shock wave in a laser experiment", *JETP Lett.*, **109**(8), 516–520 (2019).
- [14] K. K. Maevskii, "Thermodynamic parameters of mixtures with silicon nitride under shock-wave loading", *Math. Montis.*, **45**, 52–59 (2019).
- [15] A. A. Samokhin, P. A. Pivovarov, and A. L. Galkin, "Modeling of transducer calibration for pressure measurement in nanosecond laser ablation", *Math. Montis.*, **48**, 58–69 (2020).
- [16] V. I. Mazhukin, M. M. Demin, A. V. Shapranov, and A. V. Mazhukin, "Role of electron pressure in the problem of femtosecond laser action on metals", *Appl. Surf. Sci.*, **530**, 147227 (2020).
- [17] A. G. Kulikovskii, N. V. Pogorelov, and A. Yu. Semenov, *Mathematical Aspects of Numerical Solution of Hyperbolic Systems*, Monographs and Surveys in Pure and Applied Mathematics, Vol. 118, Boca Raton, FL: Chapman & Hall/CRC, (2001).
- [18] K. V. Khishchenko, "The equation of state for magnesium at high pressures", *Tech. Phys. Lett.*, 30(10), 829–831 (2004).
- [19] K. V. Khishchenko, "Equation of state for tungsten over a wide range of densities and internal energies", J. Phys.: Conf. Ser., 653, 012081 (2015).
- [20] K. V. Khishchenko, "Equation of state for titanium at high energy densities", J. Phys.: Conf. Ser., 774, 012001 (2016).
- [21] R. Courant, E. Isaacson, and M. Rees, "On the solution of nonlinear hyperbolic differential equations by finite differences", *Commun. Pure Appl. Math.*, **5**(3), 243–255 (1952).
- [22] V. I. Vovchenko, I. K. Krasyuk, P. P. Pashinin, and A. Yu. Semenov, "Wide-range ablation pressure scaling law for laser experiments", *Dokl. Akad. Nauk*, 338(3), 322–324 (1994).
- [23] I. K. Krasyuk, A. Yu. Semenov, I. A. Stuchebryukhov, and K. V. Khishchenko, "Experimental verification of the ablation pressure dependence upon the laser intensity at pulsed irradiation of metals", *J. Phys.: Conf. Ser.*, **774**, 012110 (2016).

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# ALE-MHD TECHNIQUE FOR MODELING THREE-DIMENSIONAL MAGNETIC IMPLOSION OF A LINER

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**Summary.** The article is devoted to the methodology for modeling current-carrying plasma in a Z-pinch studied in pulsed-power experiments. We discuss simulation performed via moving Lagrangian-Euler difference grid. The difference scheme approximating the hydrodynamic equations of a high-temperature medium possesses a "complete conservation" property and includes energy balances between the plasma components taking into account electromagnetic field – matter interaction and conductive (electronic, ionic) as well as radiative heat transfer. Numerical experiments provide quantitative estimates of physical effects which lead to essential distortions of a plasma shell during its magnetically-driven implosion. Performed simulations show the effect of instabilities on the final pinch structure, mainly, the hydrodynamic Rayleigh-Taylor instability and instability of a temperature-inhomogeneous plasma.

## **1 INTRODUCTION**

Difference schemes of summarised approximation [1], schemes of physical splitting [2] and their modifications are widely used since they allow reproducing accurately specific feature of studied physical processes and perform calculations economically. This is why such schemes are widely used in application codes designed for multiphysics simulations (see e.g., [3, 4]). In the monograph [5], algorithms for successive accounting physical processes are constructed for Lagrangian difference schemes of gasdynamics (GD) and magnetic gasdynamics (MHD). The advantage of the completely conservative difference schemes presented in [5] is the numerical approximation of the basic conservation laws (mass, momentum and energy) as well as additional balance equations, important for simulation of fast plasma-dynamic processes. These include the intensive energy transfer from external sources, the significant role of heat transfer by radiation, electron-ion energy relaxation, etc.

In this paper, we present a numerical technique based on the summarised approximation scheme developed for simulation of magnetoaccelerated plasma, primarily for various types of Z-pinches [6, 7].

Electrodynamic compression caused by the action of a current pulse on a plasma body in the form of a liner or a shell was first proposed for achieving thermonuclear fusion conditions [8]. Currently, such experimental schemes are mainly studied in order to generate soft x-ray radiation pulses via kinetic-to-thermal energy conversion at the stage of an accelerated shell collapse [6, 9, 10]. The development of high-current generators with the pulse duration about 100 nanoseconds and the peak current up to several MA, used in modern Z-pinch experiments, allows new prospects in this research area. High power soft x-ray sources up to several TW can be used not only in basic research, but also in industrial applications:

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materials with gradient properties, x-ray photolithography, short-wave lasers etc. The problem of current-carrying plasma stabilization is actively studied. In the ongoing research, much attention is paid to the design (material and geometry) of imploding liners. Fitting of the liner parameters with the electrical parameters of the generator is important to ensure high efficiency transformation of the electricity into the kinetic energy of the liner [10-12].

The article consists of two parts.

The first part is devoted to the construction of Lagrangian-Eulerian numerical method and algorithms for solving the MHD in the form of conservation laws.

Implicit completely conservative difference scheme (CCDS) [1, 2] in Lagrangian variables is considered as a base. The Lagrangian-Eulerian approach provides opportunities for combining explicit and implicit approximations of convective flows.

The algorithm developed in this paper employs local splitting of physical processes. For two-dimensional MHD problems, similar algorithms were considered in [14]. The system of difference equations is divided into groups, and each group is solved by its own iterative process. Local iterative processes are assembled into an overall cycle, with the convergence controlled by the overall energy balance.

It is possible to remap computed Lagrangian values to a modified grid with mass, momentum, and total energy conservation. We also check the balances of internal and magnetic energy.

We use two-level temporal approximations of convective terms to ensure the CCDS for the numerical MHD system. Homogeneity of calculations for flows with strong discontinuities is achieved by introducing artificial viscosity [5], taking into account recommendations [15] for its adaptation to flow properties.

The second part of the paper gives an example of modeling the dynamics of a Z-pinch compression. The liner is formed during ablation and subsequent implosion of a wire array under the impact of a powerful current pulse. In computational experiments, we study typical instabilities that have the most significant effect on the magnetic implosion. Namely, we observe the hydromagnetic Rayleigh – Taylor instability along with instabilities of temperature-inhomogeneous plasma. The last may lead to matter overheating or radiative collapse depending on disbalance between Joule heating and radiation losses. The Conclusion summarizes the main results of the numerical experiments.

## 2 GOVERNING MHD SYSTEM

We use the common notation for the MHD equations in Cartesian coordinates: *t* is the time,  $\mathbf{U} = (u, w, v)$  is the substance velocity,  $\rho$  is the density, *P* is the gas pressure, *T* is the temperature,  $\varepsilon$  is the specific internal energy,  $\mathbf{W} = (W_x, W_y, W_z)$  is the heat flux,  $\mathbf{B} = (B_x, B_y, B_z)$  is the magnetic induction,  $\mathbf{E} = (E_x, E_y, E_z)$  is the electric field strength,  $\mathbf{j} = (j_x, j_y, j_z)$  is the electric current density, *c* is speed of light in vacuum,  $\sigma$  and  $\kappa$  are the coefficients of electrical and thermal conductivity.

The kinematic equations for fluid particle positions:

$$\frac{dx}{dt} = u; \frac{dy}{dt} = w; \frac{dz}{dt} = v;$$
(1)

The continuity equation:

$$\frac{d\rho}{dt} + \rho \,\frac{\partial u}{\partial x} + \rho \,\frac{\partial w}{\partial y} + \rho \,\frac{\partial v}{\partial z} = 0 \tag{2}$$

The momentum equation projections on the coordinate directions:

$$\rho \frac{du}{dt} = -\frac{\partial}{\partial x} \left( P + \frac{B^2}{8\pi} \right) + \frac{1}{4\pi} \left( \frac{\partial \left( B_x^2 \right)}{\partial x} + \frac{\partial \left( B_x B_y \right)}{\partial y} + \frac{\partial \left( B_x B_z \right)}{\partial z} \right),$$

$$\rho \frac{dw}{dt} = -\frac{\partial}{\partial y} \left( P + \frac{B^2}{8\pi} \right) + \frac{1}{4\pi} \left( \frac{\partial \left( B_x B_y \right)}{\partial x} + \frac{\partial \left( B_y^2 \right)}{\partial y} + \frac{\partial \left( B_y B_z \right)}{\partial z} \right),$$

$$\rho \frac{dv}{dt} = -\frac{\partial}{\partial z} \left( P + \frac{B^2}{8\pi} \right) + \frac{1}{4\pi} \left( \frac{\partial \left( B_x B_z \right)}{\partial x} + \frac{\partial \left( B_y B_z \right)}{\partial y} + \frac{\partial \left( B_z^2 \right)}{\partial z} \right),$$
(3)

The hydrodynamic pressure in (3) is equal to the sum of the partial pressures  $P = P_e + P_i$ . The equations for the internal energies of the components:

$$p\frac{d\varepsilon_{e}}{dt} = -\rho P_{e} \frac{\partial (1/\rho)}{\partial t} - \frac{\partial (W_{e})_{x}}{\partial x} - \frac{\partial (W_{e})_{y}}{\partial y} - \frac{\partial (W_{e})_{z}}{\partial z} + Q_{ei} + G_{j} + G_{e}$$

$$p\frac{d\varepsilon_{i}}{dt} = -\rho P_{i} \frac{\partial (1/\rho)}{\partial t} - \frac{\partial (W_{i})_{x}}{\partial x} - \frac{\partial (W_{i})_{y}}{\partial y} - \frac{\partial (W_{i})_{z}}{\partial z} - Q_{ei} + G_{i}$$
(4)

Here  $G_{e,i}$  are sources (sinks) of electronic and ionic energy,  $G_j$  is the mass energy density of the Joule heating:

$$G_{j} = \frac{1}{4\pi} \left( E_{x} j_{x} + E_{y} j_{y} + E_{z} j_{z} \right)$$

$$j_{x} = \frac{\partial B_{z}}{\partial y} - \frac{\partial B_{y}}{\partial z} - \frac{1}{c^{2}} \frac{\partial}{\partial t} \left( E_{x} + vB_{y} - wB_{z} \right)$$

$$j_{y} = \frac{\partial B_{x}}{\partial z} - \frac{\partial B_{z}}{\partial x} - \frac{1}{c^{2}} \frac{\partial}{\partial t} \left( E_{y} + vB_{x} - uB_{z} \right)$$

$$j_{z} = \frac{\partial B_{y}}{\partial x} - \frac{\partial B_{x}}{\partial y} - \frac{1}{c^{2}} \frac{\partial}{\partial t} \left( E_{z} + uB_{y} - wB_{x} \right)$$

$$(5)$$

 $\varepsilon_{e,i}$  are the internal energies of the electronic and ionic components per unit mass,  $W_{e,i} = ((W_{e,i})_x, (W_{e,i})_y, (W_{e,i})_z)$  are the electron and ion heat fluxes, c is speed of light in vacuum.

Heat fluxes are defined by ion and electron temperature gradients:

$$\begin{pmatrix} W_{e,i} \end{pmatrix}_{x} = -(\kappa_{e,i})_{xx} \frac{\partial T_{e,i}}{\partial x} - (\kappa_{e,i})_{xy} \frac{\partial T_{e,i}}{\partial y} - (\kappa_{e,i})_{xz} \frac{\partial T_{e,i}}{\partial z}$$

$$\begin{pmatrix} W_{e,i} \end{pmatrix}_{y} = -(\kappa_{e,i})_{yx} \frac{\partial T_{e,i}}{\partial x} - (\kappa_{e,i})_{yy} \frac{\partial T_{e,i}}{\partial y} - (\kappa_{e,i})_{yz} \frac{\partial T_{e,i}}{\partial z}$$

$$\begin{pmatrix} W_{e,i} \end{pmatrix}_{z} = -(\kappa_{e,i})_{zx} \frac{\partial T_{e,i}}{\partial x} - (\kappa_{e,i})_{zy} \frac{\partial T_{e,i}}{\partial y} - (\kappa_{e,i})_{zz} \frac{\partial T_{e,i}}{\partial z}$$

$$(7)$$

where

$$\left(\kappa_{e,i}\right)_{\xi\xi} = \left(\kappa_{e,i}\right)_{\parallel} \left(\frac{B_{\xi}}{B}\right)^2 + \left(\kappa_{e,i}\right)_{\perp} \left(1 - \left(\frac{B_{\xi}}{B}\right)\right)^2, \quad \xi = x, y, z$$

$$\left(\kappa_{e,i}\right)_{\xi\zeta} = \left(\kappa_{e,i}\right)_{\zeta\xi} = \left[\left(\kappa_{e,i}\right)_{\parallel} - \left(\kappa_{e,i}\right)_{\perp}\right] \frac{B_{\xi}B_{\zeta}}{B^2}, \quad \xi = x, y, z; \ \zeta = x, y, z; \ \xi \neq \zeta$$

The equations of the electromagnetic field are applied in the following form:

$$\rho \frac{d}{dt} \left( \frac{B_x}{\rho} \right) = \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} + \left( B_x \frac{\partial u}{\partial x} + B_y \frac{\partial u}{\partial y} + B_z \frac{\partial u}{\partial z} \right),$$

$$\rho \frac{d}{dt} \left( \frac{B_y}{\rho} \right) = \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} + \left( B_x \frac{\partial w}{\partial x} + B_y \frac{\partial w}{\partial y} + B_z \frac{\partial w}{\partial z} \right),$$

$$\rho \frac{d}{dt} \left( \frac{B_z}{\rho} \right) = \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} + \left( B_x \frac{\partial v}{\partial x} + B_y \frac{\partial v}{\partial y} + B_z \frac{\partial v}{\partial z} \right),$$

$$E_{\xi} = \frac{1}{4\pi\sigma_{\perp}} j_{\xi} + \frac{\sigma_{\perp} - \sigma_{\parallel}}{4\pi\sigma_{\perp}\sigma_{\parallel}} \frac{B_{\xi}}{B^2} (j, B); \quad \xi = x, y, z; \quad (j, B) = j_x B_x + j_y B_y + j_z B_z.$$
(9)

The MHD system (1) - (9) is closed by the plasma equation of state (EOS).

To solve the MHD initial-boundary-value problem, the usual boundary conditions [13] are added to equations (1) - (9), which determine the hydrodynamic fluxes of mass, energy, and momentum, temperature or heat fluxes, and the conditions for the components of the electromagnetic field.

## **3 COMPUTATIONAL ALGORITHM**

The difference model is built using staggered grid functions. Thermodynamic parameters (density, pressure, internal energy) as well as magnetic induction are defined in the grid cells. The components of the velocity and electric field strength are defined in the nodes. The difference equations of continuity, energy, momentum, and magnetic induction are derived by approximating the corresponding differential balance for control volume. The control volumes are either grid cells (for continuity and energy equations), or "nodal" volumes (for momentum balance equations), which form a grid conjugate to the original one. Time-dependent pressure forces, ponderomotive forces, flows, etc. are included as a linear combination of the corresponding spatial approximations at two consecutive time layers. Weighting factors in time-weighted difference formulas were chosen to ensure complete

conservativeness of the scheme. For the dissipative processes (thermal conductivity, field diffusion), homogeneous flux schemes were constructed. The theoretical foundations of such schemes are considered in [14] for the 2D case. Here we present a 3D version of the technique [14].

The numerical solution of the governing MHD system is performed according to the twostage algorithm which is analogues to that first proposed in [16] and used in many successive works. The movement of matter is calculated in the coordinate system ( $\alpha$ ,  $\beta$ ,  $\gamma$ ), which is moving relative to the laboratory system (x, y, z).

If  $\mathbf{U} = (u, w, v)$  is the velocity of a material particle in the laboratory coordinate system, then  $\tilde{\mathbf{U}} = (\tilde{U}_x, \tilde{U}_y, \tilde{U}_z) = (u - dx/dt, w - dy/dt, v - dz/dt)|_{(\alpha, \beta, \gamma|) = \text{const}}$  is its velocity in the moving system.

The time-advance begins by solving the main system of equations in Lagrange variables (i.e., without taking into account convective flows), then, if necessary, the Lagrangian grid is corrected, and the computed values are recalculated to a new difference grid.

The first (Lagrangian) stage includes solving the grid equations, provided that the grid moves at the speed of the substance. In this case, the Jacobian **J** changes according to the equation  ${}^{(\mathbf{J})}_t = \mathbf{J}\nabla \mathbf{U}$ , and the original system of equations is supplemented by the kinematic

relation  $\frac{d\mathbf{r}(\alpha,\beta,\gamma,t)}{dt} = \mathbf{U}(\mathbf{r})$  (**r** is the radius vector of the material particle). At the end of the

Lagrangian stage of calculating the position of the grid nodes, they can be redefined based on the solution strategy. In this case, the second (Eulerian) stage is performed that is the calculation of convective fluxes in the "grid" coordinate system and the consequent changes in the grid functions.

The above decomposition of the solution of the general system of equations into stages can be represented in the form of a summarized approximation scheme, or a physical splitting scheme. The advantage of the proposed algorithm is the possibility to use an implicit Lagrangian scheme and an explicit Eulerian scheme. This combination allows a larger time integration step without loss of stability.

The overall iterative cycle is based on the sequential computation of physical processes. It includes several nested cycles for the subsystems of the general system. The Lagrangian stage can be considered as iterations of the force and energy balances. At this stage the MHD system is solved coupled with the equations for the nodes coordinates moving in physical space with the speed of the matter. In turn, the Lagrangian stage itself is split into the ideal MHD (hyperbolic type subsystem) and the dissipative processes (parabolic type equations).

Lagrangian grids simulate the motion of liquid particles or liquid contours. This approach allows very simple and convenient form of the continuity equations, freezing of the field in the MHD equations, and lastly, an effective rapidly converging iterative algorithm for solving a system of grid equations corresponding to an implicit difference scheme. The convergence of the algorithm was studied in [14].

The Eulerian stage returns the nodes of the moving grid to their start-of-the-time-step positions. This is understood as the up-flow shift of the Lagrangian grid, due to which the substance moves through the edges of the cells. At this stage, changes in the grid functions ( $\rho$ , **U**,  $\varepsilon$ , **B**) caused by convection processes are calculated. Note that the return of the grid to its

previous position is optional, which allows lower numerical diffusion and improving the deformations of the moving grid.

The power and energy balances are interconnected. The plasma momentum  $\rho U(x, y, z, t)$  is determined by the pressure gradient and electromagnetic force dependent, in particular, on the temperature of the medium. In turn, the temperature field T(x, y, z, t) depends on the work of the pressure forces and the energy flows, i.e. the plasma velocity. Therefore, the individual steps of solving the complete system of MHD grid equations are combined into an overall iterative cycle.

The system we solve includes difference equations of ideal MHD coupled with energy balance equations of the plasma components in a non-divergent (entropy) form and multigroup radiative transfer equations. The difference scheme of the Lagrangian stage is arranged in such a way that a difference analogue of the plasma – electromagnetic field integral energy balance is satisfied. This property is used to monitor the convergence of iterations at the Lagrangian stage and the quality of the solution in general.

The time derivatives of any function f in the moving coordinate system are calculated

according to the relation  $\dot{f} = f_t + \mathbf{U}\nabla f$ .

## **4** COMPUTATIONAL GRID, DISCRETIZATION, DIFFERENCE EQUATIONS

The approximation on a moving grid is implemented via mapping a single-connected region with a piecewise-smooth boundary  $D \subset R^3(x,y,z)$  to the unit cube  $D' \subset R^3(\alpha,\beta,\gamma)$  [4, 9, 10]. In general the coordinate transformation formulas are time dependent. At any point of time the map is defined as:

$$x = x(\alpha, \beta, \gamma), \quad y = y(\alpha, \beta, \gamma), \quad z = z(\alpha, \beta, \gamma)$$

$$(x, y, z) \in D, \quad (\alpha, \beta, \gamma) \in D'$$

$$(10)$$

We suppose the positivity of the coordinate mapping Jacobian:

$$\mathbf{J} = \frac{\partial(x, y, z)}{\partial(\alpha, \beta, \gamma)} > 0, (\alpha, \beta, \gamma) \in D'$$

The volume of a cell in the physical space (x, y, z) is approximated as the volume of its image in the reference space of the variables  $(\alpha, \beta, \gamma)$  multiplied by the average value of the Jacobian  $\langle \mathbf{J} \rangle$  in the cell.

#### 4.1 System of difference equations

The MHD system (1) - (9) is approximated on a moving (Lagrangian) difference grid by a completely conservative difference scheme.

The corresponding numerical model is as follows.

A uniform in each direction grid is introduced in the cube  $D'(\alpha, \beta, \gamma)$ :

$$\alpha_{i} = ih_{\alpha}, \ i = 0, NM, \ h_{\alpha} = 1/NM,$$
  
$$\omega_{h}: \quad \beta_{j} = jh_{\beta}, \ j = \overline{0, NL}, \ h_{\beta} = 1/NL,$$
  
$$\gamma_{k} = kh_{\gamma}, \ k = \overline{0, NN}, \ h_{\gamma} = 1/NN.$$

We denote by  $\omega$  the set of cells of the computational grid  $\omega_h$ ,  $\Omega$  is the set of nodes,  $\theta$  is the set of faces. Accordingly, we introduce the spaces of grid functions defined in the cells  $H_{\omega}$ , in the nodes  $H_{\Omega}$ , and in the faces  $H_{\theta}$ . We use the indices (i, j, k) for the grid functions  $f \in H_{\Omega}$ :  $f_{i,j,k} = f \in H_{\Omega}$ , and indices (m, l, n) for the grid functions  $\varphi \in H_{\omega}$ :  $\varphi_{min} \in H_{\omega}$ . The functions  $\psi \in H_{\theta}$  will be marked with indices (i, l, n), (m, j, n) and (m, l, k).

The grid in the region D obtained by the mapping (10) consists of hexagons.

- The difference equations below use grid templates  $\Xi_1$ ,  $\Xi_2$ ,  $\Xi_3$ :
- $\Xi_1$  is the cell template, it includes the incident nodes;
- $\Xi_2$  is the node template, it includes the incident cells;
- $\Xi_3$  is the pattern of faces incident to the cell (*m*, *l*, *n*).

Equations (1) - (9) are approximated on the grid  $H_{\omega}$  by a completely conservative implicit difference scheme. The difference balance equations for the mass, momentum, and energy in a control volume are constructed using the partial derivatives of the cell volumes with respect to the node coordinates (for theoretical grounds see [17, 26]):

$$x_t = u^{(0.5)}; \ y_t = w^{(0.5)}; \ z_t = v^{(0.5)}$$
(11)

$$\Delta m = \rho \left\langle \mathbf{J} \right\rangle h_{\alpha} h_{\beta} h_{\gamma} = \rho V = \hat{\rho} \hat{V}, \qquad (12)$$

$$P = P_e + P_i + q \tag{13}$$

$$M u_{t} = \sum_{r \in \Xi_{2}} \left( \frac{\partial \hat{V}_{r}}{\partial x} \right) \left( \hat{P}_{r} + \frac{B_{r} \hat{B}_{r}}{8\pi} \right) - \frac{1}{4\pi} \sum_{r \in \Xi_{2}} B_{x_{r}}^{(0.5)} \partial B_{x}$$

$$M w_{t} = \sum_{r \in \Xi_{2}} \left( \frac{\partial \hat{V}_{r}}{\partial y} \right) \left( \hat{P}_{r} + \frac{B_{r} \hat{B}_{r}}{8\pi} \right) - \frac{1}{4\pi} \sum_{r \in \Xi_{2}} B_{y_{r}}^{(0.5)} \partial B_{y}$$

$$M v_{t} = \sum_{r \in \Xi_{2}} \left( \frac{\partial \hat{V}_{r}}{\partial z} \right) \left( \hat{P}_{r} + \frac{B_{r} \hat{B}_{r}}{8\pi} \right) - \frac{1}{4\pi} \sum_{r \in \Xi_{2}} B_{z_{r}}^{(0.5)} \partial B_{z}$$

$$\partial B_{\xi} = \sum_{r \in \Xi_{1}} \frac{\partial \hat{V}_{r}}{\partial \xi} \hat{B}_{\xi_{r}}, \quad \xi = x, y, z, \quad M = \frac{1}{8} \sum_{r \in \Xi_{2}} \Delta m_{r}$$

$$(V B_{x})_{t} = \sum_{\xi = x, y, z} \hat{B}_{\xi} \sum_{r \in \Xi_{1}} \frac{\partial \hat{V}}{\partial \alpha_{r}} u_{r}^{(0.5)} + \sum_{r \in \Xi_{1}} \left[ \left( \frac{\partial \hat{V}}{\partial z_{r}} \right) \hat{E}_{z_{r}} - \left( \frac{\partial \hat{V}}{\partial y_{r}} \right) \hat{E}_{z_{r}} \right]$$

$$(V B_{z})_{t} = \sum_{\xi = x, y, z} \hat{B}_{\xi} \sum_{r \in \Xi_{1}} \frac{\partial \hat{V}}{\partial \alpha_{r}} w_{r}^{(0.5)} + \sum_{r \in \Xi_{1}} \left[ \left( \frac{\partial \hat{V}}{\partial x_{r}} \right) \hat{E}_{z_{r}} - \left( \frac{\partial \hat{V}}{\partial z_{r}} \right) \hat{E}_{x_{r}} \right]$$

$$(15)$$

$$\hat{E}_{\xi} = \frac{1}{4\pi\hat{\sigma}_{\perp}} \hat{j}_{\xi} + \frac{\hat{\sigma}_{\perp} - \hat{\sigma}_{\parallel}}{4\pi\hat{\sigma}_{\perp}\hat{\sigma}_{\parallel}} \frac{\hat{B}_{\xi}}{\hat{B}^{2}} B^{***}, \quad \xi = x, y, z$$

$$B^{***} = \hat{B}_{x} \tilde{j}_{x} + \hat{B}_{y} \tilde{j}_{y} + \hat{B}_{z} \tilde{j}_{z}$$

$$\tilde{j}_{x} = -\frac{1}{\hat{V}} \sum_{r \in \Xi_{2}} \left[ \frac{\partial V_{r}}{\partial y} \hat{B}_{z_{r}} - \frac{\partial V_{r}}{\partial z} \hat{B}_{y_{r}} \right] - \frac{1}{c^{2}} (E_{x} + vB_{y} - wB_{z})_{t}$$

$$\tilde{j}_{y} = -\frac{1}{\hat{V}} \sum_{r \in \Xi_{2}} \left[ \frac{\partial V_{r}}{\partial z} \hat{B}_{x_{r}} - \frac{\partial V_{r}}{\partial x} \hat{B}_{z_{r}} \right] - \frac{1}{c^{2}} (E_{y} + wB_{z} - uB_{x})_{t}$$

$$\tilde{j}_{z} = -\frac{1}{\hat{V}} \sum_{r \in \Xi_{2}} \left[ \frac{\partial V_{r}}{\partial x} \hat{B}_{y_{r}} - \frac{\partial V_{r}}{\partial y} \hat{B}_{r} \right] - \frac{1}{c^{2}} (E_{z} + uB_{x} - vB_{y})_{t}$$

$$(\varepsilon_{e})_{t} = -\overline{P}_{e} \left( \frac{1}{\rho} \right)_{t} + \hat{Q}_{ei} + \hat{G}_{e} + \frac{1}{\Delta m} \sum_{r \in \Xi_{3}} \sum_{\xi = x, y, z} \widehat{W}_{e,\xi r} \hat{S}_{\xi r} + \hat{G}_{j}$$

$$(\varepsilon_{i})_{t} = -\left(\hat{P}_{i} + \hat{q}\right) \left( \frac{1}{\rho} \right)_{t} - \hat{Q}_{ei} + \frac{1}{\Delta m} \sum_{r \in \Xi_{3}} \sum_{\xi = x, y, z} \widehat{W}_{i,\xi r} \hat{S}_{\xi r} + \hat{G}_{i}$$

$$(17)$$

Joule heating:

$$\widehat{G}_{j} = \frac{1}{128\pi} \left[ \frac{1}{\sigma_{\perp}} \sum_{r \in \Xi_{1}} \left( \widetilde{j}_{x_{r}}^{2} + \widetilde{j}_{y_{r}}^{2} + \widetilde{j}_{z_{r}}^{2} \right) + \left( \frac{\widehat{\sigma}_{\perp} - \widehat{\sigma}_{\parallel}}{\widehat{\sigma}_{\perp} \widehat{\sigma}_{\parallel}} \right) \sum_{r \in \Xi_{1}} \frac{\widehat{B}_{x_{r}} \widetilde{j}_{x_{r}} + \widehat{B}_{y_{r}} \widetilde{j}_{y_{r}} + \widehat{B}_{z_{r}} \widetilde{j}_{z_{r}}}{\widehat{B}_{r}^{2}} \right]$$
(18)

We use index-free notation to represent the system (11)-(18) in a compact form [1].

The grid functions **U**, **E** are defined in the nodes of the difference grid, the grid functions  $\rho$ ,  $P_{e,i}$ , q, V,  $T_{e,i}$ , **B**,  $G_{e,i}$ ,  $Q_{ei}$ ,  $\kappa_{e,i}$ ,  $\sigma$  are defined in the cells (q is the volumetric artificial viscosity; V is the volume of the cell), and the grid functions  $\mathbf{W}_{e,i}$ , **S** are defined on the faces of the cells.  $\mathbf{S}_r = (S_{xr}, S_{yr}S_{zr}), r = \overline{1,6}$  are the areas of the faces of the cell (m, l, n).

The boundary values of pressure, temperature, and magnetic field are assigned to the faces of the boundary cells.

At the boundary of the computational region, for the equations of motion, the pressure and velocity, or the absence of a plasma flow condition is specified. For Maxwell's equations, the magnetic induction or the electric field strength is specified. For energy equations, the distribution of temperature or heat fluxes is specified at the boundaries.

## 4.2 Energy balance and conservation

The difference scheme (10) - (17) is completely conservative. We define the following grid functionals to prove this property and to utilize it in practical calculations:

$$\varepsilon_{kin} = \frac{1}{2} \sum_{m=1}^{NM} \sum_{l=1}^{NL} \sum_{n=1}^{NN} \Delta m_{mln} \left( u_{mln}^2 + w_{mln}^2 + v_{mln}^2 \right)$$

$$u_{mln} = \frac{1}{8} \sum_{r \in \Xi_1} u_r, \quad w_{mln} = \frac{1}{8} \sum_{r \in \Xi_1} w_r, \quad v_{mln} = \frac{1}{8} \sum_{r \in \Xi_1} v_r$$
(19)

$$E_{tot} = \sum_{mln} \Delta m_{mln} \left( \varepsilon_{e_{mln}} + \varepsilon_{i_{mln}} + \frac{u_{mln}^2 + w_{mln}^2 + v_{mln}^2}{2} + \frac{B_{x_{mln}}^2 + B_{y_{mln}}^2 + B_{z_{mln}}^2}{8\pi \rho_{mln}} \right)$$

$$u_{mln}^2 = \frac{1}{8} \sum_{r \in \Xi_1} u_r^2, \quad w_{mln}^2 = \frac{1}{8} \sum_{r \in \Xi_1} w_r^2, \quad v_{mln}^2 = \frac{1}{8} \sum_{r \in \Xi_1} v_r^2.$$
(20)

The following indices are used for energy balance relations:

(i,j,k) for boundary nodes, r' for cells adjacent to the boundary, r'' for "ghost" cells introduced into difference scheme for processing of boundary conditions:

$$\sum_{r \in \Xi_{2}} = \sum_{r' \in \Xi_{2}} + \sum_{r'' \in \Xi_{2}}$$

$$\mu'_{ijk} = \frac{1}{8M_{ijk}} \sum_{r' \in \Xi_{2}} \Delta m_{r'}, \quad \mu''_{ijk} = \frac{1}{8M_{ijk}} \sum_{r'' \in \Xi_{2}} \Delta m_{r''} = 1 - \mu'_{ijk}$$

$$\eta'_{ijk} = \frac{1}{8\hat{V}_{ijk}} \sum_{r' \in \Xi_{2}} \hat{V}_{r'}, \quad \eta''_{ijk} = 1 - \eta'_{ijk}$$
(21)

The equation of total energy balance for the coupled plasma – electromagnetic field system (22) that follows from the system of difference equations (10) - (17) can be found in Appendix.

From this we can conclude that for the difference model (11) - (18), the change in the total energy is determined by:

- 1. The work of external forces, i.e. pressure and ponderomotive force;
- 2. The influx (outflow) of heat trough the border of the region, including radiative heat transfer;
- 3. The influx of magnetic energy through the outer boundary;
- 4. The action of energy sources and sinks.

## 4.3 Combined iterative method for the system of difference equations

The difference equations (11) - (18) represent a system of nonlinear algebraic equations. An iterative method is used with separate solving groups of equations for different physical processes.

The procedure for solving system (11) - (18) is as follows:

1. The auxiliary values of velocity, density, temperature, and magnetic induction at the time layer (n + 1) are computed.

2. With the fixed temperature, the equations of motion and the Maxwell equations are solved. The auxiliary values of the velocity, density, and electromagnetic field parameters are computed.

3. With the fixed velocity, density and electromagnetic field, the system of energy equations is solved. The auxiliary values of the electron and ion temperature at the time layer (n + 1) are computed. The equation of state is a link between the equations of the "first group" (equations of dynamics and electromagnetic field) and the "second group" (energy balance equation).

4. The satisfaction of the energy conservation law (22) is verified. If the required accuracy is achieved, the values of the functions at time t = (n + 1) are considered to be found.

Otherwise we correct the coefficient of the system and repeat the step 1 to 3.

5. If necessary, the grid is corrected after solving the system (11) - (18). The grid functions found at the Lagrangian stage are recalculated to the adjusted grid. For this, the conversion algorithm developed in [5,6] is used.

The steps 2 and 3 are detailed below.

#### 4.4 Coupled dynamics and electrodynamics equations

At the step 2, the subsystem of difference equations (11) - (16) is split by physical processes: first, the motion of a substance is calculated under the frozen magnetic field assumption, and then the diffusion of the magnetic field is accounted. The equations are solved by the Newton method with the reduction of unknown quantities [4]. The convergence of this procedure is considered, e.g., in [18]. Advancing from iteration (s) to iteration (s+1), we assume that all the variables in the equations of motion depend only on the velocity components  $u_{ijk}$ ,  $w_{ijk}$ ,  $v_{ijk}$ , and the thermal pressure is locally barotropic. The transition formulae from iteration (s) to iteration (s+1) are the following:

$$u_{ijk}^{s+1} = u_{ijk}^{s} + \delta u_{ijk}$$

$$w_{ijk}^{s+1} = w_{ijk}^{s} + \delta w_{ijk}$$

$$v_{ijk}^{s+1} = v_{ijk}^{s} + \delta v_{ijk}$$

$$x_{ijk}^{s+1} = x_{ijk}^{s} + \delta x_{ijk} = x_{ijk}^{s} + \frac{\partial x_{ijk}}{\partial u_{ijk}} \delta u_{ijk} = x_{ijk}^{s} + \frac{\Delta t}{2} \delta u_{ijk}$$

$$y_{ijk}^{s+1} = y_{ijk}^{s} + \delta y_{ijk} = y_{ijk}^{s} + \frac{\partial y_{ijk}}{\partial w_{ijk}} \delta w_{ijk} = y_{ijk}^{s} + \frac{\Delta t}{2} \delta w_{ijk}$$

$$z_{ijk}^{s+1} = z_{ijk}^{s} + \delta z_{ijk} = z_{ijk}^{s} + \frac{\partial z_{ijk}}{\partial v_{ijk}} \delta v_{ijk} = z_{ijk}^{s} + \frac{1}{2} \delta v_{ijk}$$

$$\Phi_{mln}^{s+1} = \Phi_{mln}^{s} + \delta \Phi_{mln} = \Phi_{mln}^{s} + \sum_{r \in \Xi_1} \left( \frac{\partial \Phi_{mln}}{\partial u_r} \delta u_r + \frac{\partial \Phi_{mln}}{\partial w_r} \delta w_r + \frac{\partial \Phi_{mln}}{\partial v_r} \delta v_r \right)$$
(23)

Here  $\Phi_{mln}$  is for cell functions  $P_{mln}$ ,  $q_{mln}$ ,  $B_{mln}$ , and superscripts are for the iteration number.

Substituting the values (23) into the equations (14) and neglecting the squares of the increments of the functions, we obtain a system of linear algebraic equations with respect to the increments of the velocity components  $\delta u_{ijk}$ ,  $\delta w_{ijk}$ ,  $\delta v_{ijk}$ :

$$\sum_{k_{1}=-1}^{1}\sum_{k_{2}=-1}^{1}\sum_{k_{3}=-1}^{1}\left(a_{1ijk}^{(k_{1}k_{2}k_{3})}\delta u_{i+k_{1}j+k_{2}k+k_{3}}+b_{1ijk}^{(k_{1}k_{2}k_{3})}\delta w_{i+k_{1}j+k_{2}k+k_{3}}+c_{1ijk}^{(k_{1}k_{2}k_{3})}\delta v_{i+k_{1}j+k_{2}k+k_{3}}\right)=F_{ijk}^{(1)}$$

$$\sum_{k_{1}=-1}^{1}\sum_{k_{2}=-1}^{1}\sum_{k_{3}=-1}^{1}\left(a_{2ijk}^{(k_{1}k_{2}k_{3})}\delta u_{i+k_{1}j+k_{2}k+k_{3}}+b_{2ijk}^{(k_{1}k_{2}k_{3})}\delta w_{i+k_{1}j+k_{2}k+k_{3}}+c_{2ijk}^{(k_{1}k_{2}k_{3})}\delta v_{i+k_{1}j+k_{2}k+k_{3}}\right)=F_{ijk}^{(2)}$$

$$\sum_{k_{1}=-1}^{1}\sum_{k_{2}=-1}^{1}\sum_{k_{3}=-1}^{1}\left(a_{3ijk}^{(k_{1}k_{2}k_{3})}\delta u_{i+k_{1}j+k_{2}k+k_{3}}+b_{3ijk}^{(k_{1}k_{2}k_{3})}\delta w_{i+k_{1}j+k_{2}k+k_{3}}+c_{3ijk}^{(k_{1}k_{2}k_{3})}\delta v_{i+k_{1}j+k_{2}k+k_{3}}\right)=F_{ijk}^{(3)}$$

$$i=\overline{1,NM}, \quad j=\overline{1,NL}, \quad k=\overline{1,NN}$$

$$(24)$$

Here  $a_{1,2,3ijk}^{(k_1k_2k_3)}$ ,  $b_{1,2,3ijk}^{(k_1k_2k_3)}$ ,  $c_{1,2,3ijk}^{(k_1k_2k_3)}$ ,  $F_{ijk}^{(1,2,3)}$  are numeric factors. System of equations (24) has a block structure matrix.

To solve equations (24), we use iterative method [29].

After finding the velocity increment at the iteration (s+1), the values  $\delta u_{ijk}$ ,  $\delta v_{ijk}$ ,  $\delta v_{ijk}$ ,  $V_{mln}$ ,  $\rho_{mln}$ ,  $P_{mln}$ ,  $q_{mln}$  are computed, and the intermediate value of the magnetic induction  $\tilde{\mathbf{B}}$ :

$$\tilde{\mathbf{B}}_{mln} = \mathbf{B}(\rho_{mln}^{s+1}, \mathbf{E}^{s})$$

The next step is to solve the system of equations describing the electric and magnetic fields with finite conductivity of the medium (15) – (16). The intermediate value  $\tilde{\mathbf{B}}$  is used for calculating the conductivity coefficient:

$$\sigma_{mln}^{s+1} = \sigma_{mln} \left( \rho_{mln}^{s+1}, \tilde{\mathbf{B}}_{mln}, T_{mln}^{s} \right)$$

Then the system of difference equations with respect to  $\mathbf{B}^{s+1}$ ,  $\mathbf{E}^{s+1}$  is linear. Because some rarefied plasma areas may have close to zero conductivity, it is advisable to solve the system of field equations by excluding the magnetic induction **B**. The result is a system of linear equations with respect to  $E_x$ ,  $E_y$ ,  $E_z$ :

$$\sum_{k_{1}=-1}^{1}\sum_{k_{2}=-1}^{1}\sum_{k_{3}=-1}^{1}\left(\overline{a}_{1ijk}^{(k_{1}k_{2}k_{3})}(\widehat{E}_{x})_{i+k_{1}j+k_{2}k+k_{3}}+\overline{b}_{1ijk}^{(k_{1}k_{2}k_{3})}(\widehat{E}_{y})_{i+k_{1}j+k_{2}k+k_{3}}+\overline{c}_{1ijk}^{(k_{1}k_{2}k_{3})}(\widehat{E}_{z})_{i+k_{1}j+k_{2}k+k_{3}}\right)=\overline{F}_{ijk}^{(1)}$$

$$\sum_{k_{1}=-1}^{1}\sum_{k_{2}=-1}^{1}\sum_{k_{3}=-1}^{1}\left(\overline{a}_{2ijk}^{(k_{1}k_{2}k_{3})}(\widehat{E}_{x})_{i+k_{1}j+k_{2}k+k_{3}}+\overline{b}_{2ijk}^{(k_{1}k_{2}k_{3})}(\widehat{E}_{y})_{i+k_{1}j+k_{2}k+k_{3}}+\overline{c}_{2ijk}^{(k_{1}k_{2}k_{3})}(\widehat{E}_{z})_{i+k_{1}j+k_{2}k+k_{3}}\right)=\overline{F}_{ijk}^{(2)}$$

$$\sum_{k_{1}=-1}^{1}\sum_{k_{2}=-1}^{1}\sum_{k_{3}=-1}^{1}\left(a_{3ijk}^{(k_{1}k_{2}k_{3})}(\widehat{E}_{x})_{i+k_{1}j+k_{2}k+k_{3}}+b_{3ijk}^{(k_{1}k_{2}k_{3})}(\widehat{E}_{y})_{i+k_{1}j+k_{2}k+k_{3}}+c_{3ijk}^{(k_{1}k_{2}k_{3})}(\widehat{E}_{z})_{i+k_{1}j+k_{2}k+k_{3}}\right)=\overline{F}_{ijk}^{(3)}$$

$$i=\overline{1,NM}, \quad j=\overline{1,NL}, \quad k=\overline{1,NN}$$

$$(25)$$

Here  $\overline{a}_{1,2,3ijk}^{-(k_1k_2k_3)}$ ,  $\overline{b}_{1,2,3ijk}^{(k_1k_2k_3)}$ ,  $\overline{c}_{1,2,3ijk}^{-(k_1k_2k_3)}$ ,  $\overline{F}_{ijk}^{(1,2,3)}$  are numeric factors.

The system of linear equations (25) has a block structure. After finding the electric fields, we have:

$$\mathbf{B}_{mln}^{s+1} = \mathbf{B}\left(\boldsymbol{\rho}_{mln}^{s+1}, \mathbf{E}^{s+1}\right)$$

The system of equations (11) - (16) is solved if the increments of velocities at the iteration satisfy the conditions:

$$\begin{aligned} \left| \delta u_{ijk} \right| &\leq \varepsilon_{\mu} \left| u_{ijk} \right| + u_{\min} \\ \left| \delta_{W_{ijk}} \right| &\leq \varepsilon_{\mu} \left| w_{ijk} \right| + w_{\min} \\ \left| \delta_{V_{ijk}} \right| &\leq \varepsilon_{\mu} \left| v_{ijk} \right| + v_{\min} \end{aligned}$$
(26)

Here  $\varepsilon_{\mu}$  is the relative velocity error, and  $u_{min}$ ,  $v_{min}$ ,  $w_{min}$  are the absolute velocity errors.

## 4.5 Energy Balance

The energy balance equations are solved in terms of electron and ion temperature (17).

Energy equations are solved via the Newton iterations. The transition formulae from iteration (s) to iteration (s+1) are the following:

$$(T_{e,i})_{mln}^{s+1} = (T_{e,i})_{mln}^{s} + \delta(T_{e,i})_{mln}$$

$$(P_{e,i})_{mln}^{s+1} = (P_{e,i})_{mln}^{s} + \delta(P_{e,i})_{mln} = (P_{e,i})_{mln}^{s} + \left(\frac{\partial P_{e,i}}{\partial T_{e,i}}\right)_{mln} \delta(T_{e,i})_{mln}$$

$$(Q_{ei})_{mln}^{s+1} = (Q_{ei})_{mln}^{s} + \left(\frac{\partial Q_{ei}}{\partial T_{e}}\right)_{mln} \delta(T_{e})_{mln} + \left(\frac{\partial Q_{ei}}{\partial T_{i}}\right)_{mln} \delta(T_{i})_{mln}$$

$$(K_{e,i})_{g}^{s+1} = (K_{e,i})_{g}^{s} + \sum_{r \in \Xi_{4}} \frac{(\partial K_{e,i})_{g}}{(\partial T_{e,i})_{r}} \partial(T_{e,i})_{r}$$

$$(27)$$

 $\Xi_4$  is a template of the cells adjacent to the face g.

Substituting increments of functions at the iteration (s+1) into the energy equations and neglecting the squares of the increments, we obtain a system of linear algebraic equations with respect to the temperature increments  $\delta(T_e)_{mln}$ ,  $\delta(T_i)_{mln}$ :

$$\sum_{k_{1}=-1}^{1} \sum_{k_{2}=-1}^{1} \sum_{k_{3}=-1}^{1} \left( \frac{=(k_{1}k_{2}k_{3})}{a_{mln}} \left( \delta T_{e} \right)_{m+k_{1}l+k_{2}n+k_{3}} \right) + \frac{=(0,0,0)}{b_{mln}} \left( \delta T_{i} \right)_{mln} = \overline{F}_{mln}^{(1)}$$

$$= \frac{(0,0,0)}{c_{mln}} \left( \delta T_{i} \right)_{mln} + \sum_{k_{1}=-1}^{1} \sum_{k_{2}=-1}^{1} \sum_{k_{3}=-1}^{1} \left( \frac{=(k_{1}k_{2}k_{3})}{a_{mln}} \left( \delta T_{i} \right)_{m+k_{1}l+k_{2}n+k_{3}} \right) = \overline{F}_{mln}^{(2)}$$
(28)

Here  $a_{mln}^{=(k_1k_2k_3)}$ ,  $\overline{b}_{mln}^{=(0,0,0)}$ ,  $\overline{c}_{mln}^{=(k_1k_2k_3)}$ ,  $\overline{F}_{mln}^{(1,2)}$  are the coefficients obtained in the linearization procedure.

Similar equations at the boundary are obtained in accordance with the type of boundary conditions. For example, with a fixed temperature, all the temperature increments at the boundary are set equal to  $\theta$ .

The system of difference equations (28) is solved similarly to systems (24) and (25).

The energy equations are solved if the temperature increments satisfy the conditions

$$\left|\delta(T_{e/i})_{mln}\right| \le \varepsilon_T (T_{e/i})_{mln} + T_{\min}, \ m = \overline{1, NM - 1}, \ l = \overline{1, NL - 1}, \ n = \overline{1, NN - 1}$$
(29)

Here  $\varepsilon_T$  and  $T_{min}$  are the relative and absolute temperature errors.

## 5 SIMULATION OF A Z – PINCH IMPLOSION DYNAMICS

The described technique was applied to simulations of Z – pinch plasmas experiments with the use of pulsed-power facilities. Three-dimensional modeling was carried out by means of the RMHD code MARPLE-3D [22]. We have studied the Z – pinch produced by a multiwire array heated in a powerful electric discharge. The aim of simulations was to assess the current-carrying plasma instabilities that occur at the final stage of pinch formation and their development up to the final stage of compression of the plasma compression. The spatial perturbations of matter and magnetic flux distribution inside the wire array and their evolution at various stages of pinch compression were investigated. The simulation results are compared with the experimental data obtained at the Angara-5-1 facility (Troitsk Institute for Innovative and Thermonuclear Investigations – TRINITI, Moscow, Russia). The calculations were performed for multiwire configurations described, e.g., in [24]. Multiwire arrays proved to be a very effective electric load due to possibility of flexible adjustment of its parameters to that of a pulsed-power electric generator. However, as a wire-array has inhomogeneous structure, the resulting Z-pinch is subjected to MHD instabilities.

The magnetic flux breakthrough into various multiwire arrays (tungsten, molybdenum, copper, and aluminum) during their implosion was studied experimentally at the Angara-5-1 facility [25]. It is shown that breakthroughs develop in the final stage of plasma production from the wires and occur near the initial wire position. The spatial distribution of the azimuthal magnetic field  $B_{\phi}(z, t)$  was measured using magnetic probes. The characteristic dimensions of the regions with a nonuniform magnetic field at the outer boundary of the wire array plasma were determined and compared with those of the regions with depressed plasma radiation observed in frame and time-integrated X-ray images. The dynamics of the nonuniform magnetic field was compared with the pinch radiation at different stages of implosion exposed in the frame X-ray images. The plasma density in the magnetic flux breakthrough area was estimated.

The magnetic breakthrough phenomena is illustrated by the Fig.1. The experiment No. 5265 with a 40 aluminum wires array is typical for Z-pinch studies at ANGARA-5-1.



Figure 1. Experimental results (TRINITI, shot No. 5265 [25]).

At the left is the axial distributions of the azimuthal magnetic field inside the wire array measured at different instants of time ( $t_1$ =30ns, ...  $t_7$ =90ns,  $t_8$ =110ns) by the probe installed at  $r_p = 0.89$ cm. The coordinates z = 0 and z = 1.4 cm correspond to the cathode and anode, respectively. At the right is the time integrated pinhole image (negative) of the wire array plasma recorded behind a Mylar film (hv >100 eV). To the left of the axis, the image is absent because of the diaphragming of the input aperture of the pinhole camera. The anode is on the top, and the cathode is on the bottom.

The modeling was carried out by means of 3D RMHD code MARPLE, developed in KIAM RAS [22]. MARPLE is a full-scale multiphysics research code using the state-of-theart physics and numeric techniques. MARPLE provides a platform for high performance computing and functionality for solving the initial-boundary value problems using unstructured computational meshes. MARPLE physics includes: one-fluid two-temperature MHD model with electron-ion energy relaxation; general Ohm's law; anisotropic resistivity and heat conductivity in the magnetic field; radiative energy transfer (diffusion model, multigroup spectral model); multi-component convection-diffusion; wide-range equations of state (EOS), transport and kinetic coefficients, opacity and emissivity [23]. MARPLE main numerics are: mixed unstructured / block meshes (tetrahedral, hexahedral, prismatic elements and their combinations); high-resolution explicit TVD approximations to the ideal MHD equations; implicit FV/FE/DG techniques for dissipative processes; splitting scheme for RMHD system (elemental solvers for different physical processes, additive approximation scheme, conservation laws); 2-nd order predictor-corrector time-advance scheme. MARPLE is designed for high performance distributed computations using domain decomposition and MPI parallelism. The computing environment includes a set of service functions: data IO; mesh processing; parallel computations support; dynamic processing of computation objects (solvers, approximations, boundary conditions, matter properties); configurable recovery points writing and automated backup; advanced events logging. We use the open-source products: CAD-CAE platform SALOME [30] for complex computational domains (geometry description, setting boundary and subregions attributes, mesh generation and refinement), and multi-platform data analysis and visualization application ParaView [31].

The purpose of the simulation was to study the plasma instabilities at the final stage of imploded plasma stagnation. We present here the results of a plasma implosion simulation in accordance with the conditions of the experiment No. 5265. We studied a 20mm diameter 14mm high array made of 40 15 $\mu$ m diameter Al wires with a total linear mass of 220  $\mu$ g/cm.

The computational domain was a cylindrical sector  $45^{\circ}$  with periodic boundary conditions at  $\varphi = 0$  and  $\varphi = \pi/4$  (1/8 of the discharge chamber volume with 5 wires). The sector height was 3mm (~1/5 of the array height). See Fig. 2, left. The grid contained 1.2 million cells (hexahedra and prisms). The grid in the (x, y) plane was refined from  $h_x = h_y \approx 80\mu$ m near the initial position of the wires to  $h_x = h_y \approx 17\mu$ m near the axis, the grid along the z axis was uniform,  $h_z = 30 \mu$ m. The electrodes were considered ideally conducting. At the outer wall of the discharge chamber, the boundary condition was set for the magnetic induction  $B_{\varphi} = 2I/R$ , where R is the external radius of the discharge chamber, I=I(t) is the total generator current through the array (experimental data, see Fig. 4).

Plasma emission from exploded wires was simulated using the model of prolonged plasma creation [21]. The rate of plasma production was calculated by the formula

$$\dot{m}(t) = \begin{cases} k B(t)^{2}, & t < t_{\alpha}, \\ \frac{k B(t_{\alpha})^{2}}{M_{0}(1-\alpha)} (M_{0} - m(t)), & t \ge t_{\alpha}. \end{cases}$$

Here *m* is the ablated mass,  $M_0$  is the total mass of the array,  $t_\alpha$  is defined from the condition  $m(t_\alpha) = \alpha M_0$ . The coefficient k = 2 was chosen in accordance with the experimental data, so that the wire ablation ended approximately 10ns before the current maximum.

Spatial modulation of the plasma formation rate was introduced in accordance with the experimental data [25] by the formula

$$\alpha = 0.9(1 - 0.45[1 + \sin(2\pi z/\lambda)]), \ 0 \le z \le z_{\max},$$

<u>ہ</u>

which corresponds to the experimentally observed electrical explosion inhomogeneities with a characteristic wavelength  $\lambda \sim 100 \mu m$ .

The data tables of opacities and matter properties (equation of state) for the aluminum plasma were previously calculated using the TERMOS code developed in KIAM RAS [32].

A volumetric artificial (mathematical) viscosity was introduced into the difference scheme to ensure calculation of flows with strong radiative shocks. The viscosity value was regulated according the recommendations [15].

The calculations were performed on the supercomputers MVS-100K (JSCC RAS) and K-100 (KIAM RAS). A typical run using 240 computing cores required up to 70 hours.



Figure 2. Left: The computational domain (sketch) with the initial positions of the wires. Right: Plasma density distribution in two sections (*R*-*Z* and *R*- $\varphi$  planes in cylindrical coordinates, g·cm<sup>-3</sup>)

The results of a plasma implosion simulation are summarized below.

At the beginning of ablation the main processes are Joule heating and radiation losses. At the temperature  $T_e \sim 10\text{-}20\text{eV}$ , the plasma conductivity increases due to ionization approximately linearly with the temperature, while the emissivity increases faster, approximately by the factor  $\sim 2$  [23]. Thus, the condition for the existence of thermal (overheating) instability [17, 24] cannot be satisfied. Therefore, at the early stage the temperature perturbations correspond to an initial density perturbation level of  $\sim 10\%$ .

By the time  $t_5 \sim 70$  ns, the current increases up to 1.5MA, and correspondingly the magnetic pressure increases enough to force the plasma implosion (i.e. active acceleration toward the axis). A shock wave appears at the first phase of acceleration. As some part of energy is spent to ionization and radiation ("ionization-radiation barrier" [17]), the matter

compression behind the shock wave front is rather high ( $p/p_0 \gtrsim 10$ ).

Ablation of wires creates inhomogeneous plasma distribution (see Fig. 2, right). The plasma density and magnetic field are modulated in the azimuthal direction. The magnetic force lines bend around the denser areas where the current density increases. The elasticity of the magnetic field lines leads to additional acceleration of plasma.

Noticeable perturbations of density at the outer plasma boundary (Fig. 2, right) produce Rayleigh-Taylor hydromagnetic instability. However, this instability is damped due to sufficiently large aspect ratio of the formed plasma shell, the compressibility of the substance, and smoothing of the energy density gradient of the magnetic field, which is partially transferred together with the plasma to the axis,. The instability of the inner plasma boundary is not expressed too.

The inhomogeneity of current density and plasma creates the conditions for the development of overheating (thermal) instability in the regions where the Joule heating surpasses the radiation losses. Estimation of the instability increment according to [17] gives a characteristic overheating time  $\tau \sim 10$ -20ns. As a result of the instability, at  $t \sim 30$ ns the electron temperature in the spots near the plasma boundary is significantly higher than that in the surrounding matter. The computed values are:  $T_e = 45$ eV in the spots, and  $T_e = 20$ eV in the surrounding plasma.

The thermal instability causes a change in the plasma dynamics. The magnetic field penetrates through the plasma to the skin depth. Due to plasma overheating, the skin layer in the hot spots is much thinner than in the surrounding plasma.

Magnetic force lines take the appearance of "arches" which bend around hot spots. The initial inhomogeneity increases, while the thermal pressure is less than the magnetic one

 $(\beta = B^2/8\pi P \sim 0.1)$  due to radiation cooling. Thus the thermal pressure cannot prevent the development of azimuthal perturbations. The distorted shock wave triggers the instability of a strongly radiative thermally inhomodeneous plasma.

By the time  $t_7 \sim 80-90$ ns, the plasma velocity in the shock wave reaches  $2.2 \cdot 10^7$  cm/s. Ions are heated up to  $T_i \sim 1$ keV, and electron temperature is  $T_e \sim 200$ eV. The density/temperature perturbations lead to the magnetic field breakthrough, thus violating the uniformity of a plasma shell compression (Fig. 3). This also causes the development of instability in a "thermally inhomogeneous plasma" [19, 20] and the pressure difference reaches  $p_{max}/p_{min} \sim 2$ . The development of non-isothermic instability lasts approximately 20-30ns. The intensive motion leads to equalizing the pressure in the central core and smoothing the other perturbations.

At  $t_7 \sim 90$  ns the first plasma portions reach the axis and the process of stagnation begins. The average parameters of the "near-axis" plasma are the following: velocity  $\sim 5 \cdot 10^7$  cm/s, electron temperature  $T_e \sim 100$  eV, ion temperature  $T_i \sim 300$  eV, density varies between  $\sim 5 \cdot 10^{-2} - 10^{-1}$  g/cm<sup>3</sup>, which is in good agreement with the experimental data [25]. Thus, it is shown that the model of prolonged plasma creation [21] correctly describes the rate of plasma input into the region of the forming pinch.

Due to the fast implosion of the evaporated material of the wires and the intense process of radiation cooling of the stagnated plasma, its density in the axial zone significantly exceeds the density in the peripheral zone. The formation of the central pinch replaces the shell structure of the plasma. This process is activated at the time  $t_8 \sim 110$ ns, when the current pulse reaches its maximum, and the entire plasma mass moves to the axis. At this point, the stagnation of the plasma bulk is observed, its warming up, and a sharp increase in the soft X-ray radiation yield, which is shown in Fig. 4.



Figure 3. Numerical results: Axial distributions of the azimuthal magnetic field and plasma density inside the wire array at  $r_p = 0.89$ cm.



Figure 4. SXR pulse: experiment No 5265 TRINITY [25] (left) and the simulation result (right).  $t_0$  is the moment of completion of plasma ablation.

## **6** CONCLUSIONS

The methods presented here for solving the equations of the Lagrangian-Eulerian RMHD model were tested by various computational experiments reproducing wave processes in a magnetized medium, e.g. Alfvén waves, magnetosonic waves, decays of MHD discontinuities [14, 27], flows with uniform deformation occurring in the vicinity of the zero line of the magnetic field [28], etc. It was shown by computational experiments and application

simulations, that it is advisable to use the method of physical processes splitting, if the thermal pressure is greater than the magnetic one  $p \ge B^2/8\pi$  during the entire simulated process. In the opposite situation, the method of combined iterations is more resource saving.

The splitting method is easier to implement and allows saving about 40-50% of arithmetic operations as compared to the combined iterations method. However, when magnetic pressure prevails the thermal one  $(B^2/8\pi) > p$ , the separate accounting of physical processes demands the restriction on the integration time step, similar to that obtained in [14] for the 2D case:

$$\Delta t < \frac{Ah}{\sqrt{\frac{B^2}{8\pi\rho} + (\gamma - 2)\frac{p}{\rho}}}, h = V/S_{\max}, A = const \sim 1.$$
(30)

Here V is the mesh cell volume,  $S_{\text{max}}$  is the maximum value of the side face area.

In simulations of imploding current-carrying plasma accompanied by strongly radiating shock waves, the method of adaptable artificial viscosity [15] appeared to be a resource saving and robust numerical tool. It was indicated, that this method makes possible simulation of transient plasma flows with a significant ion-electron temperature difference. It provides good practical accuracy, which allows comparison with experimental results. Note also that the method is well suitable for the use of real life wide-range EOS.

The developed numerical technique was applied to simulations of Z-pinch implosion at Angara-5-1 facility. The magnetic flux breakthrough into an array made of thin aluminum wires was studied. The numerical results are in good agreement with the experimental data on the basic parameters such as the time when the pinch reached its final state (plasma cumulation near the axis of the system) and the soft x-ray radiation power. Thus we can conclude that it is possible to use the proposed method based on the completely conservative difference scheme for solving plasma dynamics problems, and carry out predictive simulation of experiments with plasma accelerated by electromagnetic force produced by a powerful current pulses. At the same time, the numerical simulation substantially supplements the experimental data, since it provides information on the dynamics of magnetic implosion, which cannot be obtained in the experiment due to the limited capabilities of diagnostics.

Let us take up the liner implosion in cylindrical coordinates. Then, in the (R-z) plane perpendicular to the azimuthal magnetic field force lines, the Rayleigh-Taylor instability causes the most serious perturbations. In the  $(R-\varphi)$  plane, the instabilities of thermally inhomogeneous plasma are of importance due to disbalances of Joule heating and radiation losses. For further clarification of the instability effect, we need a detailed examination of the initial perturbations evolution by individual harmonics in a certain spectral range, including perturbations of an arbitrary form (superposition of harmonics), various initial amplitudes, transition to a nonlinear stage, etc. Here we concentrate on the fact that although the problem of instability in many cases is considered as "purely mechanical", the energy aspect is very important concerning the dynamics of Z-pinch plasmas. The rate of instability depends on the rate of plasma acceleration as well as on the aspect ratio of a plasma shell formed due to wire ablation. The process in whole is determined by the energy exchange between the electromagnetic field and the plasma, as well as the energy balance in the plasma, where the radiation transfer is the largest contributor. The performed simulation, even with a mild Rayleigh-Taylor instability, shows that at the final stage of compression, the distribution of density and temperature is substantially homogeneous in space. The radiation absorption

coefficient, which is inversely proportional to the mean free path, varies by several orders of magnitude in the computational domain. The radiation is locked in the central region of the pinch, as a result it radiates like a surface source.

The computations were carried out on the supercomputers MVS-100K (JSCC RAS) and K-100 (KIAM RAS).

## APPENDIX

The equation of total energy balance for the coupled plasma – electromagnetic field system:

$$\begin{split} \hat{E}_{tot} &- E_{tot} = -\Delta t \sum_{min} \left( \hat{G}_{e_{min}} + \hat{G}_{i_{min}} \right) \hat{V}_{min} + \\ & \left[ -u_{ijk}^{(0.5)} \left( \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} - \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} \right) \left( \frac{\partial \hat{V}_{r}}{\partial x_{ijk}} \right) \left( \hat{P}_{r} + \frac{\hat{B}_{r} B_{r}}{8\pi} \right) \\ & - w_{ijk}^{(0.5)} \left( \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} - \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} \right) \left( \frac{\partial \hat{V}_{r}}{\partial y_{ijk}} \right) \left( \hat{P}_{r} + \frac{\hat{B}_{r} B_{r}}{8\pi} \right) \\ & - v_{ijk}^{(0.5)} \left( \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} - \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} \right) \left( \frac{\partial \hat{V}_{r}}{\partial z_{ijk}} \right) \left( \hat{P}_{r} + \frac{\hat{B}_{r} B_{r}}{8\pi} \right) \\ & + \frac{u_{ijk}^{(0.5)}}{4\pi} \left( \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} - \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} \right) B_{xr}^{(0.5)} \left( \left( \frac{\partial \hat{V}_{r}}{\partial x_{ijk}} \right) \hat{B}_{xr} + \left( \frac{\partial \hat{V}_{r}}{\partial y_{ijk}} \right) \hat{B}_{yr} + \left( \frac{\partial \hat{V}_{r}}{\partial z_{ijk}} \right) \hat{B}_{zr} \right) \\ & + \Delta t \sum_{ijk \in D} + \frac{w_{ijk}^{(0.5)}}{4\pi} \left( \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} - \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} \right) B_{yr}^{(0.5)} \left( \left( \frac{\partial \hat{V}_{r}}{\partial x_{ijk}} \right) \hat{B}_{xr} + \left( \frac{\partial \hat{V}_{r}}{\partial y_{ijk}} \right) \hat{B}_{yr} + \left( \frac{\partial \hat{V}_{r}}{\partial z_{ijk}} \right) \hat{B}_{zr} \right) \right] \\ & + \frac{2 \lambda t}{4\pi} \left( \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} - \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} \right) B_{zr}^{(0.5)} \left( \left( \frac{\partial \hat{V}_{r}}{\partial x_{ijk}} \right) \hat{B}_{xr} + \left( \frac{\partial \hat{V}_{r}}{\partial y_{ijk}} \right) \hat{B}_{yr} + \left( \frac{\partial \hat{V}_{r}}{\partial z_{ijk}} \right) \hat{B}_{zr} \right) \right] \\ & + \frac{2 \lambda t}{4\pi} \left( \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} - \sum_{r' \in \Xi_{2}} \mu^{\prime \prime}_{ijk} \right) B_{zr}^{(0.5)} \left( \left( \frac{\partial \hat{V}_{r}}{\partial x_{ijk}} \right) \hat{B}_{zr} - \left( \frac{\partial \hat{V}_{r}}{\partial z_{ijk}} \right) \hat{B}_{zr} \right) \right] \\ & + \frac{2 \lambda t}{4\pi} \left( \sum_{r' \in \Xi_{2}} \eta^{\prime \prime}_{ijk} - \sum_{r' \in \Xi_{2}} \eta^{\prime \prime}_{ijk} \right) \left( \left( \frac{\partial \hat{V}_{r}}{\partial y_{ijk}} \right) \hat{B}_{zr}^{(0.5)} - \left( \frac{\partial \hat{V}_{r}}{\partial z_{ijk}} \right) \hat{B}_{zr} \right) \right) \\ & + \frac{2 \lambda t}{4\pi} \left( \sum_{r' \in \Xi_{2}} \eta^{\prime \prime}_{ijk} - \sum_{r' \in \Xi_{2}} \eta^{\prime \prime}_{ijk} \right) \left( \left( \frac{\partial \hat{V}_{r}}{\partial y_{ijk}} \right) \hat{B}_{zr}^{(0.5)} - \left( \frac{\partial \hat{V}_{r}}{\partial z_{ijk}} \right) \hat{B}_{zr}^{(0.5)} \right) \right) \\ & + \frac{2 \lambda t}{4\pi} \left( \sum_{r' \in \Xi_{2}} \eta^{\prime \prime}_{ijk} - \sum_{r' \in \Xi_{2}} \eta^{\prime \prime}_{ijk} \right) \left( \left( \frac{\partial \hat{V}_{r}}{\partial y_{ijk}} \right) \hat{B}_{zr}^{(0.5)} - \left( \frac{\partial \hat{V}_{r}}{\partial z_{i$$

#### REFERENCES

- [1] A.A. Samarskii, *The theory of difference schemes*, New York Basel. Marcel Dekker, Inc, (2001).
- [2] G.I. Marchuk, Metody rasshscepleniia, Moscow: Nauka (1988).
- [3] A. K. Alekseev, A.E. Bondarev, A.E. Kuvshinnikov, "Comparative analysis of the accuracy of OpenFoam solvers for the oblique shock wave problem", *Math. Montis*, **45**, 95-106 (2019).
- [4] I.N. Konshin, K.M. Terekhov and Yu.V. Vassilevski, "Numerical modeling via INMOST software platform", *Math. Montis*, **47**, 75-86 (2020).
- [5] A.A. Samarskii, Yu.P. Popov, *Raznostnye metody resheniia zadach gazovoi dinamiki*, Moscow: Nauka (1992).
- [6] V.P. Smirnov, "Fast liners for inertial fusion", *Plasma Phys. Controlled Fusion*, **33**, 1697 (1991).
- [7] Michael A. Liberman, John S. De Groot, Arthur Toor, Rick B. Spielman, *Physics of highdensity Z-pinch plasmas*, Springer (1998).
- [8] James J. Duderstadt, Gregory A. Moses, *Inertial Confinement Fusion*, John Wiley and Sons, New York (1982).
- [9] V.I. Oreshkin, *Radiation of High-temperature Plasma*. *Pinch-effect*, LAP Lambert Academic Publishing, Saarbrukken (2012).
- U. Shumlak, B. A. Nelson, R. P. Golingo, [10] Y. Zhang, T. R. Weber, A. D. Stepanov, E. L. Claveau, E. G. Forbes, Z. T. Draper, J. M. Mitrani, H. S. McLean, K. K. Tummel, D. P. Higginson and C. M. Cooper, "Sustained Neutron Production from a Sheared-Flow 135001 Stabilized Ζ Pinch", Phys. Rev. Lett.. 122, (2019).doi:10.1103/PhysRevLett.122.135001.
- [11] M. R. Gomez, et al, "Assessing Stagnation Conditions and Identifying Trends in Magnetized Liner Inertial Fusion". *IEEE Transactions on Plasma Science*. *IEEE Transactions on Plasma Science*, 47(5), 2081–2101 (2019).
- [12] V.V. Aleksandrov, A.V. Branitski, E.V. Grabovskiy, A.N. Gritsuk, K.N. Mitrofanov, I.N. Frolov, V.A. Gasilov, O.G. Olkhovskaya, P.V. Sasorov, "Study of interaction between plasma flows and the magnetic field at the implosion of nested wire arrays", *Plasma Physics and Controlled Fusion*, **61** (3), 035009 (2019).
- [13] G.A Kulikovskiy, A.G Lyubimov, Magnitnaya gidrodinamika, Moscow: Logos (2011).
- [14] A.Yu. Krukovskiy, V.A. Gasilov, Yu.A. Poveschenko, Yu. S. Sharova, L.V. Klochkova, "Implementation of the iterative algorithm for numerical solution of 2D magnetogasdynamics problems", *Matem. Mod.*, **32** (1), 50–70 (2020). doi: 10.20948/mm-2020-01-04.
- [15] I.V. Popov, I.V. Friazinov, Metod adaptivnoi iskusstvennoi viazkosti chislennogo resheniia uravnenii gazovoi dinamiki, Moscow: Krasand (2015).
- [16] C.W. Hirt, A.A. Amsden and J.L. Cook, "An arbitrary Lagrangian-Eulerian computing method for all ow speeds", *J. Comput. Phys.*, **14**, 227–253 (1974).
- [17] A.A. Samarskii, A.P. Mikhailov, *Principles of Mathematical Modeling. Ideas, Methods, Examples*, London and New York. Taylor and Francis, (2002).
- [18] A.A. Samarskii, A.V. Gulin, *Chislennye metody*, Moscow: Nauka (1989).
- [19] R. Benattar, P. Ney, A. Nikitin, S.V. Zakharov, A.A. Otochin, A.N. Starostin, A.E. Stepanov, A.F. Nikiforov, V.G. Novikov, A.D. Solomyannaya, V.A. Gasilov and A.Yu. Krukovskii, "Implosion Dynamics of a Radiative Z-Pinch", *IEEE Transactions on Plasma Science*, 26 (4) (special issue on Z-pinch plasmas), 1210-1223 (1998).
- [20] A.S. Boldarev, E.A. Bolkhovitinov, I.Yu. Vichev, G.S. Volkov, V.A. Gasilov, E.V. Grabovskii, A.N. Gritsuk, S.A. Dan'ko, V.I. Zaitsev, V.G. Novikov, G.M. Oleinik, O.G. Olkhovskaya, A.A. Rupasov, M.V. Fedulov, A.S. Shikanov, "Methods and Results of Studies of the

Radiation Spectra of Megampere Z-Pinches at the Angara-5-1 Facility", *Plasma Physics Reports*, **41** (2), 178-181 (2015).

- [21] V. V. Aleksandrov, A.V. Branitskii, G.S. Volkov, E.V. Grabovskii, M.V. Zurin, S.L. Nedoseev, G.M. Oleinik, A.A. Samokhin, P.V. Sasorov, V.P. Smirnov, M.V. Fedulov, I.N. Frolov, "Dynamics of Heterogeneous Liners with Prolonged Plasma Creation", *Plasma Physics Reports*, 27 (2), 89–109 (2001).
- [22] V.A. Gasilov, A.S. Boldarev, S.V. D'yachenko, O.G. Olkhovskaya, E.L. Kartasheva, S.N. Boldyrev, G.A. Bagdasarov, I.V. Gasilova, M.S. Boyarov, V.A. Shmyrov, "Program package MARPLE3D for simulation of pulsed magnetically driven plasma using high performance computing", *Matem. Mod.*, 24 (1), 55–87 (2012).
- [23] A.F. Nikiforov, V.G. Novikov, V.B. Uvarov, Quantum-Statistical Models of Hot Dense Matter. Methods for Computation Opacity and Equation of State, Basel, Berlin: Birkhauser Verlag (2005).
- [24] V.V. Alexandrov, E.V. Grabovsky, M.V. Zurin, I.V. Krasovsky, K.N. Mitrofanov, S.L. Nedoseev, G.M. Oleinik, I.Yu. Porofeev, A.A. Samokhin, V.P. Smirnov, M.V. Fedulov, I.N. Frolov, P.V. Sasorov, "Characteristics of high-power radiating imploding discharge with cold start" *Journal of Experimental and Theoretical Physics*, **99** (6), 1150-1172 (2004).
- [25] K.N. Mitrofanov, V.V. Aleksandrov, E.V. Grabovski, E.A. Ptichkina, A.N. Gritsuk, I.N. Frolov, Y.N. Laukhin, "Study of the termination phase of plasma production and the formation of magnetic flux breakthroughs during wire array implosion", *Plasma Physics Reports*, **40** (9), 779-806 (2014).
- [26] A. A. Samarskii, "Some results of the theory of difference methods.", *Differentsial'nye Uravneniya*, **16** (7), 1155–1171, 1348 (1980).
- [27] K.V. Brushlinskiy, *Matematicheskiye i vychislitel'nyye zadachi magnitnoy gazodinamiki*, Moscow: BINOM (2020). (in Russian)
- [28] E. Priest and T. Forbes, *Magnetic Reconnection*, Cambridge, UK: Cambridge University Press, (2007).
- [29] Linear Solver: https://trilinos.github.io/linear\_solver.html (Accessed December 19, 2020)
- [30] SALOME: http://www.salome-platform.org/ (Accessed December 19, 2020)
- [31] ParaView: <u>https://www.paraview.org/</u> (Accessed December 19, 2020)
- [32] THERMOS: <u>http://keldysh.ru/cgi/thermos/navigation.pl?en,home</u> (Accessed December 19, 2020)

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# GERMANIUM AND GERMANIUM–GOLD ALLOYS UNDER SHOCK-WAVE LOADING

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**Summary.** The results of numerical experiments upon modeling thermodynamic parameters such as value of pressure and compression of germanium and its alloys with gold are presented. The calculations were performed using the model TEC (thermodynamic equilibrium components). The model allows us to take into account the phase transition of germanium under shock-wave action. The interest in investigating of the compressibility for such materials is related both to the possibility of creating materials with the necessary properties and to the properties of the materials themselves. The results of calculations are compared with the known experimental results of different authors. The value of pressure and compression for shock wave loading of pure germanium and alloys with germanium as a component of various compositions are calculated.

## **1 INTRODUCTION**

The researches of shock loading on heterogeneous materials are of interest for many problems of modern science, which causes the emergence of new models for describing the thermodynamic parameters of mixtures, alloys and composites [1–4]. It is preferable to use a fairly simple model of the equation of state given a large number of components with different properties. The construction of equations of state has been carried out for many years, while taking into account the complexity and diversity of the materials studied, the problem of creating simple equations of state with a small number of parameters is relevant [5–13]. Modern approaches to the choice of equations of state of a condensed medium are given in [14]. A significant change in the volume in the phase transition region of the components that make up the mixtures makes it possible to expand the range of changes in the thermodynamic parameters of mixtures under shock-wave loading.

The interest in researching the compressibility of alloys that include germanium as a component is related to its properties, in particular, the presence of a phase transition under shock-wave

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action [15, 16]. The alloys containing germanium [17] and materials including germanium in their composition are being investigated [18].

## **2** CALCULATION MODEL

The thermodynamically equilibrium model of shock-wave loading, taking into account the presence of gas in the pores, was used to describe the thermodynamic parameters of alloys and mixtures under shock-wave action [19–21]. The model is based on the assumption that all components of the mixture, including the gas in the pores, have equal values of velocities, pressures and temperatures. The equations of state of Mie–Grüneisen type are used to describe the behavior of condensed phases. The equations are written out:

$$P(\rho, T) = P_C(\rho) + P_T(\rho, T), \qquad E(\rho, T) = E_C(\rho) + E_T(T),$$
(1)

$$P_T(\rho, T) = \Gamma \rho E_T(T), \qquad E_T(T) = c_V(T - T_0).$$
 (2)

Here  $P_C$  and  $E_C$  are potential components of the pressure and specific energy;  $P_T$  and  $E_T$  are thermal components;  $c_V$  is the specific heat capacity;  $T_0$  is the initial temperature; The initial energy  $E_0$  of the substance under normal conditions is neglected, taking into account the range of pressure values greater than 5 GPa for this model.  $c_V$  is assumed to be a constant value, by analogy with [22]. The function  $\Gamma = P_T V/E_T$  that determines the contribution of the thermal component depends explicitly only on the temperature  $\Gamma(T)$  in the model [19–21]. Therefore, the thermal and caloric forms of the equation of state for a condensed component with current density  $\rho$  and initial density  $\rho_0$  are as follows:

$$P(\boldsymbol{\rho},T) = A\left[\left(\boldsymbol{\rho}/\boldsymbol{\rho}_0\right)^k - 1\right] + \Gamma \boldsymbol{\rho} c_V(T - T_0), \tag{3}$$

$$E(\rho,T) = A/\rho_0 \left[ 1/(k-1) \left( \rho/\rho_0 \right)^{k-1} + \rho_0/\rho - k/(k-1) \right] + E_T.$$
(4)

The ideal gas equation of state is taken for a gas. The conditions of conservation of the mass flux for each component of the material and the conditions of conservation of momentum and energy fluxes for the media considered as a whole are written at the wave front. The obtained equations, together with the equations of state of each component, are sufficient to find dependences P(U) or D(U) (P, U, and D are pressure, mass and wave velocities; A, k are coefficients in the equations of state of condensed component). The following expression can be obtained for a material with n condensed components ( $\mu_{i0}$  is the volume fraction of *i*-th condensed component):

$$P = \frac{\sum_{i=1}^{n} \frac{\mu_{i0}}{\sigma_i} A_i \left[ \left( h_i - \frac{k_i + 1}{k_i - 1} \right) \sigma_i^{k_i} + \frac{2k_i \sigma_i}{k_i - 1} - h_i - 1 \right]}{\sum_{i=1}^{n} \frac{\mu_{i0}}{\sigma_i} h_i + \frac{h_g}{\sigma_g} \left( 1 - \sum_{i=1}^{n} \mu_{i0} \right) - 1}.$$
(5)



Figure 1: The shock adiabat of germanium: solid line corresponds to calculations taking into account the phase transition, dash-dotted line for low pressure phase, dotted line for high pressure phase; markers—experimental data (1-[24]; 2-[15]; 3-[17]; 4-[25]).

Here  $h_i = 2/\Gamma_i + 1$ , i = 1, ..., n;  $h_g = 2/(\gamma - 1) + 1$ ;  $\sigma_i = \rho_i/\rho_{i0}$ ,  $\sigma_g = \rho_g/\rho_{g0}$  are the compression ratios of the corresponding component,  $\mu_{i0}$  are the volume fraction,  $\rho_{i0}$ ,  $\rho_i$  are the density of the *i*-th phase of the substance ahead of the shock wave front and behind it, respectively (i = 1, ..., n, and g);  $\gamma = 1.41$  (ratio of specific heats). By adding to equation (5) relationships that follow from the equations of state of components and expressing equality in temperatures of all components, we finally have equations which allow us to construct the shock adiabat of investigated material. In the case of calculation for solid material, we assume that  $\sum_{i=1}^{n} \mu_{i0} = 1$ .

The phase transition of components under shock-wave action is taken into account in this model. Germanium is considered as the mixture of low-pressure phase and high-pressure phase in the phase transition region. The conditions of dynamic compatibility are written on the shock wave front taking into account the phase transition [23].

#### **3 MODELING RESULTS**

The results of modeling for germanium and the data from experiments [15, 17, 24, 25] are shown in figure 1 in the variables pressure–mass velocity, in figure 2 in the variables wave-mass velocities. As noted in [26], the transition pressure of germanium depends on how close the ap-



Figure 2: The shock adiabat of germanium: the notation is similar to figure 1.

plied pressure is to the hydrostatic pressure and on the presence of shear stress components. The phase transformation of germanium I–II was determined at pressure about 9 GPa with a volume decrease of 19%. This transition was investigated at shear stresses and high pressures [27–36]. The coefficients of the equation of state (3) and (4) for germanium I (low-pressure phase) are as follows:  $\rho_0 = 5.328 \text{ g/cm}^3$ , A = 17.25 GPa, k = 4.0,  $c_V = 375 \text{ J/(kg K)}$ ; for germanium II (high-pressure phase):  $\rho_0 = 6.572 \text{ g/cm}^3$ , A = 18.5 GPa, k = 4.0,  $c_V = 375 \text{ J/(kg K)}$ . The beginning of the phase transition for germanium in the calculations according to the author's model is also assumed at a pressure value of 9 GPa. The curve break at 30 GPa corresponds to the end of the phase transition. A reliable description of the available data is obtained. There is a lot of work on the definition of phase transitions in germanium at the moment. However, the presence of drop-down points confirms the need for further work in this direction.

The parameters that made it possible to reliably describe the thermodynamic parameters of germanium in a wide range of pressure and compression values made it possible to describe the shock wave loading of gold and germanium alloys with experimental accuracy. It is necessary to know only the composition and density of the alloy to describe its dynamic loading. The following parameters are determined for gold with a density of  $\rho_0 = 19.302 \text{ g/cm}^3$ , A = 47.9 GPa, k = 4.0,  $c_V = 277 \text{ J/(kg K)}$ .



Figure 3: The shock adiabats of gold–germanium alloys: curves correspond to the present calculations for  $\rho_0 = 16.851 (1), 16.111 (2)$  and  $15.536 \text{ g/cm}^3 (3)$ ; markers—experimental data (4, 5, 6—[37]).

The simulation results and available experimental data are shown in figure 3. For three alloys of gold in combination with germanium with mass fractions wt % Au(94.2)Ge (5.8), respectively,  $\rho_0 = 16.851$  g/cm<sup>3</sup>; Au(92.1)Ge(7.9),  $\rho_0 = 16.111$  g/cm<sup>3</sup>; Au(90.7)Ge (9.3),  $\rho_0 = 15.536$  g/cm<sup>3</sup> [37]. For clarity, the calculations and data are shown with a pressure shift of 50 GPa. It is assumed that the phase transition of germanium in the alloy begins under the same conditions as for pure germanium. Due to the fact that the calculation was carried out for alloys with low porosity, the assumed pressure values for the beginning of the phase transition can be considered justified. This assumption was confirmed in the calculations of mixtures with two components experiencing a phase transition [38].

It can be concluded that the proposed scheme for describing thermodynamic parameters under dynamic loads allows us to describe the behavior of pure germanium and materials with it as a component. The calculations correspond well to the data of experiments for germanium-gold alloys. The deviation of the calculated points from the experimental data is probably due, in particular, to the influence of other phase transitions for germanium. Only the phase transformation of germanium I–II was considered in this paper.

## **4** CONCLUSIONS

Thus, the model allows calculating thermodynamic parameters of germanium and alloys with germanium as a component under shock wave loading. The Mie–Grüneisen equation of state, together with the condition of thermodynamic equilibrium of the mixture components under shock-wave loading, gives a closed system of equations that determines the parameters under dynamic loads. The assumption of thermodynamic equilibrium allows us to take into account the interaction of components with each other, which becomes essential when using materials experiencing a phase transition at high dynamic loads. The simulation results show that it is possible to determine the thermodynamic parameters of heterogeneous materials taking into account the phase transition of its components under shock-wave loading.

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## REFERENCES

- B. R. Krueger and T. Vreeland, "A Hugoniot theory for solid and powder mixtures", *J. Appl. Phys.*, 69, 710–716 (1991).
- [2] B. Nayak and S. V. G. Menon, "Non-equilibrium theory employing enthalpy-based equation of state for binary solid and porous mixtures", *Shock Waves*, **28**, 141–151 (2018).
- [3] E. A. Strebkova, M. N. Krivosheina, and Ya. V. Mayer, "Features of the processes of elastic deformation in cubic crystals", *Math. Montis.*, **46**, 91–104 (2019).
- [4] K. K. Maevskii, "Numerical simulation of thermodynamic parameters of lithium deuteride and its mixtures under shock wave loading", *AIP Conf. Proc.*, **2051**, 020181 (2018).
- [5] K. V. Khishchenko, "Equation of state for magnesium hydride under condition of shock loading", *Math. Montis.*, **43**, 70–77 (2018).
- [6] W. B. Holzapfel, "Equations of state for Cu, Ag, and Au and problems with shock wave reduced isotherms", *High Pressure Res.*, **30**, 372–394 (2010).
- [7] M. A. Kadatskiy and K. V. Khishchenko, "Theoretical investigation of the shock compressibility of copper in the average-atom approximation", *Phys. Plasmas*, **25**, 112701 (2018).
- [8] D. V. Minakov, M. A. Paramonov, and P. R. Levashov, "Consistent interpretation of experimental data for expanded liquid tungsten near the liquid–gas coexistence curve", *Phys. Rev. B*, 97, 024205 (2018).
- [9] E. I. Kraus and I. I. Shabalin, "Calculation of elastic modules behind strong shock wave", J. Phys.: Conf. Ser., 774, 012009 (2015).
- [10] M. N. Krivosheina and E. V. Tuch, "Equations of state in materials beyond the assumption of isotropy of volume compressibility", *J. Phys.: Conf. Ser.*, **1128**, 012102 (2018).
  [11] A. V. Ostrik and D. N. Nikolaev, "Construction of the equations of state for polycrystalline solids
- [11] A. V. Ostrik and D. N. Nikolaev, "Construction of the equations of state for polycrystalline solids for the purpose of the numerical solution of problems of continuous medium mechanics", *J. Mat. Phys. Mech.*, **1392**, 012017 (2019).
- [12] K. V. Khishchenko, "Equation of state for niobium at high pressures", *Math. Montis.*, 47, 119–123 (2020).
- [13] K. K. Maevskii, "Thermodynamic parameters of lithium deuteride in pressure range 5–1000 gigapacals", *Math. Montis.*, 41, 123–130 (2018).
- [14] I. V. Lomonosov and S. V. Fortova, "Wide-range semiempirical equations of state of matter for numerical simulation on high-energy processes", *High Temp.*, 55, 585–610 (2017).

- [15] M. N. Pavlovskii, "Formation of metallic modifications of germanium and silicon under conditions of shock compression", *Fiz. Tverd. Tela*, **9**, 3192–3197 (1967).
- [16] M. N. Magomedov, "State equations and properties of various polymorphous modifications of silicon and germanium", *Phys. Solid State*, **59**, 1085–1093 (2017).
- [17] R. G. McQueen, S. P. Marsh, J. W. Taylor, J. N. Fritz, and W. J. Carter, "The equation of state of solids from shock wave studies", in: *High Velocity Impact Phenomena* ed. by R. Kinslow, New York: Academic Press, pp. 293–417, 515–568 (1970).
- [18] C. Zhang, Y. Jin, P. Kong, S. Li, S. Chen, W. Zhang, S. Cheng, K. He, and W. Dai, "Theoretical investigations on the structural stability, structural and physical properties, and bonding feature for RuX (X = Si, Ge, Sn) with B20 and B2 phases", *Mater. Today Commun.*, 24, 101116 (2020).
- [19] K. K. Maevskii and S. A. Kinelovskii, "Thermodynamic parameters of mixtures with silicon nitride under shock-wave impact in terms of equilibrium model", *High Temp.*, **56**, 853–858 (2018).
- [20] K. K. Maevskii and S. A. Kinelovskii, "Numerical simulation of thermodynamic parameters of high-porosity copper", *Tech. Phys.*, **64**, 1090–1095 (2019).
- [21] K. K. Maevskii, "Thermodynamic parameters of shock wave loading of carbides with various stoichiometric compositions", *AIP Conf. Proc.*, **2167**, 020204 (2019).
- [22] A. V. Ostrik and A. V. Utkin, "Calculation of a shock adiabatic curve for syntactic foam taking into account presence of gas component localized in hollow microspheres", J. Mat. Phys. Mech., 31, 48–51 (2017).
- [23] K. K. Maevskii, "Modelling of polymorphic phase transitions under shock wave loading", AIP Conf. Proc., 2103, 020009 (2019).
- [24] S. P. Marsh (ed.), LASL Shock Hugoniot Data, Berkeley, CA: University of California Press, (1980).
- [25] M. van Thiel (ed.), *Compendium of Shock Wave Data*, Lawrence Livermore Laboratory Report UCRL-50108, Livermore, CA, (1977).
- [26] Yu. E. Tonkov and E. G. Ponyatovsky, *Phase Transformations of Elements under High Pressure*, Boca Raton, FL: CRC Press, (2005).
- [27] J. C. Jamieson, "Crystal structures at high pressures of metallic modifications of silicon and germanium", *Science*, **139**, 762–764 (1963).
- [28] L. F. Vereshcliagin, E. V. Zubova, and K. P. Burdina, "Dense modifications of Ge and Si under high pressure and shear stress", *Dokl. Akad. Nauk SSSR*, 168, 314–315 (1966).
- [29] B. Okai and T. Yoshimoto, "Stress-induced phase change of single-crystalline GaSb, InAs and Ge", J. Phys. Soc. Jpn., 45, 1887–1890 (1978).
- [30] Yu. F. Shul'pyakov and A. N. Dremin, "Shear-stress and high-pressure effects on electro-conductivity of Si and Ge single-crystals", *Fiz; Tverd. Tela*, 25, 1989–1993 (1983).
- [31] S. B. Qadri, E. F. Skelton, and A. W. Webb, "High pressure studies of Ge using synchrotron radiation", J. Appl. Phys., 54, 3609–3611 (1983).
- [32] C. S. Menoni, J. Z. Hu, and I. L. Spain, "Germanium at high pressures", *Phys. Rev. B*, 34, 362–368 (1986).
- [33] C. Meade and R. Jeanloz, "Acoustic emissions and shear instabilities during phase transformations in Si and Ge at ultrahigh pressures", *Nature*, **39**, 616–618 (1989).
- [34] F. X. Zhang and W. K. Wang, "Crystal structure of germanium quenched from the melt under high pressure", *Phys. Rev. B*, **52**, 3113–3116 (1995).
- [35] M. Imai, T. Mitamura, K. Yaoita, and K. Tsuji, "Pressure-induced phase transition of crystalline and amorphous silicon and germanium at low temperatures", *High Pressure Res.*, **15**, 167–189 (1996).
- [36] E. Principi, F. Decremps, A. Di Cicco, F. Datchi, S. De Panfilis, A. Filipponi, and A. Polian, "Pressure induced phase transitions in amorphous Ge", *Phys. Scr.*, **T115**, 381–383 (2005).
- [37] P. R. Levashov, K. V. Khishchenko, I. V. Lomonosov, and V. E. Fortov, "Database on shock-wave experiments and equations of state available via Internet", *AIP Conf. Proc.*, **706**, 87–90 (2004).
- [38] K. K. Maevskii, "Thermodynamic parameters of mixtures with silicon nitride under shock-wave loading", *Math. Montis.*, **45**, 52–59 (2019).

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