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Hamiltonian dynamics of boolean networks

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HAMILTONIAN DYNAMICS OF BOOLEAN NETWORKS*

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Abstract. This article examines the impact of Hamiltonian dynamics on the interaction graph of Boolean networks. Three types of dynamics are considered: maximum height, Hamiltonian cycle, and an intermediate dynamic between these two. The study addresses how these dynamics influence the connectivity of the graph and the existence of variables that depend on all other variables in the system. Additionally, a family of regulatory Boolean networks capable of describing these three Hamiltonian behaviors is introduced, highlighting their specific properties and limitations. The results provide theoretical tools for modeling complex systems and contribute to the understanding of dynamic interactions in Boolean networks.

Key words. Boolean networks, Hamiltonian dynamics, self-dual networks, regulatory networks.

MSC codes. 68-XX, 93-XX

1. Introduction.

Boolean networks are a widely used mathematical model for representing complex systems composed of variables, where each variables can assume one of two possible states: 0 or 1. These networks have proven to be valuable tools in various fields such as biology [21], genetics [10, 13, 20], and social network theory [9], among others. By reducing problems to a binary context, Boolean networks enable the modeling, simulation, and analysis of nonlinear interactions, as well as the study of the dynamic behavior of systems with multiple interdependent variables.

A significant portion of existing studies has focused on specific complex systems, emphasizing the interaction between variables to infer dynamic properties. Notable examples include the analysis of interaction graphs with bounded in-degree and their implications on dynamics [2], the existence of fixed points [1, 3], limit cycles [8, 16], and the determination of the maximum length of limit cycles in certain families of Boolean networks [4, 12].

However, most of these works rely on restrictions imposed on the interaction graph to infer dynamic properties, leaving the study of conditions induced in the interaction graph by a given dynamic largely unexplored.

The primary objective of this paper is to analyze the properties induced by Hamiltonian dynamics [23], characterized by a unique trajectory capable of visiting all states of the system. This analysis includes cases of maximum height, maximum limit cycle length, and dynamics intermediate to the two aforementioned cases.

Additionally, we address the problem: given a Hamiltonian digraph G_Γ, is it possible to construct a regulatory Boolean network whose dynamics is isomorphic to G_Γ? To understand this question, we explore certain families of Boolean networks capable of exhibiting Hamiltonian cycle behaviors in neural networks [17, 14] and their implications for self-dual networks. From this, we present a family of Hamiltonian regulatory Boolean networks, self-dual and non-neural.

This document is organized as follows: section 2 introduces the fundamental def-

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initions and notations. section 3 focuses on the analysis of maximum in-degree and connectivity in interaction graphs. In section 4, a family of Hamiltonian regulatory Boolean networks is introduced, and finally, section 5 presents the conclusions, discussing the obtained results and future work.

2. Definitions and notation. A directed graph $G = (V, A)$, where V is the set of vertices and A is the set of arcs. The in-degree of a vertex $j \in V$ is denoted as $d^-_G(j)$, and when there is no ambiguity, the subscript G is omitted. A directed graph is said to have a **source component** if it is a component with no incoming arcs from other components of the graph, while a **sink component** is a component with no outgoing arcs to other components. Finally, two components are considered **independent** if there is no directed path between them in G. For a more detailed description of graph-related concepts, we recommend consulting [5, 22].

A **Boolean network** $f : \{0,1\}^n \to \{0,1\}^n$, where $n \in \mathbb{N}$, is a dynamic system defined in discrete time and space, consisting of n binary variables x_j, with $j \in [n] := \{1, 2, \ldots, n\}$. The network is described by Boolean functions $f = (f_1, f_2, \ldots, f_n)$, called **local activation functions**, where $x_j(t + 1) = f_j(x(t))$ determines the temporal evolution of each variable.

The temporal evolution of the system is represented by a directed graph called the **state transition graph** or **dynamics** of f, defined as follows:

$$\Gamma(f) = (\{0,1\}^n, \{(x, f(x)) : x \in \{0,1\}^n\}).$$

Since f is a function, each vertex has an out-degree of one. We denote by $\mathcal{G}(n)$ the family of digraphs isomorphic to the dynamics of a Boolean network with n variables, described as follows:

$$\mathcal{G}(n) = \{(V, A) \text{ digraph} : |V| = 2^n \text{ and for all } u \in V,\ d^+(u) = 1\}.$$

The study of graphs $G_\Gamma \in \mathcal{G}(n)$ aims to identify properties common to all Boolean networks with the dynamic behavior G_Γ. The set of Boolean networks whose dynamics are isomorphic to G_Γ is denoted by $\mathcal{F}(G_\Gamma)$:

$$\mathcal{F}(G_\Gamma) = \{f : f \text{ is a Boolean network and } \Gamma(f) \cong G_\Gamma\}.$$

We focus on digraphs $G_\Gamma \in \mathcal{G}(n)$ that possess a directed path capable of visiting all their vertices, with the goal of analyzing the properties of the family of Boolean networks $\mathcal{F}(G_\Gamma)$.

The configurations $\vec{0}, \vec{1}, e_i \in \{0,1\}^n$ are defined as those with all zeros, all ones, and all zeros except for a one in component $i \in [n]$, respectively. Additionally, $\oplus$ denotes the modulo two sum operator, generalized to configurations in $\{0,1\}^n$ by applying the operator component-wise.

For a Boolean network f with n variables and a configuration $x \in \{0,1\}^n$, the following terms are defined: A **Garden of Eden** is a configuration x such that $f^{-1}(\{x\}) = \emptyset$. A configuration x is a **fixed point** if $f(x) = x$, and it is **periodic** if there exists $k \in \mathbb{N}$ such that $f^k(x) = x$. Otherwise, x is called **transient**. A **limit cycle** is a cycle in $\Gamma(f)$ of length at least two, and an **attractor** of the network is any fixed point or limit cycle.

Moreover, the **period** of f, denoted as $p(f)$, is the least common multiple of the lengths of all its limit cycles. The **height** of f, denoted as $h(f)$, is the smallest $k \in \mathbb{N}$ such that, for any $x \in \{0,1\}^n$, $f^k(x)$ is a periodic point. Finally, a **trajectory** R of

f is a path in $\Gamma(f)$ that does not repeat arcs, and $|R|$ is the length of the trajectory, corresponding to the number of arcs.

We say that the local activation function f_j depends on the variable x_i, or on the index i, if there exists a configuration $x \in \{0,1\}^n$ such that $f_j(x) \neq f_j(x \oplus e_i)$. The **interaction graph** or **dependency graph** of the Boolean network f, denoted by $G(f)$, is a directed graph with n vertices representing the network variables, where an edge (i,j) indicates that f_j depends on x_i.

Additionally, the **local interaction graph** at z, denoted by $G_z(f)$, is a subgraph of $G(f)$ restricted to dependencies on a specific configuration $z \in \{0,1\}^n$. The interaction and local interaction graphs are formally defined as:

$$G(f) = ([n], \{(i,j) \in [n] \times [n] : f_j \text{ depends on the variable } x_i\})$$
$$G_z(f) = ([n], \{(i,j) \in [n] \times [n] : f_j(z) \neq f_j(z \oplus e_i)\})$$

A source component isolates a set of variables whose dynamics can be analyzed independently of the rest of the network. Let f be a Boolean network of n variables, $x \in \{0,1\}^n$, and $I \subsetneq [n]$ a set inducing a source component in $G(f)$. The configuration $x_I \in \{0,1\}^{|I|}$ is defined as the projection of x onto the components indexed by I, while $\overline{x}^I \in \{0,1\}^n$ is the negation of x on the components indexed by I. Finally, the **subnetwork of** f induced by I is the Boolean network $f_I : \{0,1\}^{|I|} \to \{0,1\}^{|I|}$, defined as $f_I(x) = f(x,y)_I$, for any $y \in \{0,1\}^{n-|I|}$.

EXAMPLE 2.1. *Let f be the Boolean network of 3 variables described by the local activation functions and the network dynamics presented in Figure 1.*

$$f_1(x) = (x_1 \wedge \overline{x}_2 \wedge \overline{x}_3) \vee (x_1 \wedge x_2 \wedge x_3)$$
$$f_2(x) = (x_1 \wedge x_3) \vee (\overline{x}_2 \wedge x_3) \vee (x_1 \wedge \overline{x}_2)$$
$$f_3(x) = x_3$$

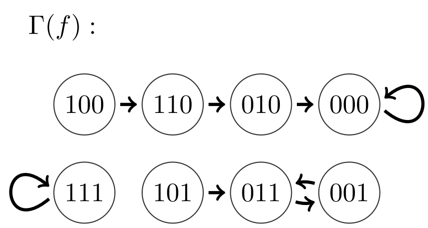

Fig. 1: Local activation functions and dynamics of the Boolean network f from Example 2.1.

In this case, the configurations $(1,0,0)$ and $(1,0,1)$ are Garden of Eden states, while $(0,0,0)$ and $(1,1,1)$ are fixed points. The network's limit cycle is $[(0,1,1), (0,0,1)]$, with a period $p(f) = 2$ and a height $h(f) = 3$.

Note that f_1 and f_2 depend on all variables. On the other hand, (2.1) shows that the local activation function f_3 depends only on variable x_3, since for any other index $i \neq 3$, $f_3(x) = f_3(x \oplus e_i)$ holds.

$$f_3(1,1,1) \neq f_3((1,1,1) \oplus e_3) \tag{2.1}$$

The interaction graph $G(f)$ along with $G_{(1,1,0)}(f)$ is shown in Figure 2.

DEFINITION 2.1. *For $x, y \in \{0,1\}^n$, we define $x \leq y$ if, for every component, $x_i \leq y_i$ holds. Given f, a Boolean network with $n \in \mathbb{N}$ variables, the local activation function f_j is said to be:*

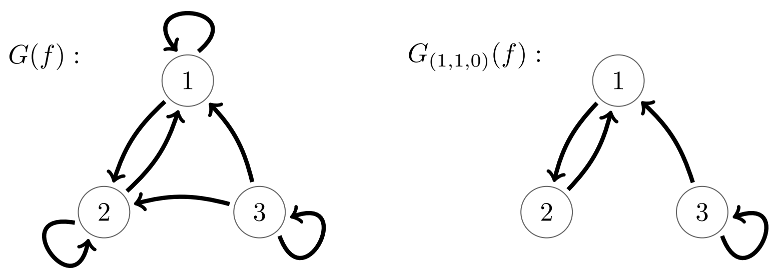

Fig. 2: Interaction graph and local interaction graph at $(1,1,0)$ for f in Example 2.1.

- ***Increasing in component*** *$i \in [n]$, if for any configuration x such that $x_i = 0$, it holds that $f_j(x) \leq f_j(x \oplus e_i)$.*
- ***Decreasing in component*** *$i \in [n]$, if for any configuration x such that $x_i = 0$, it holds that $f_j(x) \geq f_j(x \oplus e_i)$.*

*Additionally, f_j is called **unate** if it is either increasing or decreasing in each of its components $i \in [n]$. The network is said to be **regulatory** if all its local activation functions are unate. Furthermore, the network is said to be **monotone** if all its local activation functions are increasing in each of its components $i \in [n]$.*

The arcs of the interaction graph of a regulatory Boolean network can be labeled with **signs** $\sigma(i,j) \in \{+1,-1\}$, which indicate the nature of the relationship between the variables. A positive sign $(+1)$ implies that f_j is increasing with respect to x_i, while a negative sign (-1) indicates that f_j is decreasing with respect to x_i.

DEFINITION 2.2. *A Boolean network f is said to be **Hamiltonian** if its dynamics possess a trajectory that reaches all configurations. A Hamiltonian Boolean network f is classified as **maximum height** if its only attractor is a fixed point; **intermediate height** if its only attractor is a limit cycle of length $k \in \{2,3,\ldots,2^n-1\}$; or a **Hamiltonian cycle** if its dynamics form a limit cycle of length 2^n. Similarly, a digraph $G_\Gamma \in \mathcal{G}(n)$ is classified as Hamiltonian of maximum height, intermediate height, or Hamiltonian cycle if $G_\Gamma \cong \Gamma(f)$ and f belongs to the corresponding classification.*

EXAMPLE 2.2. *Let $f = (f_1, f_2, f_3)$ be a Boolean network with local activation functions and the interaction graph described in Figure 3. The Boolean network is Hamiltonian of maximum height, and its dynamics are shown in Figure 4.*

EXAMPLE 2.3. *Given the Boolean network $f = (f_1, f_2, f_3)$ defined in Figure 5, along with its interaction graph, we observe that the network is Hamiltonian of intermediate height, as reflected in its dynamics described in Figure 6.*

$$f_1(x) = x_3$$
$$f_2(x) = \overline{x}_1 \vee (x_1 \wedge x_2 \wedge \overline{x}_3)$$
$$f_3(x) = (x_2 \wedge x_3) \vee (\overline{x}_2 \wedge \overline{x}_3)$$

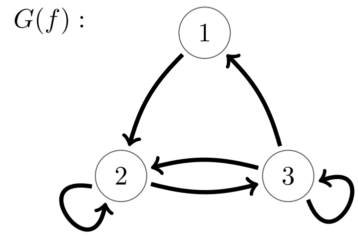

Fig. 3: Local activation functions and interaction graph of f from Example 2.2.

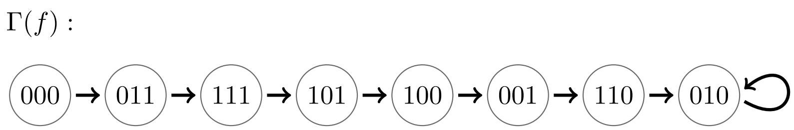

Fig. 4: Hamiltonian dynamics of maximum height from Example 2.2.

$$f_1(x) = \overline{x}_1$$
$$f_2(x) = (\overline{x}_2 \wedge x_3) \vee (\overline{x}_1 \wedge x_3) \vee (x_1 \wedge x_2)$$
$$f_3(x) = \overline{x}_2$$

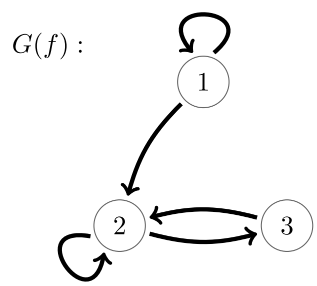

Fig. 5: Local activation functions and interaction graph of f from Example 2.3.

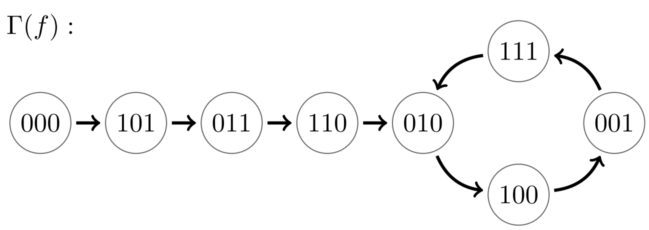

Fig. 6: Intermediate height Hamiltonian dynamics of Example 2.3.

EXAMPLE 2.4. *Given $f = (f_1, f_2, f_3)$, described by the local activation functions and the interaction graph shown in Figure 7, note that f is Hamiltonian with a cycle since its dynamics form a cycle of length 2^3, as depicted in Figure 8.*

$$f_1(x) = \overline{x}_1$$
$$f_2(x) = (\overline{x}_2 \wedge x_3) \vee (\overline{x}_1 \wedge x_3) \vee (x_1 \wedge x_2 \wedge \overline{x}_3)$$
$$f_3(x) = \overline{x}_2$$

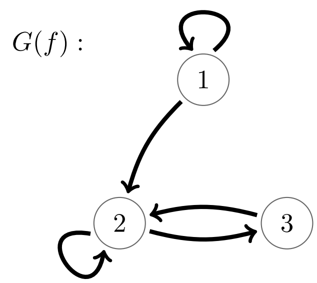

Fig. 7: Local activation functions and interaction graph of f from Example 2.4.

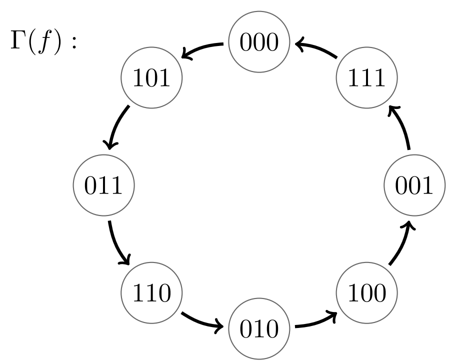

Fig. 8: Hamiltonian cycle dynamics of Example 2.4.

Our objective is on the properties of a Boolean network with Hamiltonian dynamic. Next, we define a partition of the configuration space to identify patterns in the variable behavior that will be useful in the following results.

DEFINITION 2.3 ([7]). *Given f, a Boolean network with n variables, and $j \in [n]$, the set $T(f_j) \subseteq \{0,1\}^n$ is defined as the set of true points, and $F(f_j) \subseteq \{0,1\}^n$ as the set of false points of f_j. These sets are defined as follows:*

$$T(f_j) = \{x \in \{0,1\}^n : f_j(x) = 1\} \tag{2.2}$$

$$F(f_j) = \{x \in \{0,1\}^n : f_j(x) = 0\} \tag{2.3}$$

*If, for every $j \in [n]$, it holds that $|T(f_j)| = |F(f_j)| = 2^{n-1}$, the Boolean network f is said to be **balanced**.*

The sets of true and false points establish a partition of $\{0,1\}^n$, implying that for any $j \in [n]$, $|T(f_j)| + |F(f_j)| = 2^n$ holds. Henceforth, results concerning the set T will also apply to the set of false points F.

3. In-degree and connectivity of the interaction graph. In [6], it is established that any digraph $G_\Gamma \in \mathcal{G}(n)$, other than the constant and identity digraphs, admits a Boolean network $f \in \mathcal{F}(G_\Gamma)$ with interaction graph K_n, a complete digraph including loops. However, it does not analyze whether the existence of a digraph G_Γ imposes common properties on all networks with dynamics isomorphic to G_Γ. To address this question, Lemma 3.1 establishes a necessary condition on the in-degree of the interaction graph, linking Boolean networks with their dynamic behavior.

LEMMA 3.1 ([19], [23]). *Let f be a Boolean network with $n \in \mathbb{N}$ variables and $j \in [n]$ such that $|T(f_j)|$ is odd. Then, the in-degree of vertex j in the interaction graph is n.*

Proof. Suppose $|T(f_j)|$ is odd and that f_j does not depend on the index $i \in [n]$. From the definition of dependence, it follows that for any configuration $x \in T(f_j)$, $x \oplus e_i \in T(f_j)$. This contradicts the hypothesis that $|T(f_j)|$ is odd, completing the proof. □

It is important to note that the converse implication of Lemma 3.1 is not true: in Example 2.4, $T(f_2)$ is a set of even cardinality, although variable 2 has maximum in-degree. On the other hand, if $G_\Gamma \in \mathcal{G}(n)$ has a unique vertex with in-degree zero, the associated dynamics differ in exactly one image compared to a bijective behavior, motivating Theorem 3.2.

THEOREM 3.2. *If $G_\Gamma \in \mathcal{G}(n)$ (not necessarily connected) has exactly one vertex with in-degree zero, then for any Boolean network $f \in \mathcal{F}(G_\Gamma)$, there exists a component $j \in [n]$ such that $d^-(j) = n$ in its interaction graph.*

Proof. Suppose G_Γ has exactly one vertex with in-degree zero. By definition, the out-degree of every vertex in G_Γ is one. Consequently, $2^n - 2$ vertices have in-degree one, one vertex has in-degree zero, and one vertex has in-degree two.

For an arbitrary Boolean network $f \in \mathcal{F}(G_\Gamma)$, denote $u, v \in \{0,1\}^n$ as the Garden of Eden and the configuration with two preimages, respectively. Since these are distinct configurations, there exists a component $j \in [n]$ such that $u_j \neq v_j$. Let us analyze the cases based on the value of component j of u.

- If $u_j = 1$, given that the dynamics have $2^n - 2$ configurations with exactly one preimage and $v_j = \overline{u_j} = 0$, it follows that $|T(f_j)| = 2^{n-1} - 1$, which is odd.
- If $u_j = 0$, it follows that $|T(f_j)| = 2^{n-1} + 1$, which is also odd.

In both cases, $T(f_j)$ has odd cardinality, and by Lemma 3.1, it is concluded that for any Boolean network $f \in \mathcal{F}(G_\Gamma)$, there exists a vertex $j \in [n]$ with in-degree $d^-(j) = n$ in $G(f)$. □

Theorem 3.2 provides a sufficient condition to guarantee the existence of a variable with in-degree n in $G(f)$ for Hamiltonian Boolean networks of maximum and intermediate height. However, this result does not apply to Hamiltonian cycle Boolean networks, as there exists a counterexample where no variable reaches this degree communicated by Florian Bridoux.

The proof of the theorem allows the identification of variables with in-degree n, using the labels assigned to both the Garden of Eden and the configuration with an odd number of preimages.

COROLLARY 3.3. *Every Boolean network whose dynamics possess a unique Garden of Eden has a connected interaction graph. Moreover, if the Garden of Eden and the configuration with an odd number of preimages are negated configurations of each* *other, then* $G(f) = K_n$.

Proof. Follows directly from Theorem 3.2. ∎

In Hamiltonian Boolean networks, there is a relationship between global dynamics and the type of induced subnetworks. In particular, this relationship extends to any $G_\Gamma \in \mathcal{G}(n)$ that possesses a sufficiently long trajectory.

LEMMA 3.4. *Let f be a Boolean network with $n \geq 2$ variables, and let $I \subsetneq [n]$ be a set that induces a subnetwork of f. If the network has a trajectory in its dynamics of length greater than $2^n - 2^{n-|I|}$, then f_I is Hamiltonian cycle.*

Proof. Let P be a trajectory in $\Gamma(f)$ of length greater than $2^n - 2^{n-|I|}$, and let $z \in \{0,1\}^n$ be the initial configuration of the trajectory. Let $k \in \mathbb{N}$ be the smallest value such that $(f_I)^k(z_I) = z_I$. We can prove that $k = 2^{|I|}$. Since P does not repeat internal vertices and z_I can appear at most $2^{n-|I|}$ times in the trajectory, the length of P is bounded as described in (3.1):

$$2^n - 2^{n-|I|} < |P| < k \cdot 2^{n-|I|}. \tag{3.1}$$

Since $2^n - 2^{n-|I|} = (2^{|I|} - 1) \cdot 2^{n-|I|}$, it follows that $k > 2^{|I|} - 1$, implying that f_I is Hamiltonian cycle. ∎

We name the **quasi-Hamiltonian** Boolean networks, whose dynamics consist of a cycle of length $2^n - 1$ and a fixed point. Although this network is neither strictly Hamiltonian nor connected, it satisfies Lemma 3.4 and is of theoretical interest for being modelable with a bounded interaction graph [2].

COROLLARY 3.5. *Let f be a Hamiltonian or quasi-Hamiltonian Boolean network with $n \geq 2$ variables, and let $I \subsetneq [n]$ be a set that induces a subnetwork of f. Then f_I is Hamiltonian cycle.*

Proof. Follows directly from Lemma 3.4. ∎

Lemma 3.4 strengthens the connection between the dynamics digraph and the resulting interaction graph, highlighting how the global properties of a network influence the characteristics of its induced subnetworks. Next, we explore how these properties affect the connectivity of the interaction graph in Hamiltonian Boolean networks.

PROPOSITION 3.6. *If G_Γ is a Hamiltonian cycle, then for any $f \in \mathcal{F}(G_\Gamma)$, $G(f)$ is guaranteed to be connected.*

Proof. Suppose G_Γ is a Hamiltonian cycle, and consider $f \in \mathcal{F}(G_\Gamma)$. By contradiction, assume $G(f)$ is not connected. This implies that $G(f)$ has $k \geq 2$ connected components, denoted as $G(f)[S_1], G(f)[S_2], \ldots, G(f)[S_k]$, with $S_i \subsetneq [n]$ for $i \in \{1, 2, \ldots, k\}$. Since $G(f)[S_i]$ has no incoming or outgoing edges to other components, by Lemma 3.4, each subnetwork induced by S_i is a Hamiltonian cycle.

Let $d \in \mathbb{N}$ denote the least common multiple described in (3.2). Since f_{S_i} is a Hamiltonian cycle, its period $p(f_{S_i})$ is a power of two, and the least common multiple of these periods corresponds to the largest of these powers:

$$d = \operatorname{lcm}\{p(f_{S_i}) : i \in \{1, 2, \ldots, k\}\} \tag{3.2}$$
$$= \max\{2^{|S_i|} : i \in \{1, 2, \ldots, k\}\}. \tag{3.3}$$

Since $|S_i| < n$, it follows that $d < 2^n$. For an arbitrary configuration $x \in \{0,1\}^n$, note that $(f_{S_i})^d(x_{S_i}) = x_{S_i}$ for all $i \in \{1, 2, \ldots, k\}$. This implies that the period

$p(f) \leq d < 2^n$, contradicting the assumption that f is a Hamiltonian cycle. Thus, for any $f \in \mathcal{F}(G_\Gamma)$, the digraph $G(f)$ must be connected. ◻

Example 2.3 and 2.4 present Hamiltonian cycle and intermediate height Boolean networks with interaction graphs that are not strongly connected. In contrast, for maximum height, intermediate height, and quasi-Hamiltonian dynamics, the lenght of the attractor plays a crucial role in variable dependence, leading to greater interaction graph connectivity as shown in the following proposition.

Proposition 3.7. *Let f be a Hamiltonian Boolean network of maximum height, quasi-Hamiltonian, or intermediate height, with $p(f)$ being odd. Then $G(f)$ is strongly connected.*

Proof. Let f be a Hamiltonian Boolean network of maximum height. By Corollary 3.3, the digraph $G(f)$ is connected. By contradiction, assume $G(f)$ is not strongly connected. Denote $G(f)[I]$ as a source component of $G(f)$ induced by $I \subsetneq V(G(f))$. By Lemma 3.4, f_I is a Hamiltonian cycle with period $p(f_I) = 2^{|I|}$, which contradicts the existence of a fixed point in f's dynamics, thus proving that $G(f)$ is strongly connected.

Now, consider f as a quasi-Hamiltonian or intermediate height network with an odd period. By contradiction, assume $G(f)$ is not strongly connected, and let $I \subsetneq [n]$ be the set inducing a source component in $G(f)$. Then, f_I is a Hamiltonian cycle by Lemma 3.4.

Let $y \in \{0,1\}^n$ be an arbitrary configuration. For all $a \in \mathbb{N}$, it holds that $(f_I)^{a \cdot p(f_I)}(y_I) = y_I$. For any periodic configuration $x \in \{0,1\}^n$ of f, it follows that $x = f^{p(f)}(x)$. Projecting onto the components in I gives (3.4):

$$x_I = f^{p(f)}(x)_I = (f_I)^{p(f)}(x_I). \tag{3.4}$$

The equality implies that $p(f)$ is a multiple of $p(f_I)$. However, since $p(f_I) = 2^{|I|}$, $p(f)$ must be even. This contradicts the assumption that $p(f)$ is odd, proving that $G(f)$ is strongly connected. ◻

Hamiltonian Boolean networks satisfy $p(f) + h(f) = 2^n$, which allows Proposition 3.7 to be reformulated in terms of height. On the other hand, if $G(f)$ is not strongly connected, then Hamiltonian cycle and intermediate height dynamics induce an ordering among the components. This highlights the absence of independent components in the interaction graph and limits the number of source and sink components.

Definition 3.8. *A digraph is **unilaterally connected** if, for every pair of vertices, there exists at least one directed path between them.*

It is straightforward to observe that a digraph is unilaterally connected if and only if it has no independent components. This fact is fundamental to the proof of Theorem 3.9, which establishes the connection between Hamiltonian dynamics and the structure of the interaction graph.

Theorem 3.9. *Let f be a Boolean network with Hamiltonian cycle or intermediate height dynamics. The interaction graph of f is unilaterally connected.*

Proof. Assume, by contradiction, that f has an interaction graph that is not unilaterally connected. Then, there exist two vertices in $G(f)$ with no directed path between them, implying they belong to independent components induced by $A, B \subsetneq [n]$.

Let $M \subsetneq [n]$ be a set inducing a subnetwork of f that has edges directed to vertices in A and B in $G(f)$ but not the other way around. This implies that $M \cup A$, $M \cup B$, and $M \cup A \cup B =: D$ induce Hamiltonian cycle subnetworks due to Corollary 3.5.

Denote $g = f_D$ and let $s = \max\{p(f_{M\cup A}), p(f_{M\cup B})\} < 2^{|D|}$. Since $p(f_{M\cup A})$ and $p(f_{M\cup B})$ are multiples of a power of two, for any configuration $x \in \{0,1\}^{|D|}$, it holds:

$$g^s(x) = (g^s(x)_A, (g_{M\cup B})^s(x_{M\cup B})) = (g^s(x)_A, x_{M\cup B}) = (g^s(x)_A, x_M, x_B), \tag{3.5}$$

$$g^s(x) = ((g_{M\cup A})^s(x_{M\cup A}), g^s(x)_B) = (x_{M\cup A}, g^s(x)_B) = (x_A, x_M, g^s(x)_B). \tag{3.6}$$

Equating (3.5) and (3.6), we obtain $g^s(x) = x$, implying that the period of g is less than $2^{|D|}$. This contradicts the assumption that g is a Hamiltonian cycle, proving that $G(f)$ is unilaterally connected. □

Theorem 3.9 implies several relevant results. In particular, it establishes that the interaction graph has at most one source component and one sink component, guarantees that any pair of components is connected by a directed path, and ensures that the component graph of $G(f)$ contains a Hamiltonian path. It is conjectured that if f has Hamiltonian cycle or intermediate height dynamics, the components of $G(f)$ form a topological ordering with all possible edges between them.

4. Regulatory family of Hamiltonian Boolean networks. Since not all families of Boolean networks can exhibit Hamiltonian behaviors, this section focuses on the construction of Hamiltonian-type regulatory Boolean networks.

From the literature, it is known that monotone networks without constant local activation functions have at least two fixed points: $\vec{0}$ and $\vec{1}$. Additionally, the length of their limit cycles $|C| \in \mathbb{N}$ cannot reach 2^n, as it is upper-bounded by the number of incomparable vectors with n components [4, 18]. This bound is presented in (4.1):

$$|C| \leq \binom{n}{\lfloor \frac{n}{2} \rfloor} < 2^n. \tag{4.1}$$

On the other hand, conjunctive and disjunctive networks have a height upper-bounded by $h(f) \leq 2n^2 - 3n + 2$ [11]. If the interaction graph is strongly connected, these networks also have at least two fixed points. Additionally, Hamiltonian cycle Boolean networks are balanced in each of their local activation functions, a property not satisfied by certain types of networks, such as conjunctive, disjunctive, or canalizing networks with more than one variable.

In contrast, [17] states that Hamiltonian cycle Boolean networks can be modeled using neural networks, a subfamily of regulatory Boolean networks, and demonstrates that self-duality is a necessary condition to describe bijective behaviors. Along these lines, we will prove the existence of regulatory, non-neural Boolean networks that describe Hamiltonian dynamics of maximum height, intermediate height, and Hamiltonian cycle.

4.1. Self-dual Boolean networks. In this section, we explore self-duality, formally described in Definition 4.1. It is conjectured that self-duality constitutes a necessary condition for a Hamiltonian cycle Boolean network to be regulatory, derived from the properties it induces and empirical results in the literature [15].

DEFINITION 4.1. *A Boolean network f with $n \in \mathbb{N}$ variables is said to be* ***self-dual*** *in $I \subseteq [n]$, with $I \neq \emptyset$, if for any configuration $x \in \{0,1\}^n$, it holds that $f(x) = \overline{f(\overline{x}^I)}^I$.*

LEMMA 4.2. *Let $I \subseteq [n]$ be non-empty. The Boolean network f is self-dual in I if and only if, for any $x \in \{0,1\}^n$ and $k \in \mathbb{N}$, it holds that:*

$$f^k(x) = \overline{f^k(\overline{x}^I)}^I.$$

Proof. Let f be self-dual in I. As shown in (4.2), applying the definition of self-duality twice proves the case $k = 2$.

$$f^2(x) = f(f(x)) = f(\overline{f(\overline{x}^I)}^I) = \overline{f(f(\overline{x}^I))}^I = \overline{f^2(\overline{x}^I)}^I. \tag{4.2}$$

Proceed by induction on $k \in \mathbb{N}$. Suppose that for all $x \in \{0,1\}^n$, $f^k(x) = \overline{f^k(\overline{x}^I)}^I$. We prove the case for $k+1$:

$$f^{k+1}(x) = f(f^k(x)) = f(\overline{f^k(\overline{x}^I)}^I) = \overline{f(f^k(\overline{x}^I))}^I = \overline{f^{k+1}(\overline{x}^I)}^I. \tag{4.3}$$

For the reverse implication, consider $k = 1$, which corresponds to the definition of self-duality. Thus, the property holds for all $k \in \mathbb{N}$, completing the proof. ◻

A notable result is the relationship between self-duality and the distance between configurations in a Hamiltonian cycle dynamic. This is formally established in the following lemma.

LEMMA 4.3. *Let f be a Hamiltonian cycle Boolean network with $n \in \mathbb{N}$ variables and $I \subseteq [n]$, with $I \neq \emptyset$. The network f is self-dual in I if and only if, for any configuration $x \in \{0,1\}^n$, it holds that:*

$$f^{2^{n-1}}(x) = \overline{x}^I.$$

Proof. Suppose f is self-dual in I. By contradiction, assume there exists a configuration x such that $f^{2^{n-1}}(x) \neq \overline{x}^I$. Let $k < 2^{n-1}$ be the smallest value such that $f^k(x) = \overline{x}^I$. By Lemma 4.2, we deduce:

$$f^k(\overline{x}^I) = \overline{f^k(x)}^I = x. \tag{4.4}$$

This implies that the distance between $\overline{x}^I$ and x in the dynamics is k. However, this contradicts the fact that f has a cycle of length 2^n. Therefore, for any $x \in \{0,1\}^n$, it holds that $f^{2^{n-1}}(x) = \overline{x}^I$.

For the converse, if every configuration $x \in \{0,1\}^n$ satisfies $f^{2^{n-1}}(x) = \overline{x}^I$, the bijectivity of the network allows us to take $x = f(y)$, yielding $f(\overline{y}^I) = \overline{f(y)}^I$, which is equivalent to the definition of self-duality. ◻

A relevant result for our study is associated with local dependency. In the case where a configuration $x \in \{0,1\}^n$ induces an edge in $G_x(f)$, we can prove that such dependency is also induced by $\overline{x}$.

LEMMA 4.4. *Any self-dual Boolean network f in $[n]$ satisfies, for every $x \in \{0,1\}^n$, the equality:*

$$(G_x(f), \sigma_f) = (G_{\overline{x}}(f), \sigma_f).$$

Proof. Let $i, j \in [n]$ be arbitrary, and suppose that the edge (i, j) belongs to the digraph $G_x(f)$. By the self-duality of f, the following chain of equivalences holds:

$$\begin{aligned}
(i,j) \in A(G_x(f)) &\Leftrightarrow (f_j(x) < f_j(x \oplus e_i)) \vee (f_j(x) > f_j(x \oplus e_i)) \\
&\Leftrightarrow (\overline{f_j(\overline{x})} < \overline{f_j(\overline{x \oplus e_i})}) \vee (\overline{f_j(\overline{x})} > \overline{f_j(\overline{x \oplus e_i})}) \\
&\Leftrightarrow (f_j(\overline{x}) > f_j(\overline{x} \oplus e_i)) \vee (f_j(\overline{x}) < f_j(\overline{x} \oplus e_i)) \\
&\Leftrightarrow (i,j) \in A(G_{\overline{x}}(f)).
\end{aligned}$$

Therefore, both local interaction graphs are equal, i.e., $G_x(f) = G_{\overline{x}}(f)$.

If $\sigma_x(i, j) \in \{+1, -1\}$, this label implies a value for x_i in the chain of equivalences, establishing an increasing or decreasing behavior of f_j with respect to index i. Evaluating at $\overline{x}$, the value in component j is inverted, and the inequalities switch from strictly greater to strictly lesser, and vice versa. Hence, $\sigma_x(i, j) = \sigma_{\overline{x}}(i, j)$. Consequently, we prove that $(G_x(f), \sigma_f) = (G_{\overline{x}}(f), \sigma_f)$, completing the proof. ∎

Self-duality in I for Hamiltonian cycle Boolean networks ensures maximum in-degree for such components. This is because self-duality guarantees that for arbitrary $x, \overline{x}^I \in \{0, 1\}^n$, one belongs to the set of true points and the other to the set of false points.

Definition 4.5. *Let f be a Boolean network with n variables, $i, j \in [n]$, and $a \in \{0, 1\}$. We denote $T(f_j, x_i = a) = \{x \in T(f_j) : x_i = a\}$ as a subset of the set of true points of f_j consisting of configurations such that x_i takes the value a. Similarly, $F(f_j, x_i = a) = \{x \in F(f_j) : x_i = a\}$ is defined for the set of false points.*

Theorem 4.6. *Let f be a Boolean network with $n \geq 3$ variables, $i, j \in [n]$, and suppose that the set of true points $T(f_j)$ is a multiple of four and non-empty. If there exists some $a \in \{0, 1\}$ such that $|T(f_j, x_i = a)|$ is odd, then f_j depends on all variables.*

Proof. First, let us prove that if the cardinalities of $T(f_j, x_i = 0)$ and $T(f_j, x_i = 1)$ differ, this implies that $i \in N^-(j)$. By contraposition, suppose that f_j does not depend on x_i. In this case, for any configuration $x \in T(f_j)$, it also holds that $x \oplus e_i \in T(f_j)$. However, this implies that the cardinalities of $T(f_j, x_i = 0)$ and $T(f_j, x_i = 1)$ are equal.

On the other hand, if there exists $a \in \{0, 1\}$ such that $|T(f_j, x_i = a)|$ is odd, we can prove that $N^-(j) \supseteq [n] \setminus \{i\}$. By contradiction, assume that there exists $k \in [n] \setminus \{i\}$ such that $k \notin N^-(j)$. This implies that for any configuration $x \in T(f_j, x_i = a)$, it also holds that $x \oplus e_k \in T(f_j, x_i = a)$, which contradicts the odd cardinality of $|T(f_j, x_i = a)|$.

Finally, since $|T(f_j)|$ is a multiple of four, the cardinalities of $T(f_j, x_i = 0)$ and $T(f_j, x_i = 1)$ must both be odd and different, as their sum must be a multiple of four. If these cardinalities were equal, their sum would be a multiple of two but not of four. This proves that $N^-(j) = [n]$, implying that f_j depends on all variables. ∎

Proposition 4.7. *If a Hamiltonian cycle Boolean network f with $n \in \mathbb{N} \setminus \{2\}$ variables is self-dual in $I \subseteq [n]$, then, for any $j \in I$, it holds that $d^-(j) = n$.*

Proof. Let $j \in I$ be arbitrary, and denote by P and Q the directed paths in $\Gamma(f)$ from $\vec{0} \in \{0, 1\}^n$ to the configuration $\vec{0} \oplus e_I \in \{0, 1\}^n$ and vice versa, respectively. From Lemma 4.3, we know that $\vec{0}$ and $\vec{0} \oplus e_I$ are at a distance of 2^{n-1}, implying that $|P| = |Q| = 2^{n-1}$. Moreover, since the network is a Hamiltonian cycle, these paths cover all edges in the dynamics.

The path P must contain at least one configuration $z \in T(f_j, x_j = 0)$ to transition the value of j from 0 to 1. In particular, if P contains $k \in \mathbb{N}$ configurations in $T(f_j, x_j = 0)$, then P contains exactly $k-1$ configurations $w \in F(f_j, x_j = 1)$, as these transitions are necessary for the change in the value of j along P.

If $w \in F(f_j, x_j = 1)$ is arbitrary, the self-duality of f implies that $f_j(w) \neq f_j(\overline{w}^I)$, which in turn establishes that $w \in F(f_j, x_j = 1)$ if and only if $\overline{w}^I \in T(f_j, x_j = 0)$. This means that $w \in F(f_j, x_j = 1)$ belongs to the trajectory P if and only if $\overline{w}^I \in T(f_j, x_j = 0)$ belongs to the trajectory Q.

Finally, the cardinality of $T(f_j, x_j = 0)$ is obtained as the sum of the configurations $z, \overline{w}^I \in T(f_j, x_j = 0)$, resulting in an odd quantity as described in (4.5).

$$|T(f_j, x_j = 0)| = k + (k-1) = 2k - 1. \tag{4.5}$$

Applying Theorem 4.6, it is concluded that the index $j \in I$ has in-degree n in $G(f)$, completing the proof. ∎

It is not difficult to observe that if the Hamiltonian cycle Boolean network is self-dual in $[n]$, by the previous result, its interaction graph is K_n.

4.2. Family of Hamiltonian cycle Boolean networks. Initially, let us analyze the case $n = 1, 2$. From Lemma 4.8, given f as a Hamiltonian cycle Boolean network described by a regulatory Boolean network, it has a unique interaction graph $G(f)$ with edges labeled with different signs. Figure 9 presents an example of such an interaction graph with signs and details how $f^{[2]}$ is constructed from the base case $f^{[1]} = (\overline{x}_1)$, a network of a single variable that is regulatory and has a Hamiltonian cycle.

LEMMA 4.8. *If f is a Hamiltonian cycle, regulatory Boolean network with $n = 2$ variables, then its interaction graph with signs $(G(f), \sigma_f)$ is a cycle without loops, with edges labeled as $\sigma_f(i,j) = +1$ and $\sigma_f(j,i) = -1$, where $i \neq j \in [2]$.*

Proof. An exhaustive analysis is carried out considering all possible configurations of a regulatory Hamiltonian cycle Boolean network with $n = 2$ variables. ∎

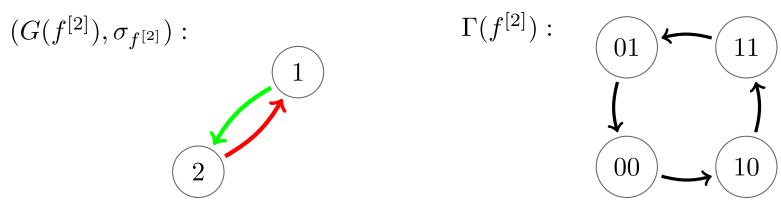

Fig. 9: Interaction graph with signs for $f^{[2]}(x_1, x_2) = (\overline{x}_2, x_1)$ and its dynamics.

To extend this construction to the case $n+1$, we use $f^{[n]}$ a Hamiltonian cycle Boolean network with n variables.

DEFINITION 4.9. *Let $f^{[1]} = (\overline{x}_1)$ be a Boolean network with a single variable. Recursively, networks $h^{[n+1]}, f^{[n+1]} : \{0,1\}^{n+1} \to \{0,1\}^{n+1}$ are constructed from $f^{[n]}$,*

$n \in \mathbb{N}$. *Specifically, if* $z^{[n+1]} =: z \in \{0,1\}^{n+1}$ *such that* $f^{[n]}(z_{[n]}) = \vec{0}$ *and* $z_{n+1} = 0$, *then:*

$$h^{[n+1]}(x) = (f^{[n]}(x_{[n]}), x_{n+1}),$$
$$f_i^{[n+1]}(x) = (h_i^{[n+1]}(x) \wedge d_{\overline{z}^{[n+1]}}(x)) \vee c_{z^{[n+1]}}(x)$$

where $i \in [n]$, *the Boolean functions* $c_z, d_{\overline{z}} : \{0,1\}^{n+1} \to \{0,1\}$ *are conjunctive and disjunctive clauses defined as* $c_z(z) = 1$, $d_{\overline{z}}(\overline{z}) = 0$, *and take the opposite value otherwise.*

Figure 10 shows $f^{[2]}(x_1, x_2) = (\overline{x}_2, x_1)$ and the associated auxiliary network $h^{[3]}(x_1, x_2, x_3) = (\overline{x}_2, x_1, x_3)$.

By modifying the auxiliary network, swapping the preimages of $\vec{0} \in \{0,1\}^{n+1}$ and $\vec{1} \in \{0,1\}^{n+1}$, a new Boolean network $f^{[n+1]}$ is constructed, which is a Hamiltonian cycle, regulatory, and self-dual in $[n+1]$. Figure 11 illustrates $f^{[3]}$, a self-dual Boolean network in [3] defined by swapping preimages in the auxiliary network $h^{[3]}$.

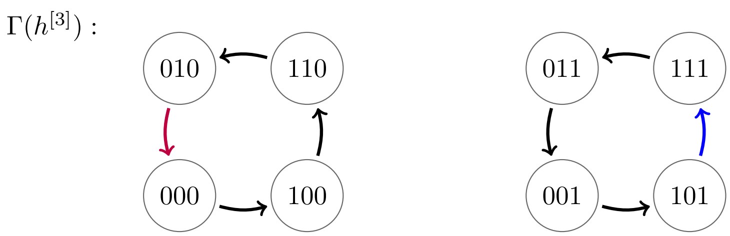

Fig. 10: Dynamics of $h^{[3]}(x_1, x_2, x_3) = (\overline{x}_2, x_1, x_3)$, the auxiliary network.

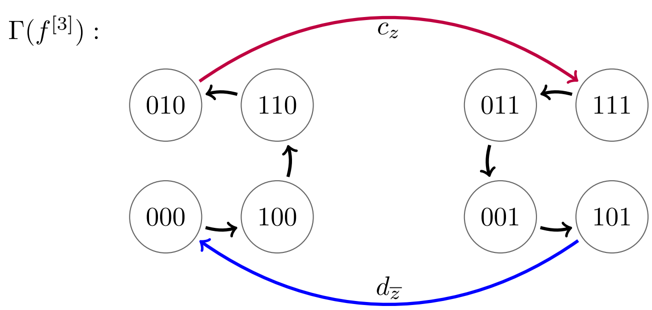

Fig. 11: Dynamics of the network $f^{[3]}$ constructed from the auxiliary network h in Figure 10.

Lemma 4.10. *For any* $n \in \mathbb{N}$, *the Boolean network* $f^{[n]}$ *is a Hamiltonian cycle and self-dual in* $[n]$.

Proof. **Base Case** $n = 1, 2, 3$: For $n = 1$, the network $f^{[1]} = (\overline{x}_1)$ is trivially a Hamiltonian cycle and self-dual in [1]. It is explicitly verified that $f^{[2]}$ and $f^{[3]}$ are

Hamiltonian cycles and self-dual in [2] and [3], respectively, according to the local activation functions:

$$
\begin{aligned}
f_1^{[2]}(x) &= \overline{x}_2, \\
f_2^{[2]}(x) &= x_1, \\
f_1^{[3]}(x) &= (\overline{x}_1 \wedge \overline{x}_2) \vee (\overline{x}_2 \wedge \overline{x}_3) \vee (\overline{x}_1 \wedge \overline{x}_3), \\
f_2^{[3]}(x) &= (x_1 \wedge x_2) \vee (x_1 \wedge \overline{x}_3) \vee (x_2 \wedge \overline{x}_3), \\
f_3^{[3]}(x) &= (\overline{x}_1 \wedge x_3) \vee (x_2 \wedge x_3) \vee (\overline{x}_1 \wedge x_2).
\end{aligned}
$$

Induction for $n \geq 3$: Assume that $f^{[n]}$ is a Hamiltonian cycle and self-dual in $[n]$, and prove that $f^{[n+1]}$ is as well.

Hamiltonian Cycle: Let $c_z, d_{\overline{z}}$ be the clauses defined for $f^{[n+1]}$. Note that:

$$f^{[n+1]}(z) = \vec{1}, \quad f^{[n+1]}(\overline{z}) = \vec{0}.$$

For $x \in \{0,1\}^{n+1} \setminus \{z, \overline{z}\}$, the network reduces to:

$$f^{[n+1]}(x) = (f^{[n]}(x_{[n]}), x_{n+1}). \tag{4.6}$$

Since $f^{[n]}$ is a Hamiltonian cycle, the configuration $\vec{0}_{[n]}$ reaches all configurations $u \in \{0,1\}^{n+1}$ with $u_{n+1} = 0$. Similarly, $\vec{1}_{[n]}$ reaches all configurations $v \in \{0,1\}^{n+1}$ with $v_{n+1} = 1$. Finally, since $f^{[n+1]}(z) = \vec{1}$ and $f^{[n+1]}(\overline{z}) = \vec{0}$, the dynamics are strongly connected, and $f^{[n+1]}$ is a Hamiltonian cycle.

Self-Duality: Let $x \in \{0,1\}^{n+1}$ be arbitrary. Using (4.6) and the inductive hypothesis, we prove self-duality in $[n+1]$:

$$
\begin{aligned}
f^{[n+1]}(x) &= (f^{[n]}(x_{[n]}), x_{n+1}), \\
&= \overline{(f^{[n]}(\overline{x}_{[n]}), \overline{x}_{n+1})}, \\
&= \overline{f^{[n+1]}(\overline{x})}.
\end{aligned}
$$

Hence, $f^{[n+1]}$ is a Hamiltonian cycle and self-dual in $[n+1]$. ∎

A distinctive feature of the networks in Definition 4.9 is that, except for $n = 2$, they always generate complete digraphs including loops. This result, derived from the self-dual structure of these networks, is formalized below.

COROLLARY 4.11. *Any Boolean network $f^{[n]}$ with $n \in \mathbb{N} \setminus \{2\}$ variables has a complete interaction graph K_n, including loops.*

Proof. For $n = 1$, the result is immediate, as $f^{[1]} = (\overline{x}_1)$.

For $n \geq 3$, Lemma 4.10 establishes that $f^{[n]}$ is self-dual in $[n]$. By Proposition 4.7, it is concluded that for all $j \in [n]$, the in-degree satisfies $d^-(j) = n$, implying $G(f^{[n]}) = K_n$. ∎

From this construction, certain properties justify the regulatory nature of the network. Describing $f_j^{[n]}$, with $j \in [n]$, as the concatenation of a conjunctive and a disjunctive clause of size $k \in \{j, j+1, \ldots, n\}$ over the variable x_j, it is possible to infer the value of $f_j^{[n]}$ when evaluated at an arbitrary configuration. This requires projecting the first k variables of the configuration to be evaluated. By a case analysis, given $z \in \{0,1\}^n$ such that $f^{[n]}(z) = \vec{1}$, the cases where there exist $i, j \in [n]$ satisfying the inequality $f_j^{[n]}(z) \neq f_j^{[n]}(z \oplus e_i)$ are summarized in Table 1.

	$i > j$		$i = j$		$i < j$	
	i even	i odd	i even	i odd	j even	j odd
n even	True	False	False	True	True	False
n odd	False	True	True	False	False	True

Table 1: Summary of the proposition: There exist $i, j \in [n]$ such that $f_j^{[n]}(z) \neq f_j^{[n]}(z \oplus e_i)$.

It is important to emphasize that, due to the definition of $f^{[n]}$, the conjunctive and disjunctive clauses of size n in $f_j^{[n]}$ dominate the rest of the local activation function. For instance, we know that for any $j \in [n]$, $f^{[n]}(z) = \vec{1}$. This holds because each local activation function contains a conjunctive clause c_z that fixes its value. Similarly, when evaluating $f^{[n]}$ at $\overline{z}$, each $f_j^{[n]}$ includes a disjunctive clause $d_{\overline{z}}$ that sets the value to zero when evaluated at $\overline{z}$. This behavior extends to clauses of sizes $k \in \{j, j+1, \ldots, n-1\}$ when not evaluated at $z, \overline{z}$, enabling characterization of these clauses. Following this direction, we generalize Table 1 to arbitrary configurations.

Definition 4.12. *Given $k \in \mathbb{N}$, the configuration $t_k \in \{0,1\}^k$ is defined as one that oscillates in its values by components, i.e., $t_k = (0, 1, 0, \ldots)$ or $t_k = (1, 0, 1, \ldots)$. For $x \in \{0,1\}^n$, $k_x \in \mathbb{N}$ denotes the largest value such that $x_{[k_x]} = t_{k_x}$.*

The recursive construction of $f^{[n]}$ incorporates clauses defined from the configuration $z^{[n]}$. The following result demonstrates that $z^{[n]} = t_k$, contributing to understanding the construction of $f^{[n]}$.

Lemma 4.13. *The configurations $z^{[n]}$ and $\overline{z}^{[n]}$ from Definition 4.9 are of type t_k and $\overline{t_k}$, respectively. This establishes conjunctive clauses c_{t_k} and disjunctive clauses $d_{\overline{t_k}}$ at each recursive step of the construction.*

Proof. For the base case $n = 2$, these clauses are induced from $z^{[2]} = (1, 0)$ and its negation. Assume by induction on $n \geq 2$ that for all $k \leq n$, $z^{[k]} = t_k$. By construction, the last component of any $z^{[k]}$ has value zero, and by the induction hypothesis $z^{[n]} = t_n = (t_{n-1}, 0)$. Given that $f^{[n+1]}(\overline{z}^{[n]}, 0) = \vec{1}$, it follows that $z^{[n+1]} = (\overline{z}^{[n]}, 0) = (\overline{t_n}, 0) = t_{n+1}$, completing the proof. ∎

From Lemma 4.13, the relationship between $z^{[i]}$ and $z^{[n]}$, $i \in [n]$, is established, along with understanding the indices such that $f_j(z \oplus e_i) = 1$. For an arbitrary configuration $x \in \{0,1\}^n$, note that the analysis pertains to $x_{[k_x]}$. The following result classifies these effects based on the relationship between the original configuration and its modification in component i, providing a tool for further analysis.

Lemma 4.14. *Given $f^{[n]}$ described in Definition 4.9, $i \in [n]$, and $x \in \{0,1\}^n$ arbitrary:*

1. *For all $i \in [n] \setminus \{j\}$ such that $k_x, k_{x \oplus e_i} < j$, it holds that $f_j^{[n]}(x) = f_j^{[n]}(x \oplus e_i)$*

2. *$k_x, k_{x \oplus e_i} < i$ if and only if $k_x = k_{x \oplus e_i}$*
3. *If $k_x = k_{x \oplus e_i}$, then for each $j \in [n] \setminus \{i\}$, it holds that $f_j^{[n]}(x) = f_j^{[n]}(x \oplus e_i)$*

Proof. (1) Suppose $k_x, k_{x \oplus e_i} < j$, noting that the conjunctive and disjunctive clauses in $f_j^{[n]}$ do not contribute to the evaluation of x and $x \oplus e_i$, as these clauses are of size j and above. Hence, the value of $f_j^{[n]}$ depends only on the variable x_j, implying:

$$f_j^{[n]}(x \oplus e_i) = (x \oplus e_i)_j = x_j = f_j^{[n]}(x).$$

(2.1) If $k_x, k_{x\oplus e_i} < i$, note that x and $x \oplus e_i$ differ only in component i. If $k_x \neq k_{x\oplus e_i}$, this implies there exists $j < i$ where x and $x \oplus e_i$ differ, leading to a contradiction. Thus, $k_x = k_{x\oplus e_i}$.

(2.2) Assume $k_x = k_{x\oplus e_i}$. If the change in component i of x does not alter the value of k_x, then $k_x, k_{x\oplus e_i} < i$, as desired.

(3) Let $k_x = k_{x\oplus e_i}$ and $j \in [n] \setminus \{i\}$.

If $j > k_x$, from (1) it follows that $f_j^{[n]}(x) = f_j^{[n]}(x \oplus e_i)$.

If $j \leq k_x$, the value of $f_j^{[n]}(x)$ is determined by x_j or the conjunctive and disjunctive clauses. By Lemma 4.13, these clauses are of type c_{t_k} and $d_{\overline{t_k}}$, with $k \geq j$. Since $k_x = k_{x\oplus e_i}$, it holds that $x_j = (x \oplus e_i)_j$, and thus the clauses of $f_j^{[n]}(x)$ and $f_j^{[n]}(x \oplus e_i)$ take the same values:

$$c_{t_k}(x) = c_{t_k}(x \oplus e_i), \quad d_{\overline{t_k}}(x) = d_{\overline{t_k}}(x \oplus e_i).$$

Therefore, $f_j^{[n]}(x) = f_j^{[n]}(x \oplus e_i)$. ∎

Lemma 4.14 is further refined considering the parity of n and the parity of the altered index in $x \in \{0,1\}^n$. Lemma 4.15 establishes how the conjunctive and disjunctive clauses interact with the size of the oscillating configuration $x_{[k_x]}$ for predicting the evaluation of the local activation function.

LEMMA 4.15. *For the Boolean network $f^{[n]}$, $j \in [n]$, and $x \in \{0,1\}^n$ such that $k_x \geq j$, it holds that:*

1. *Assuming n is even and $x_{[k_x]} = z^{[k_x]}$, or n is odd and $x_{[k_x]} = \overline{z}^{[k_x]}$, then $f_j^{[n]}(x \oplus e_p) = 0$ and $f_j^{[n]}(x \oplus e_q) = 1$.*
2. *Conversely, if n is odd and $x_{[k_x]} = z^{[k_x]}$, or n is even and $x_{[k_x]} = \overline{z}^{[k_x]}$, then $f_j^{[n]}(x \oplus e_p) = 1$ and $f_j^{[n]}(x \oplus e_q) = 0$.*

Where $p, q \in \{j+1, \ldots, k_x\}$ such that p is even and q is odd.

Proof. Let $i \in \{j+1, \ldots, k_x\}$ and note that the parity or oddness of $k_{x\oplus e_i} = i - 1$ depends on i. From the proof of Lemma 4.13, and denoting $z = z^{[n]}$, $f_j^{[n]}$ includes conjunctive clauses $c_{z_{[n]}}$, $c_{\overline{z}_{[n-1]}}$, $c_{z_{[n-2]}}$, alternating in negation up to index j. Similarly, the disjunctive clauses in $f_j^{[n]}$ alternate as $d_{\overline{z}_{[n]}}$, $d_{z_{[n-1]}}$, $d_{\overline{z}_{[n-2]}}$, also up to index j. Denoting $p, q \in \{j+1, \ldots, k_x\}$ as described in the statement:

(1) If n is even and $x_{[k_x]} = z_{[k_x]}$, this implies that $f_j^{[n]}(x \oplus e_p) = d_{z_{[p-1]}}(z) = 0$. This result follows since $(x \oplus e_p)_{[p-1]} = x_{[p-1]} = z_{[p-1]}$, and because n is even, the clause of size $p-1$ (odd) activated by evaluating $z_{[p-1]}$ corresponds to $d_{z_{[p-1]}}$. Similarly, for n odd and $x_{[k_x]} = \overline{z}_{[k_x]}$, we deduce that $f_j^{[n]}(x \oplus e_q) = c_{z_{[q-1]}}(z) = 1$.

(2) Since $f^{[n]}$ is self-dual in $[n]$, applying (1) yields the desired result. ∎

The results obtained are sufficient to demonstrate that the family of Boolean networks $f^{[n]}$ is regulatory.

THEOREM 4.16. *The Boolean network $f^{[n]}$ is regulatory.*

Proof. Suppose, by contradiction, that $f^{[n+1]}$ is not a regulatory Boolean network. Then, there exist $i, j \in [n]$, $x \in \{0,1\}^n \setminus \{z^{[n]}, z^{[n]} \oplus e_i\}$, such that $x_i = z_i^{[n]}$, and without loss of generality, satisfies (4.7) and (4.8).

$$f_j^{[n]}(z^{[n]}) > f_j^{[n]}(z^{[n]} \oplus e_i), \tag{4.7}$$

$$f_j^{[n]}(x) < f_j^{[n]}(x \oplus e_i). \tag{4.8}$$

Evaluating at $z^{[n]}$ is justified because, from Lemma 4.4, the local interaction graphs with signs for z and $\overline{z}$ coincide. Moreover, these are the only configurations with distinct images in the regulatory Boolean network $h = (f^{[n-1]}, x_n)$.

Note that the case $k_x, k_{x\oplus e_i} < i$ cannot occur, as it would contradict (4.8) by Lemma 4.14. Assuming n is even, we proceed with a case analysis on the relationship between i and j:

- **Case $i > j$:** From Table 1, it follows that i is even. Suppose $k_x > i$, so $k_{x\oplus e_i} = i - 1$, an odd value. However, Lemma 4.15 implies that $f_j^{[n]}(x \oplus e_i) = 0$, contradicting our assumption. Conversely, if $k_{x\oplus e_i} > i$, it follows that $k_x = i - 1$ (odd). Since $x_i = z_i^{[n]}$, the only possible case is $x_{[i-1]} = \overline{z}^{[i-1]}$, which returns 1 when evaluated in the network by Lemma 4.15. This contradicts (4.8), ruling out the case $i > j$.
- **Case $i = j$:** Since n is even, Table 1 implies that i is odd.

Suppose $k_x > i$ and note that $k_{x\oplus e_i} = i - 1$, an even value. However, since $i = j$, $k_{x\oplus e_i} < j$, implying that $f_j^{[n]}(x \oplus e_i) = (x \oplus e_j)_j = \overline{x}_j$ and $f_j^{[n]}(z^{[n]} \oplus e_i) = (z^{[n]} \oplus e_j)_j = \overline{z}_j^{[n]}$, values known to be equal because $x_i = z_i^{[n]}$. This contradicts (4.7) and (4.8).

Suppose $k_{x\oplus e_i} > i$, so $k_x = i - 1$, an even value. Since $i = j$, $k_x < j$, implying $f_j^{[n]}(x) = x_j$ and $f_j^{[n]}(z^{[n]}) = z_j^{[n]}$. These values are equal because $x_i = z_i^{[n]}$, contradicting (4.7) and (4.8). Therefore, the case $i = j$ is impossible.

- **Case $i < j$:** From Table 1, j is even. Since $k_{z^{[n]}\oplus e_i} = i-1 < j$, $f_j^{[n]}(z^{[n]} \oplus e_i) = z_j^{[n]}$. Furthermore, inequality (4.7) implies $z_j^{[n]} = 0$.

Analyzing j, Lemma 4.14 precludes the possibility of $k_x, k_{x\oplus e_i} < j$, as this would contradict (4.8).

If $k_x > j$, then $k_{x\oplus e_i} = i - 1 < j$, so $f_j^{[n]}(x \oplus e_i) = (x \oplus e_i)_j = x_j$, and from (4.8), $x_j = 1$. Since $x_i = z_i^{[n]}$, it follows that $x_{[k_x]} = z_{[k_x]}^{[n]}$, which contradicts $x_j \neq z_j^{[n]} = 0$.

Suppose $k_{x\oplus e_i} > j$, then $k_x = i - 1$. Since $x_i = z_i^{[n]}$, it follows that $x_{[i-1]} = \overline{z}_{[i-1]}^{[n]}$ and $(x \oplus e_i)_{[k_{x\oplus e_i}]} = \overline{z}_{[k_{x\oplus e_i}]}^{[n]}$. Noting that $i < j < k_{x\oplus e_i}$, $(x \oplus e_i)_j = x_j = \overline{z}_j^{[n]} = 1$, and since $k_x = i - 1 < j$, $f_j^{[n]}(x) = x_j = 0$, contradicting our assumption.

The case for n odd follows similarly to the even case. It is proven that $f_j^{[n]}$ is unate, and therefore, the network f is regulatory. □

A corollary extending this intermediate result between the auxiliary network $h^{[n]}$ and $f^{[n]}$ is presented below.

COROLLARY 4.17. *The Boolean networks $h^{[n]} \vee c_{z^{[n]}}$ and $h^{[n]} \wedge d_{\overline{z}^{[n]}}$, defined in (4.9) and (4.10) for all $j \in [n]$, are regulatory.*

$$(h^{[n]} \vee c_{z^{[n]}})_j(x) = (h_j^{[n]} \vee c_{z^{[n]}})(x) \tag{4.9}$$

$$(h^{[n]} \wedge d_{\overline{z}^{[n]}})_j(x) = (h_j^{[n]} \wedge d_{\overline{z}^{[n]}})(x) \tag{4.10}$$

Proof. To prove that $h^{[n]} \vee c_{z^{[n]}}$ is regulatory, we proceed analogously to the proof of Theorem 4.16. This is because the fact that $f^{[n+1]}(\overline{z}) = \vec{0}$ is not used.

For the network $h^{[n]} \wedge d_{\overline{z}^{[n]}}$, from Lemma 4.4, the local interaction graphs with signs satisfy:

$$(G_{\overline{z}}(h^{[n]} \wedge d_{\overline{z}^{[n]}}), \sigma_{g_1}) = (G_{\overline{z}}(f^{[n+1]}), \sigma_{g_2}) = (G_z(f^{[n+1]}), \sigma_{g_3}) = (G_z(h^{[n]} \vee c_{z^{[n]}}), \sigma_{g_4}),$$

Hence, $h^{[n]} \wedge d_{\overline{z}^{[n]}}$ is a regulatory network. ∎

4.3. General case of Hamiltonian Boolean networks.

Regulatory Boolean networks can model Hamiltonian behaviors because, from Corollary 4.17, we can manipulate the local activation functions to establish Hamiltonian dynamics of maximum and intermediate height.

THEOREM 4.18. *Every Hamiltonian digraph $G_\Gamma \in \mathcal{G}(n)$ has an associated regulatory Boolean network with dynamics isomorphic to G_Γ.*

Proof. Let $n \in \mathbb{N}$ and G_Γ be a Hamiltonian digraph with 2^n vertices. The case where G_Γ is a Hamiltonian cycle follows from Theorem 4.16. If G_Γ is not a Hamiltonian cycle, we can define $g^{[n]} \in \mathcal{F}(G_\Gamma)$ from $f^{[n]}$. To do so, it suffices to change the arc $(z^{[n]}, \vec{1}) \in A(\Gamma(f^{[n]}))$ to the arc $(z^{[n]}, u)$, $u \neq \vec{1}$, describing a Hamiltonian but non-cyclic Hamiltonian dynamic.

Since by definition $f^{[n]} = ((f^{[n-1]} \wedge d_{\overline{z}^{[n]}}) \vee c_{z^{[n]}}, (x_n \wedge d_{\overline{z}^{[n]}}) \vee c_{z^{[n]}})$, we can define $g^{[n]} \in \mathcal{F}(G_\Gamma)$ as described in (4.11).

$$g_j^{[n]}(x) = \begin{cases} (h_j^{[n]} \wedge d_{\overline{z}^{[n]}})(x) & \text{if } x = z^{[n]} \text{ and } u_j = 0, \\ f_j^{[n]}(x) & \text{otherwise.} \end{cases} \tag{4.11}$$

According to Theorem 4.16 and Corollary 4.17, the local activation functions $g_j^{[n]}$ are unate. If $x \in \{0,1\}^n \setminus \{z^{[n]}\}$, it follows that $g^{[n]}(x) = f^{[n]}(x)$, forming a Hamiltonian Boolean network. By definition, $g^{[n]}(z^{[n]}) = u$, proving that $g^{[n]}$ is a regulatory and Hamiltonian Boolean network of maximum height when $u = z^{[n]}$, or of intermediate height otherwise. ∎

The network $h^{[n]}$ served as an auxiliary tool for constructing Hamiltonian cycle dynamics. However, this construction can be exploited further to extend the implications of Corollary 4.17.

Transitioning from a Hamiltonian cycle to another Hamiltonian dynamic requires changing only one arc. However, we demonstrate that this can be done for both the image of $z^{[n]}$ and $\overline{z}^{[n]}$.

DEFINITION 4.19. *A directed graph $G_\Gamma \in \mathcal{G}(n)$ is called 2-Hamiltonian if all arcs of the digraph can be covered by two trajectories of length 2^{n-1}.*

2-Hamiltonian digraphs illustrate the ability to modify two images of the auxiliary network $h^{[n]}$ while maintaining the property of being a regulatory Boolean network. Examples of 2-Hamiltonian digraphs include Hamiltonian digraphs, $\Gamma(h^{[n]})$, or the one described in Figure 12, among others. For this last example, the arcs can be covered by two trajectories $P: 1,2,4,6,5$ and $Q: 8,7,5,3,3$, both of equal length, demonstrating its 2-Hamiltonian property.

Note that 2-Hamiltonian digraphs do not necessarily induce properties in the connectivity of the interaction graph. A clear example of a disconnected interaction graph is $G(h^{[n]})$.

COROLLARY 4.20. *Any 2-Hamiltonian digraph $G_\Gamma \in \mathcal{G}(n)$ has a regulatory Boolean network with dynamics isomorphic to G_Γ.*

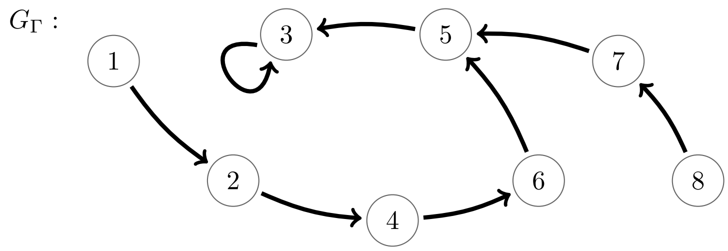

Fig. 12: Example of a 2-Hamiltonian digraph.

Proof. Let $n \in \mathbb{N}$, and suppose G_Γ is 2-Hamiltonian, distinct from a Hamiltonian cycle, with 2^n vertices. Since $f^{[n]}$ is a Hamiltonian cycle, it is also 2-Hamiltonian, with trajectories P and Q defined in (4.12) and (4.13), respectively.

$$P = \vec{1}, f^{[n]}(\vec{1}), (f^{[n]})^2(\vec{1}), \ldots, (f^{[n]})^{2^{n-1}-2}(\vec{1}), \overline{z}^{[n]}, \tag{4.12}$$

$$Q = \vec{0}, f^{[n]}(\vec{0}), (f^{[n]})^2(\vec{0}), \ldots, (f^{[n]})^{2^{n-1}-2}(\vec{0}), z^{[n]}. \tag{4.13}$$

Since G_Γ is 2-Hamiltonian, it can be covered using P and Q. Let $u, v \in \{0,1\}^n$ be the images of $\overline{z}^{[n]}$ and $z^{[n]}$ in the coverage of G_Γ, and define $g^{[n]} \in \mathcal{F}(G_\Gamma)$ as the network describing this coverage. Based on $f^{[n]}$, the arcs $(z^{[n]}, \vec{1})$ and $(\overline{z}^{[n]}, \vec{0}) \in A(\Gamma(f^{[n]}))$ are replaced with $(z^{[n]}, u)$ and $(\overline{z}^{[n]}, v)$. $g^{[n]}$ is described as shown in (4.14).

$$g_j^{[n]}(x) = \begin{cases} (h_j^{[n]} \wedge d_{\overline{z}^{[n]}})(x) & \text{if } x = z^{[n]} \text{ and } u_j = 0, \\ (h_j^{[n]} \vee c_{z^{[n]}})(x) & \text{if } x = \overline{z}^{[n]} \text{ and } v_j = 1, \\ f_j^{[n]}(x) & \text{otherwise.} \end{cases} \tag{4.14}$$

From Theorem 4.16 and Corollary 4.17, $g_j^{[n]}$ are unate local activation functions. For $x \in \{0,1\}^n \setminus \{z^{[n]}, \overline{z}^{[n]}\}$, $g^{[n]}(x) = f^{[n]}(x)$. Additionally, $g^{[n]}(z^{[n]}) = u$, $g^{[n]}(\overline{z}^{[n]}) = v$, and it follows that $g^{[n]} \in \mathcal{F}(G_\Gamma)$. ∎

5. Conclusions. In this work, Hamiltonian dynamics were addressed with the aim of contributing to the understanding of extreme dynamic behaviors, which achieve maximum possible values in parameters of interest such as height, the length of the limit cycle, and the minimum number of Garden of Eden states, among others.

The relationship between the digraph G_Γ of Hamiltonian dynamics and the associated interaction graph was demonstrated. In particular, the existence of networks that cannot be modeled using interaction graphs $G(f)$ with bounded in-degree was proven, requiring specific connectivity conditions to reproduce these dynamics (see Table 2).

Additionally, the inherent limitations of certain families of Boolean networks for modeling Hamiltonian dynamics were analyzed. As a primary contribution, a family of regulatory networks $f^{[n]}$ with Hamiltonian dynamics was presented, including cases of maximum height, intermediate height, quasi-Hamiltonian, Hamiltonian cycles, and their generalization to 2-Hamiltonian dynamics. The network $f^{[n]}$ is notable for being self-dual, suggesting that self-duality in $[n]$ may be a necessary condition for any Hamiltonian cycle network to be regulatory.

Furthermore, the network $f^{[n]}$ allows corroboration of the capacity of regulatory networks to model dynamics with an attractor of arbitrary length without requiring these networks to be bijective. This result broadens the understanding of regulatory networks and their applications in modeling dynamic systems.

Finally, although the results presented are limited to networks defined over a binary alphabet, the techniques and constructions developed in this work could be generalizable to networks with alphabets of size $q \geq 2$. This aspect opens the door to new lines of research exploring the extension of these properties to complex systems.

Type of dynamics	**Variable with total dependency**	**Type of connectivity**	**Existence of regulatory network**
Hamiltonian of maximum height	Yes	Strongly connected	Yes
Hamiltonian intermediate with even period	Yes	Unilaterally connected	Yes
Hamiltonian intermediate with odd period	Yes	Strongly connected	Yes
Hamiltonian cycle	Not necessarily	Unilaterally connected	Yes
Quasi-Hamiltonian	Not necessarily	Strongly connected	Unknown
2-Hamiltonian	Not necessarily	No restrictions	Yes

Table 2: Summary of properties present in the dynamics under study.

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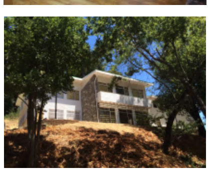

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