Journal of Automata, Languages and Combinatorics **27** (2022) 1–3, 91 – 130

MULTI-WAVE SOLITON AUTOMATA

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ABSTRACT

A soliton or solitary wave, when travelling through a molecule, for instance a polyacetylene chain, may cause changes in the bond structure. These changes can be interpreted as state changes of an automaton. In the late 1970s F. L. Carter suggested that computers could be built based on the switching of bonds by solitons. Several successful experiments were conducted at that time.

An abstract mathematical model of soliton switching, soliton automaton, was defined by Dassow and Jürgensen about 1986. A graph with weighted edges takes the rôle of the molecule, and the soliton is a kind of pebble which moves from node to node along the edges of the graph and, in doing so, changes the weights of the edges. Using this model, the logical potential of soliton-based switching has been explored. So far, the essential simplifying assumption was that only one soliton can be in the molecule at any given time.

We extend this model to include the simultaneous presence of more than one soliton. When multiple soliton waves or particles are present, their interactions have to be modelled in a physically meaningful way. Some situations are specific to the multi-soliton case and are not observed otherwise. This leads one to re-consider even the most basic concepts regarding soliton automata. In this paper we lay the foundations for this theory of multi-soliton automata, explain the modelling decisions, and discuss issues which are new when multiple solitons are considered. The new model includes the single-soliton case in a consistent manner.

Keywords: molecular computer, unconventional modes of computation, bond switching, soliton automaton, soliton wave, multiple soliton waves, finite automaton

1. Solitons

"When considering unorthodox means of computation one needs to discard any preconceived ideas, but first investigate what the new means have to offer and, after that, how to use the new features to achieve the intended goals." This was stated by one of the present authors (HJ) in the 1980s in several talks. A similar opinion is found

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A preliminary version of this paper, without proofs and details, appeared as *Soliton Automata with Multiple Waves* in the Festschrift *Computing with New Resources: Essays Dedicated to Jozef Gruska on the Occasion of His 80th Birthday* [10].

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in [61] where Mario Ruben states "to do Boolean logic with molecules is to do violence against them". This could be said about many unconventional models of computation when traditional thinking is imposed on untraditional concepts. Hence, before investigating how to implement logical gates and the like, using the unconventional model, one should explore the computational power of the model itself and, after that, how to harness it to achieve certain goals, not the other way around.

The computing model under consideration concerns the switching behaviour of bonds in a molecule when a disturbance, called a soliton in the sequel, is injected. The bonds are likely to change, leading to a different molecule. Taking these molecules as states, one obtains a system which behaves like an automaton.

Such molecules could be combined into a larger one, to form something akin to a cellular automaton. One would build a powerful computer at the size of a few hundred Ångström[1]. In our work we consider only the components of such a powerful cellular computer and their capabilities. The study of (cellular) automata based on such components can be conducted at a far higher level of abstraction and seems to belong to the traditional study of automaton compositons in general rather than that of unconventional computing devices. In [37] it was shown how all finite automata can be built as products of soliton automata. The soliton automata implement the permutation automata while their connections implement the resets, the latter required by the general theory of automaton compositions (see [48]).

Solitons can be considered as waves or particles travelling through some "substance" unhindered, without energy loss, and without interference. They travel slowly – at the speed of sound, but fast enough when only small distances need to be covered. They can, however, modify the "field" through which they travel. It has been suggested for instance, that solitons are a means by which genetic information is being transmitted (see [58] for example).

This suggests that soliton waves or particles can be used to induce computational operations. In the sequel, we consider the effects of solitons without distinguishing between waves and particles, as this is not important for the issue at hand. Moreover, we use the terms of *molecule* and *soliton* in a metaphorical sense, abstracting radically from the physical and chemical realities. We speculate about what could be achieved by the soliton effect in molecules. What can actually be achieved is for researchers in physics, chemistry and engineering to explore.

For a brief account of the history of solitons we refer to [59, pp. 18–19] and [57]. In our paper we only consider solitons in molecules. For the physics of solitons in such situations we refer to the books by Davydov [32] and by Lu [59]. The latter contains several articles by the author, 84 reprinted papers by other authors on the subject, and an extensive bibliography as of 1987. A non-technical, but quite helpful explanation of solitons, including a video, for lay persons is provided by Tong [69]. A fundamental analysis and survey as of 1988 (and still up-to-date in most respects) was given by Heeger et al. [46].

The idea of molecule-sized computers was expressed in Feynman's famous lecture *There's Plenty of Room at the Bottom* [34] and re-considered in its sequel *Infinitesi-*

[1] One Å (Ångström) is equal to 10^{-10} m or 0.1 nm.

mal Machinery [35]. By the late 1970s, much research towards molecular computing was conducted both at the theoretical and the experimental levels as witnessed, for example, by technical laboratory reports like [36, 56] or by the series of conferences on *Molecular Electronic Devices* [24, 17, 22].

In several publications Carter et al. studied the idea of soliton-based switching [16, 20, 21, 23, 13, 14, 15, 18, 19, 45]. The kind of molecules under consideration is specified below. One sends a soliton through that molecule; the binding structure of the molecule changes. Hence, if one interprets the prior and the posterior binding structures as states of a system, the molecule together with the solitons behaves as an automaton or a switching device. In the early literature these are called *soliton valves.* A formal definition of *soliton automata* based on this physical or chemical phenomenon was given by Dassow and one of us (HJ) in a 1987 conference paper [26], with an expanded version of the paper published in 1990 [28]. That work, as that of Carter and others, assumes that at any time at most one soliton is travelling through the molecule. In the present work, we remove this assumption.

The field of molecular computing has many facets. We focus on the aspect of one or more soliton waves incurring changes of the bond structure in a molecule. There is a large number of studies, beyond Carter's work, of the potential of such effects. For some still quite early work we refer to [12]. Recent research corroborates the conclusions. It also confirms ideas about the interaction of multiple solitons at the molecular level (see [60] and references cited there).

Terminological confusion may arise: There is another definition of *soliton automata,* which is completely unrelated to the one used here. It was initiated by a paper on "Soliton-Like Behavior in Automata" by Park [62]. In that sense the term *soliton automaton* is found in many papers on cellular automata as, for example, [66]. The soliton-like behaviour expresses itself in its appearance of state changes in the cells of the automaton. That work has no relation to the physics of solitons at all except that computational processes through the cellular automaton look like solitary waves.

We return to the basic idea. Not all molecules would work. Polyacetylene chains and several other types of molecules are known to have a fairly controlled reaction to solitons. Accordingly, research on soliton-based switching or automata focussed on bond changes in polyacetylene chains or polymers. In essence, one considers molecules, the basic structure of which is a sequence of carbon atoms with bonds of alternating weights connecting them and with other atoms or molecules – of not always logical, but often physical relevance – connected to the carbon atoms.

In this paper we only consider the soliton-induced state changes in polymers – more precisely, abstractions of them. In other words, we ignore physical and chemical details. In representing molecules, we show nothing but the carbon atoms and possibly some hydrogen atoms as illustrated in Figure 1. Abstracting further, we consider graphs with special properties and transformations of such graphs into others with the same topology and the same properties. Such graphs are called soliton graphs in the sequel.

In a soliton graph the nodes have degrees 1, 2 or 3. Nodes of degree 1 are said to be exterior; they form the entry and exit points for solitons. Nodes of degrees 2 or 3 are interior. The edges are undirected; there are no loops; the edges have weights 1 or 2,

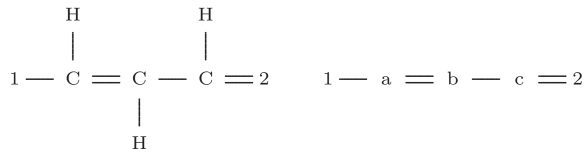


Figure 1: A very simple polyacytelene molecule before and after abstraction. Interior nodes are specified by letters when required. Exterior nodes replacing some unknown attached molecules are represented by numbers.

these representing single and double bonds, respectively. From entry to exit a soliton travels along edges of alternating weights. While it may cycle through the graph, it will never immediately turn back. Therefore, the two edges at a node of degree 2 must have different weights, and of the three edges at a node of degree 3, two have weight 1 and one has weight 2. Formal definitions of these concepts are given in Section 3 below.

Informally, a soliton transforms a soliton graph into another soliton graph. Consequently, a soliton automaton consists of an initial soliton graph as the initial state, solitons specified by their entry and exit locations as the input alphabet, the potential state changes as the transition function, and all reachable soliton graphs as the state space.

The theory of solitons in polymers suggests to study not only the effect of single solitons as proposed originally by Carter, but also to investigate the effect of multiple soliton waves. Multiple soliton waves introduce parallelism of a kind not usually encountered in computer science because soliton waves could pass each other unchanged. Processes are not synchronized – at least at a measurable level. There is no appropriate automaton theoretic model for this kind of situation. As an unconventional mode, regardless of its realization, unsynchronized computation seems to be a model worth studying both theoretically and also in terms of its rôle in natural processes.

Solitons have been described as particles, as deficiencies or as waves. Each of these models conveys a specific intuition about the underlying physical process. To our readers we recommend that of a wave, as this implies a direction, caused potentially by external sources. Particles could, in principle, oscillate. That would not be useful in a computational context. On the other hand, real soliton waves extend over molecule chains of some length. In the model we only consider the position of the peak of the wave, that is, where we assume the particle to be when it is swept on.

Our paper is structured as follows: We introduce some very basic notation in Section 2. This is followed by a review of soliton graphs and soliton paths for single solitons in Section 3 and a summary of results regarding single-soliton automata in Section 4. In Section 5 we list postulates which a mathematical model of soliton behaviour ought to satisfy. These are abstracted from reported physical observations and meant to guide the definition of the model. We then show, by several examples, where the definitions and intuition for the single-soliton case break down when multiple solitons are considered in Section 6. These examples may seem excessively long. We kept them because they show, that intuition cannot be taken for granted. A formal treatment of the multi-soliton case follows in Section 7. Several fundamental statements regarding the behaviour of multiple solitons are proved. These results can be viewed in two ways: (1) As a confirmation that the formal model is consistent with the physical theories and the intuitive ideas derived from them. (2) As a challenge to physics and chemistry to verify the consequences of the abstractions proposed in the formal model. The paper concludes with many questions in Section 8.

Many of the problems considered in this paper resulted from or were raised in the thesis [64]. A preliminary account of this work was presented in [10]; the present paper presents the complete scenario including detailed proofs and examples and also corrects mistakes made in that earlier version.

2. Notation and Basic Notions

We introduce some notation and review some basic notions.

The sets of positive integers, of non-negative integers and of integers are denoted by $\mathbb{N}$, $\mathbb{N}_0$ and $\mathbb{Z}$, respectively. We use standard notation for sets. We write $|S|$ for the cardinality of a set S. When no confusion is likely, we omit set brackets for singleton sets.

An *alphabet* is a finite non-empty set the elements of which are called *symbols*. Let Σ be an alphabet. The set of all (finite) words over Σ, including the empty word λ, is denoted by Σ^*; let $\Sigma^+ = \Sigma^* \setminus \{\lambda\}$. The length $\mathsf{lg}(w)$ of a word $w \in \Sigma^*$ is defined by

$$\mathsf{lg}(w) = \begin{cases} 0, & \text{if } w = \lambda, \\ 1 + \mathsf{lg}(v), & \text{if } w = av \text{ with } a \in \Sigma \text{ and } v \in \Sigma^*. \end{cases}$$

A *semi-automaton* is a construct $\mathcal{A} = (Q, \Sigma, \tau)$ where Q is a non-empty set, Σ is an alphabet and $\tau : Q \times \Sigma \to 2^Q$ is a mapping. The elements of Q are called states; Σ is the input alphabet of $\mathcal{A}$; τ is the transition function of $\mathcal{A}$. In this paper, we assume that Q is finite and that, for all $q \in Q$ and all $a \in \Sigma$, $\tau(q, a) \neq \emptyset$. Moreover, we drop the prefix "semi-" as we do not consider any other kind of automata.

Let $\mathcal{A} = (Q, \Sigma, \tau)$ be an automaton. The transition function τ is extended to $2^Q \times \Sigma^*$ as follows: for $R \subseteq Q$ and $w \in \Sigma^*$, let

$$\tau(R, w) = \begin{cases} R, & \text{if } w = \lambda, \\ \tau\left(\bigcup_{q \in R} \tau(q, a), v\right), & \text{if } w = av \text{ with } a \in \Sigma \text{ and } v \in \Sigma^*. \end{cases}$$

For $w \in \Sigma^*$, let τ_w be the mapping defined by $\tau_w(R) = \tau(R, w)$ for all $R \subseteq Q$. Instead of $\tau_w(R)$ we often write $R\tau_w$. With this convention, the mapping τ of Σ^* into the monoid $\mathfrak{T}_{2^Q}$ of all mappings of 2^Q into 2^Q which maps $w \in \Sigma^*$ onto τ_w is a homomorphism[2], that is, for $w = uv$ with $u, v \in \Sigma^*$ one has[3] $\tau_w = \tau_{uv} = \tau_u \tau_v$.

The automaton $\mathcal{A}$ is said to be deterministic if $|\tau_a(q)| = 1$ for all $a \in \Sigma$ and all $q \in Q$. In that case τ_a is considered as a mapping of Q into Q, that is as a

[2] Assuming $Q \cap \Sigma = \emptyset$, one could write qw and Rw instead of $q\tau_w$ and $R\tau_w$. However, in the sequel it is convenient to distinguish notationally between a word and the transformation induced by it.

[3] For two mappings τ_1 and τ_2 over a set X, the notation $\tau_1\tau_2$ refers to their composition $\tau_1\tau_2(x) = \tau_2(\tau_1(x))$, for all $x \in X$.

transformation of Q rather than of 2^Q. The set of transformations of Q induced by τ is a monoid with the multiplication defined as above, the *transition monoid* $T(\mathcal{A})$ of $\mathcal{A}$. The transformation τ_λ is the identity element[4] of $T(\mathcal{A})$. Inputs u and v of $\mathcal{A}$ are said to be equivalent if and only if $\tau_u = \tau_v$. As the transition monoid $T(\mathcal{A})$ is a submonoid of the monoid of all mappings of Q into Q, the *full transformation monoid* $\mathfrak{T}_Q$ of Q, the order (cardinality) of $T(\mathcal{A})$ is at most $|Q|^{|Q|}$. The symmetric group $\mathfrak{S}_Q$ on Q is a maximal subgroup of $\mathfrak{T}_Q$.

Let R be a non-empty subset of Q. Define $[R] = \bigcup_{w\in\Sigma^*} R\tau_w$. Here we do not assume that $\mathcal{A}$ is deterministic. The construct $([R], \Sigma, \tau)$ is the subautomaton of $\mathcal{A}$ generated by R. The set $[R]$ is the smallest subset of Q, which contains R and is closed under repeated applications of τ or, equivalently, the set of all states in Q, which can be reached from states in R.

The monoids that appear in the context of this paper are Klein's group $\mathfrak{V}_4$ with 4 elements, the symmetric group $\mathfrak{S}_n$ with $n!$ elements, and the alternating group $\mathfrak{A}_n$ with $n!/2$ elements. We consider these groups as concrete groups rather than as their isomorphism types. For example, the groups $\mathfrak{V}_4$ and $\mathfrak{S}_2 \times \mathfrak{S}_2$ are isomorphic, but as concrete groups they would be considered different. In fact, from these two isomorphic groups, only $\mathfrak{S}_2 \times \mathfrak{S}_2$ occurs in our context.

3. Soliton Graphs and Soliton Paths

We list and elaborate on, a few definitions taken from [28]. The model of soliton automata considered there assumes that only a single soliton is present at any given moment. We summarize known facts regarding the computational power of soliton automata with this restriction from [9, 26, 27, 28, 29, 30, 31, 37, 47, 49, 51]. We consider the presence of multiple solitons further below.

Many of the results summarized, but not used, in the sequel would require extensive formal definitions. Rather than copying these, we refer the reader to the original publications and supply only informal explanations here.

A *graph* is a pair $G = (N, E)$ with N the set of *nodes* and $E \subseteq N \times N$ the set of edges. We consider only finite undirected graphs. An edge connecting nodes n and n' is given both as (n, n') and (n', n). Therefore, we require that, for $n, n' \in N$, $(n, n') \in E$ if and only if $(n', n) \in E$ and that these represent the same edge. Thus, any two nodes can be connected by at most one edge.

A *weight function* for G is a mapping $w : N \times N \to \mathbb{N}_0$ satisfying

$$w(n, n') = w(n', n) \begin{cases} = 0, & \text{if } (n, n') \notin E \\ > 0, & \text{if } (n, n') \in E. \end{cases}$$

A *weighted graph* is a triple (N, E, w) such that (N, E) is a graph and w is a weight function.

For a node n, the set $V(n) = \{\, n' \mid (n, n') \in E \,\}$ is the *vicinity* of n. The *degree* of n is $d(n) = |V(n)|$, and the *weight* of n is $w(n) = \sum_{n'\in V(n)} w(n, n')$. A node n is said to be *isolated* if $d(n) = 0$, *exterior* if $d(n) = 1$, and *interior* if $d(n) > 1$.

[4] In general the identity mapping of a set into itself is denoted by ι.

Definition 1 [28]. A *soliton graph* is a weighted graph $G = (N, E, w)$ satisfying the following conditions:

(I) N is the finite, non-empty set of nodes.

(II) $E \subseteq N \times N$ is the set of undirected edges, such that $(n, n') \in E$ if and only if $(n', n) \in E$.

(III) Every node $n \in N$ has the following properties:

(A) $(n, n) \notin E$.

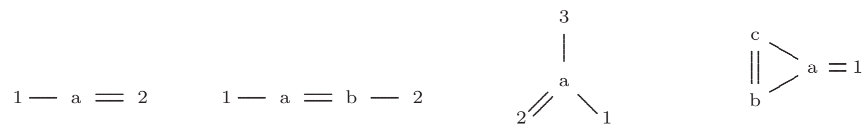
(B) $1 \leq d(n) \leq 3$.

(C) $w(n) \in \{1, 2\}$ if n is exterior, and $w(n) = d(n) + 1$ if n is interior.

(IV) Every component (maximal connected subgraph) of G has at least one exterior node.

In the sequel we assume, without special mention, that $|N| \geq 3$. This only excludes trivial cases. The conditions regarding weight and degree imply that the weight of an edge can only be 1 or 2, that the two edges at a node of degree 2 must have different weights, and that, of the three edges meeting at a node of degree 3, two must have weight 1 and one must have weight 2.

A soliton graph $G = (N, E, w)$ models a "soliton valve" as follows: Each interior node n represents a C atom if $d(n) = 3$ or a C-H group if $d(n) = 2$. An edge (n, n') represents a (CH)-chain with alternating single and double bonds which connects the C atoms of n and n' and begins and ends with a $w(n, n')$-fold bond. Exterior nodes represent the connections to surrounding structures. See [28] for further explanations. When drawing soliton graphs, we indicate the weight of an edge (n, n') (and thus the multiplicity of the bond) by $w(n, n')$ parallel lines. In Figure 2 we show examples of small soliton graphs.



(a) (b) (c) (d)

Figure 2: Examples of soliton graphs: (a) A soliton graph (tree) with $|N| = 3$. (b,c) Two soliton graphs (trees) with $|N| = 4$. (d) A soliton graph with a cycle and $|N| = 4$.

Next, we need to define which paths a soliton can take. This definition only works when the presence of a single soliton is considered. It will change in a consistent way below to accommodate the presence of more than a single soliton.

Definition 2 [28]. Let $G = (N, E, w)$ be a soliton graph. A *partial soliton* path is a sequence $n_0, n_1, \ldots, n_k$ of nodes in N with the following properties:

(I) The nodes $n_0, n_1, \ldots, n_k$ form a path in the underlying graph, that is, $(n_i, n_{i+1}) \in E$ for $i = 0, 1, \ldots, k-1$.

(II) n_0 is exterior and $n_1, \ldots, n_{k-1}$ are interior.

(iii) There are weighted graphs $G_0, G_1, \ldots, G_k$ with

$$G_i = (N, E, w_i)$$

for $i = 0, 1, \ldots, k$ with the following properties:

(a) $G_0 = G$.

(b) For $i = 0, 1, \ldots, k-2$ the graph G_{i+1} is defined if and only if G_i is defined and $w_i(n_i, n_{i+1}) \neq w_i(n_{i+1}, n_{i+2})$. Then

$$w_{i+1}(n, n') = w_{i+1}(n', n) = \begin{cases} 3 - w_i(n, n'), & \text{if } n = n_i \text{ and } n' = n_{i+1} \\ & \text{or vice versa,} \\ w_i(n, n'), & \text{otherwise.} \end{cases}$$

(c) G_k is defined if and only if G_{k-1} is defined. w_k is defined as above with $k = i + 1$.

If n_k is exterior the path is a *(total) soliton path.*

The two typical situations, according to Definition 2.iii.b permitting the formation of a soliton partial soliton path are shown in Figure 3. The special case of $i = k - 1$ just changes the weight of the last edge.

The case of $k = 0$ is included here for notational convenience.

Graph G_i	becomes G_{i+1} if $i \leq k-2$
$n_i = n_{i+1} - n_{i+2}$	$n_i - n_{i+1} - n_{i+2}$
or	
$n_i - n_{i+1} = n_{i+2}$	$n_i = n_{i+1} = n_{i+2}$

Figure 3: Typical situations in Definition 2.iii.b. In the next step, if it is possible, the weight of the edge from n_{i+1} to n_{i+2} will change.

The following observations are immediate consequences of the definitions.

Observation 3. *Let $n_0, n_1, \ldots, n_k$ be a partial or total soliton path.*

- $n_i \neq n_{i+1}$ *for* $i = 0, 1, \ldots, k-1$.
- $n_i \neq n_{i+2}$ *for* $i = 0, 1, \ldots, k-2$.

Proof. The first statement follows from the fact that G has no loops. For the second statement, suppose that G_i is defined and $n_i = n_{i+2}$. As

$$w_i(n_i, n_{i+1}) = w_i(n_{i+1}, n_i) = w_i(n_{i+1}, n_{i+2}),$$

the graph G_{i+1} is not defined. □

Observation 4. *Let G be a soliton graph, and let $n_0, n_1, \dots, n_k$ be a partial soliton path in G. For all i with $0 < i \leq k$ also $n_0, n_1, \dots, n_i$ is a partial soliton path in G.*

The terminology introduced in Definition 2 could suggest an unintended intuition. A partial or total soliton path is not a static object − like a path in an arbitrary graph, but a dynamic one which arises from a soliton traversing the soliton graph. This is illustrated in Figure 4. The traversal of a soliton path changes the weights in the original graph.

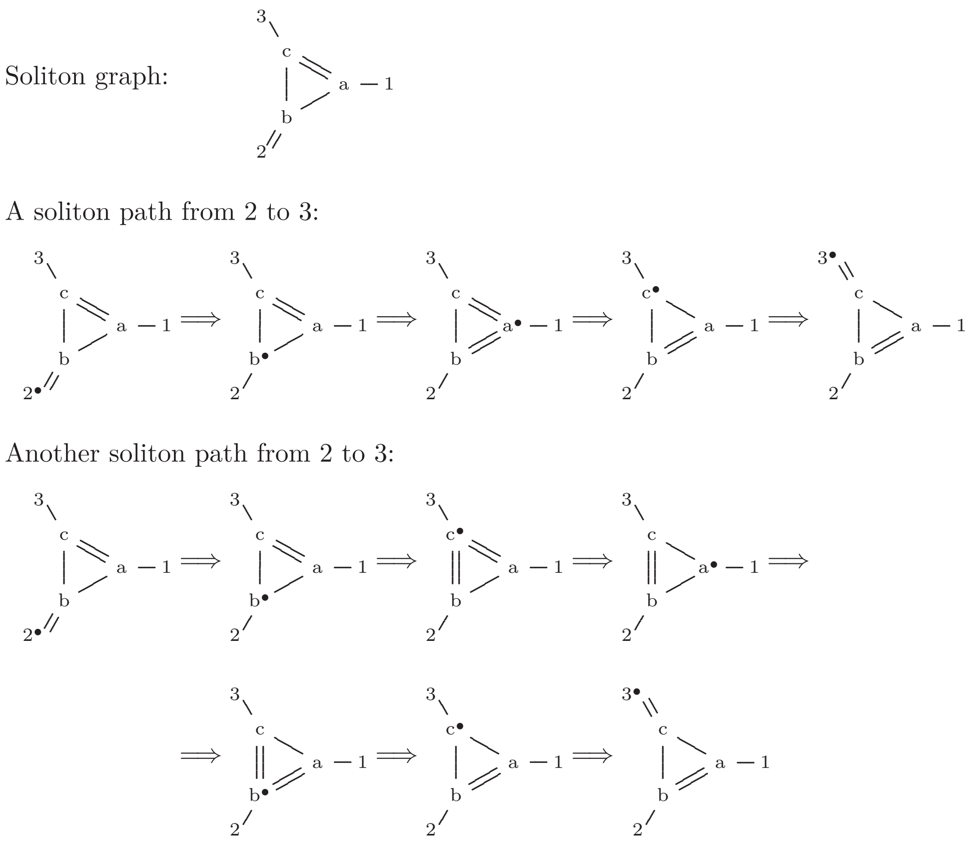


Figure 4: A soliton graph with several soliton paths between the same exterior nodes. The dots indicate the current positions of the soliton.

We use expressions like “a soliton moves from n_i to n_{i+1}” or “a soliton traverses a path” or “a soliton is at node n_i” in a metaphorical sense to indicate the sequence of changes in the sequence $G_0, G_1, \dots, G_k$ of graphs. In constructing a soliton path, the following property is helpful:

Proposition 5. *Let $G = (N, E, w)$ be a soliton graph and let $n_0 \in N$ be an exterior node. To construct a partial soliton path from n_0 one proceeds as follows:*

(I) *Let* $i = 1$*, and let* n_1 *be the unique node with* $(n_0, n_1) \in E$*. Further, let* $G_0 = (N, E, w_0) = G$*, let* P_0 *be the path of length 0 consisting only of the node* n_0*, and let* P_1 *be the path of length 1 consisting of* n_0, n_1*. Define*

$$w_1(n, n') = w_1(n', n) = \begin{cases} 3 - w_0(n, n'), & \textit{if } n = n_0 \textit{ and } n' = n_1 \\ & \quad \textit{or vice versa,} \\ w_0(n, n'), & \textit{otherwise.} \end{cases}$$

Let $G_1 = (N, E, w_1)$*.*

(II) *Suppose* $i > 0$*, that* $n_0, n_1, \ldots, n_i$ *is a path* P_i *constructed so far and that* $G_0, G_1, \ldots, G_i$ *is the sequence of weighted graphs considered in the construction. Choose a node* $n_{i+1} \in N$*, different from* n_{i-1} *and* n_i*, with* $(n_i, n_{i+1}) \in E$ *and such that* $w_i(n_i, n_{i+1})$ *differs from* $w_{i-1}(n_{i-1}, n_i)$*. If no such node exists, the construction ends. Otherwise, let* P_{i+1} *be the path* $n_0, n_1, \ldots, n_i, n_{i+1}$*. Define*

$$w_{i+1}(n, n') = w_{i+1}(n', n) = \begin{cases} 3 - w_i(n, n'), & \textit{if } n = n_i \textit{ and } n' = n_{i+1} \\ & \quad \textit{or vice versa,} \\ w_i(n, n'), & \textit{otherwise.} \end{cases}$$

Let $G_{i+1} = (N, E, w_{i+1})$*. Increase* i *by 1 and repeat this construction step.*

Each path P_i *with* $i > 0$ *is a partial soliton path. Moreover, all soliton paths originating at* n_0 *are obtained by this construction.*

Proof. We need to show that a path $n_0, n_1, \ldots, n_k$ satisfying Definition 2 can be constructed using Proposition 5 and that every path constructed according to the proposition satisfies the definition. We look at some special cases first, then use induction up to $k - 1$ and then deal with the final case separately.

In both cases, the first node is exterior. Thus one can chose n_0 to be the same in both constructions. This also settles the special case of $k = 0$.

Next, let $k = 1$. As n_0 is exterior, there is only a single node to be reached. For Proposition 5, this node is the next node in any soliton path starting at n_0. For Definition 2, using the fact that $k = 1$, this is the unique adjacent node to form a soliton path starting at n_0.

Let $k > 1$ and consider the way how the node n_1 can has been obtained. The choice of the exterior node n_0 determines n_1 uniquely. According to the first condition of Proposition 5, n_1 is the unique successor node of n_0 for that construction. Using the fact that $k > 1$ and that $n_0, n_1, \ldots, n_k$ is a soliton path according to Definition 2, one has

$$w_0(n_0, n_1) \neq w_0(n_1, n_2).$$

Therefore, n_1 is also the unique sucessor node according to the definition.

From here up to $k - 1$ we proceed by induction. Let $1 \leq i < k - 1$ and assume that the two constructions have led to the sequence $G_0, G_1, \ldots, G_i$ of weighted graphs and the corresponding sequence of nodes $n_0, n_1, \ldots, n_i$. We now consider the next step moving from i to $i + 1$.

Suppose this next step has been performed according to Definition 2. We need to show that this step could also have been performed according to Proposition 5, that is, that

$$w_{i-1}(n_{i-1}, n_i) \neq w_i(n_i, n_{i+1}).$$

Inequality in the present context means

$$w_{i-1}(n_{i-1}, n_i) = 3 - w_i(n_i, n_{i+1}).$$

In the step leading to G_i, the condition

$$w_{i-1}(n_{i-1}, n_i) \neq w_{i-1}(n_i, n_{i+1})$$

of Definition 2 was satisfied. More precisely,

$$w_{i-1}(n_{i-1}, n_i) = 3 - w_{i-1}(n_i, n_{i+1}).$$

By Observation 3,

$$w_{i-1}(n_i, n_{i+1}) = w_i(n_i, n_{i+1}).$$

Hence

$$w_{i-1}(n_{i-1}, n_i) = 3 - w_{i-1}(n_i, n_{i+1}) = 3 - w_i(n_i, n_{i+1})$$

as needed. Thus the next node in the construction according to Proposition 5 can be chosen to be n_{i+1}.

For the converse, suppose that the step has been performed using the construction of Proposition 5. Objects constructed according to Proposition 5 are denoted by 'primed' symbols like n'_j, G'_j and w'_j to avoid confusion. We need to show that the choice of the next node n'_{i+1} satisfies the conditions of Definition 2. This would imply that one can assume that $n_{i+1} = n'_{i+1}$.

The condition to be satisfied is

$$w_i(n_i, n_{i+1}) = 3 - w_i(n_{i+1}, n_{i+2}).$$

As the node n_{i+2} only appears in the condition of Definition 2, but not in the construction of G_{i+1}, any node n instead of n_{i+2} could be used as long as n has an edge connecting it to n_{i+1} and it is different from both n_i and n_{i+1}.

As $i < k - 1$ we can assume that the sequence $n'_0, n'_1, \ldots, n'_i, n'_{i+1}, n'_{i+2}$ with the corresponding graphs has been constructed using Proposition 5. By the induction hypothesis, $n'_j = n_j$ and $G'_j = G_j$ for all j with $j \leq i$. The condition to be satisfied turns into

$$w_i(n'_i, n'_{i+1}) = 3 - w_i(n'_{i+1}, n)$$

for some n subject to the conditions above. We show that this holds with $n = n'_{i+2}$. Clearly, n'_{i+2} is distinct from both n'_{i+1} and $n'_i = n_i$. According to the construction this implies that

$$w'_{i+1}(n'_{i+1}, n'_{i+2}) = w_i(n'_{i+1}, n'_{i+2})$$

and

$$w'_{i+1}(n'_{i+1}, n'_{i+2}) = 3 - w'_i(n'_i, n'_{i+1}).$$

Thus the choice of $n_{i+1} = n'_{i+1}$ is also possible according to Definition 2, and $G_{i+1} = G'_{i+1}$.

We now have to consider the final steps leading up to k.

Let $i = k - 1$. Assume the path and the sequence of graphs up to i have been obtained according to Definition 2. One proceeds as above for $k < i - 1$. On the other hand, if the path and graphs have been constructed according to Proposition 5 then any n'_k would satisfy the definition. □

In Figure 4 two kinds of non-determinism are exhibited. In general, a given pair (n, n') of exterior nodes of a soliton graph may have any number of soliton paths joining them: (1) there could be no path at all; (2) there could be two or more paths differing in terms of the direction taken by the soliton at nodes of degree 3; (3) there could be paths in which the soliton takes multiple rounds. Case (2) is illustrated by the two paths in Figure 4. Case (3) can be seen in the second path of that figure. As drawn, the soliton completes one full round of the triangle and leaves after having started a second round. Instead of leaving, it could continue around the triangle an additional even number of full rounds before leaving. Hence, in Case (3) the time between entry and exit of the soliton is unpredictable. Such situations can arise already with just a single soliton. When more than one soliton is involved, one expects even more complicated scenarios.

4. Single-Soliton Automata

Let $G = (N, E, w)$ be a soliton graph, and let X be its set of exterior nodes. For $n, n' \in X$, let $S(G, n, n')$ be the set of weighted graphs obtained by traversing a soliton path from n to n' completely[5]. If no such soliton path exists, let $S(G, n, n') = \{G\}$. Let

$$S(G, n) = \bigcup_{n' \in X} S(G, n, n').$$

Every graph in $S(G, n)$ is a soliton graph [28, Lemma 3.3].

Let $\Gamma = \Gamma(N, E)$ be the set of all soliton graphs with N and E as sets of nodes and edges, respectively. For $n, n' \in X$, define the mappings

$$\tau_{n,n'} : \Gamma \to 2^\Gamma : G \mapsto S(G, n, n')$$

and

$$\delta_n : \Gamma \to 2^\Gamma : G \mapsto S(G, n).$$

[5] The intermediate graphs obtained during the travel from n to n' are not included in $S(G, n, n')$. Only the graphs resulting from a complete traversal are in $S(G, n, n')$. As there could be more than one soliton path from n to n', the set $S(G, n, n')$ could contain more than one graph.

Let $\tau : (n, n') \mapsto \tau_{n,n'}$ and $\delta : n \mapsto \delta_n$ map $X \times X$ and X, respectively, to these mappings. The constructs $(\Gamma, X \times X, \tau)$ and (Γ, X, δ) are automata.

Definition 6 [28]. Let $G = (N, E, w)$ be a soliton graph. Let X be its set of exterior nodes. Let Γ and τ be as above. The subautomaton $\mathcal{A}(G)$ of $(\Gamma, X \times X, \tau)$ generated by G is the *soliton automaton* of G. Let $S(G)$ denote the set of states of $\mathcal{A}(G)$.

A similar definition can be formulated with respect to δ. This latter variant, which involves much nondeterminism, has not been studied in the literature so far and is not considered in the present work either. A useful visualization of soliton automata as transition graphs can be found in [28, Examples 3.8 and 3.9].

In soliton automata, two kinds of determinism can be observed:

(I) Determinism in the usual automaton theoretic sense: $|S(G', n, n')| = 1$ for all $G' \in S(G)$ and all $(n, n') \in X \times X$.

(II) *Strong determinism:* For all $G' \in S(G)$ and $(n, n') \in X \times X$, there is at most one soliton path in G' from n to n'.

The soliton automaton of Figure 4 is deterministic, but not strongly deterministic. It has four states. Its transition monoid is the group $\mathfrak{S}_2 \times \mathfrak{S}_2$ which is isomorphic with the group $\mathfrak{V}_4$. As a physical building block, a soliton automaton should be deterministic, at least. Strong determinism is preferable as the behaviour of the soliton automaton with respect to timing is nondeterministic otherwise. Hence, research focussed on deterministic soliton automata in either sense, on the graph structure implying determinism and on the computational power of deterministic soliton automata. The latter is considered in terms of the size and structure of the transition monoids of these automata.

By saying that G is deterministic or strongly deterministic, we mean that $\mathcal{A}(G)$ is deterministic or strongly deterministic, respectively.

A soliton graph G may consist of several connected components. Each component defines a soliton automaton with its own input alphabet. Thus, if G has the connected components $G_1, G_2, \ldots, G_k$, then

$$T(\mathcal{A}(G)) = T(\mathcal{A}(G_1)) \times T(\mathcal{A}(G_2)) \times \cdots \times T(\mathcal{A}(G_k)).$$

Beyond the merely graph theoretical notion of connectedness, one also needs to consider another related concept which is based on the existence or non-existence of soliton paths.

Definition 7 [28]. Let $G = (N, E, w)$ be a soliton graph and let $n, n' \in N$. A path from n to n' in the graph theoretical sense is said to be *impervious* if none of its edges occurs in a partial soliton path in any $G' \in S(G)$.

If $n_0, n_1, \ldots, n_k$ is an impervious path of the soliton graph G, then also its reverse $n_k, n_{k-1}, \ldots, n_0$ is impervious. Moreover, each impervious path can be extended to an impervious path with start and end nodes of degree 3 [28, Lemma 4.3]. In Figure 5 we show an example of a soliton graph with an impervious path. A *basic impervious path* is an impervious path with the following two properties: (a) The start and end nodes of the path have degree 3. (b) All other nodes of the path have degree 2. The path from node h to node k in Fig 5 is a basic impervious path.

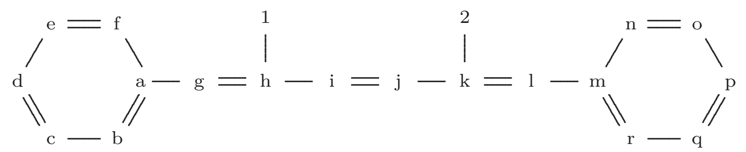


Figure 5: A soliton graph with an impervious path from node h to node k.

In the single-soliton model, basic impervious paths can be removed from the graph without change to the transition monoid. More precisely: Let G be a soliton graph with basic impervious path. Let G' be the weighted graph obtained from G by removing that path. Then G' is a soliton graph, possibly not connected, and $T(\mathcal{A}(G)) \simeq T(\mathcal{A}(G'))$ [30, Lemma 3.8]. Removal of impervious paths may increase the number of connected components. The transition monoid of the resulting *reduced soliton graph* is trivially isomorphic with that of the original soliton automaton. More precisely, if $G_1, G_2, \ldots, G_m$ are the connected components of the reduced soliton graph obtained from G, then

$$T(\mathcal{A}(G)) \simeq T(\mathcal{A}(G_1)) \times T(\mathcal{A}(G_2)) \times \cdots \times T(\mathcal{A}(G_m)).$$

Hence, one needs to consider only *indecomposable soliton graphs,* that is, soliton graphs which, after the removal of impervious paths, are connected. This holds when only a single soliton is present. We show below that the presence of more than one soliton changes the situation significantly.

We now summarize what is known about the transition monoids of soliton automata and what is not known, assuming that only a single soliton is present at any given time. For the following statements, let $G = (N, E, w)$ be an indecomposable soliton graph[6].

(I) $T(\mathcal{A}(G))$ is a group generated by involutorial elements.

(II) If G has a cycle of odd length, then it is not strongly deterministic.

(III) If G is deterministic and has a cycle of even length on which only the first and last nodes are the same, then $T(\mathcal{A}(G)) \simeq \mathfrak{S}_2$.

(IV) If G is strongly deterministic with a path as in the previous statement, then G is a chestnut[7].

(V) G is strongly deterministic if and only if G is a chestnut or a tree.

(VI) If G is a chestnut then $T(\mathcal{A}(G)) \simeq \mathfrak{S}_2$.

---

[6] A soliton graph G is indecomposable if it consists of a single connected component and does not possess impervious paths.

[7] A *chestnut* as defined in [28] is soliton graph consisting of a single cycle, the cycle having even length and some paths entering the cycle; the entry points of paths entering the cycle have even distances from each other; meeting points of paths entering the cycle have even distances from the cycle.

(vii) If G is a tree, then $T(\mathcal{A}(G))$ is a primitive group of permutations.

(viii) For every $n \in \mathbb{N}$ with $n \geq 2$, there is a soliton tree[8] G_n such that $T(\mathcal{A}(G_n)) \simeq \mathfrak{S}_n$.

(ix) Let G' be obtained from G by attaching a soliton tree to an exterior node of G. If G and G' are deterministic and if $T(\mathcal{A}(G))$ is a primitive group of permutations, then also $T(\mathcal{A}(G'))$ is a primitive group of permutations.

(x) If G is deterministic and has a single exterior node, then either G is a chestnut and $T(\mathcal{A}(G)) \simeq \mathfrak{S}_2$ or $T(\mathcal{A}(G))$ is trivial, that is, $\mathfrak{S}_1$.

Statements i–viii are proved in [28]. Statement ix is taken from [30]. Statement x is proved in [29].

Thus, strongly deterministic indecomposable soliton graphs are completely characterized as either chestnuts or trees. The transition monoids of the former are the group $\mathfrak{S}_2$, that is, their switching behaviour is that of a flip-flop. For the latter, no complete characterization of the transition monoids is known. By Statements vii and viii, the transition monoids are primitive groups of permutations and, moreover, all symmetric groups in their natural representations occur. In [31] it is shown that the transition monoids of soliton trees in which all branching points have an even distance from each other are symmetric groups; more precisely, if such a tree has n exterior nodes, then the transition monoid is the group $\mathfrak{S}_n$. The transition monoids of trees in which some branching points have an odd distance could be different from symmetric groups; the first such example was given in [28], and shown to be a subgroup of the alternating group $\mathfrak{A}_{12}$. In [31] it is proved to be the group $\mathfrak{A}_{12}$ itself, in its natural representation; the soliton tree is shown in Figure 6. By a systematic enumeration of all soliton trees up to a certain number of branching points, in addition to symmetric groups, the following alternating groups were found: $\mathfrak{A}_{12}$, $\mathfrak{A}_{20}$, $\mathfrak{A}_{28}$, $\mathfrak{A}_{32}$, $\mathfrak{A}_{36}$, $\mathfrak{A}_{44}$, $\mathfrak{A}_{48}$, $\mathfrak{A}_{52}$, all in their natural representations. No other types of groups have been found so far as transition monoids of soliton trees [49]. Recent research, supported by findings in [51], indicate that these are the only types of groups occurring, and that there is a correspondence between the structure of the tree (as composed from smaller trees) and the structure of the group; however, this correspondence seems to be significantly more complicated than originally envisaged by Bartha and one of the present authors (HJ) in [2].

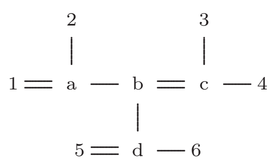


Figure 6: Tree with $\mathfrak{A}_{12}$ as transition monoid.

One can think of soliton graphs as being equivalent if and only if their soliton automata are isomorphic. For the single-soliton model this leads to the following observation.

[8] A soliton tree is a soliton graph, the underlying graph structure of which is a tree.

Observation 8. *Let $G = (N, E, w)$ be a soliton graph. Let n_0, n_1, n_2, n_3 be a path such that $d(n_1) = d(n_2) = 2$ and $(n_0, n_3) \notin E$. Let G' be the weighted graph obtained from G as follows:*

(i) *Remove n_1 and n_2 from N.*

(ii) *Remove all edges involving n_1 or n_2 from E.*

(iii) *Add (n_0, n_3) and (n_3, n_0) to the remaining edges.*

(iv) *Define the weights of these new edges as $w(n_0, n_1)$.*

The resulting graph G' is a soliton graph which is equivalent to G.

In simple words: The length of a path without branches does not matter for the logic; only the parity of the length of such a path matters. The length itself is important, of course, for the timing and, more importantly, for the physical realization. It turns out that this observation is no longer true when multiple solitons can be present as relative timing will become an important issue.

A completely graph theoretic approach to the theory of soliton automata, based on matching theory, is taken by Bartha, Krész and others [3, 4, 5, 6, 7, 8, 52, 53, 54, 55]. For the single-soliton model graph matching theory is an extremely useful framework. It did, however, not yet help in clarifying the suspected functorial connection between soliton graphs and the transition monoids of their automata [2]. For the multi-soliton model the potential rôle of matching theory is currently unknown.

A kind of switching theory for soliton automata is proposed by Groves in [39]. Design and verification rules are presented based on the experimental experience with the single-soliton model. Unfortunately, little of his important work is easily accessible. Partial publications include [38, 40, 41, 42, 43, 44]. Whether this work has a meaningful extension to the model of multi-soliton automata and how this would look like is an open question.

5. Postulates for a Discrete Model of Soliton Movement

Before going into the details of the multi-soliton model we list some basic assumptions guiding the formal definitions.

(i) One can insert and extract solitons at predetermined places: This concerns the external control of the system and is the same as in the case of single solitons.

As an alternative, only the insertion point may be determined while the target may depend on which path is free. We briefly explain this variant without pursuing it.

(ii) Solitons move at the same speed: This implies that solitons cannot overtake each other on the same path.

(iii) Solitons move at a constant speed: They cannot pause. Once in the graph, a soliton has to move in every step. The speed is measured discretely as moving from one node to a next one.

(iv) Solitons move over edges of alternating weights: If a soliton has travelled along an edge of weight w, it can only continue along an edge of weight $3 - w$.

(v) When a soliton travels along an edge of weight w, the weight of the edge changes to $3 - w$.

(vi) When solitons travel along the same edge at the same time, the effect on the weight of that edge must be defined.

Too little seems to be known about such situations. We consider these as illegal in the sequel.

(vii) A soliton does not travel along the same edge twice in immediately consecutive steps.

(viii) We consider sequences of solitons (called bursts) inserted into a molecule. A burst is successful if and only if all its solitons can have left the molecule after a finite amount of time.

This generalizes the single-soliton model: There the transition caused by a soliton is considered to be the identity if the soliton cannot leave the molecule. If one accepts partial successes, our model would have to change.

In essence our view is based on the following assumption: An input which is going to be unsuccessful is not going to be sent.

A fundamental model of soliton behaviour in polymers has been established by Heeger et al. in [46], often cited as the SSH model. Solitons behave differently, of course, at the molecular level from what can be observed in the water of canals [65]. There are, however, some striking analogies, by which assumptions required for a discrete model become justified – at least to elicit further research. Collisions of solitons in various settings have been studied many times [11, 25, 63, 67, 68]. We have not seen conclusive answers to the question of how collisions of solitons behave phenomenologically in polymers in general, but many detailed answers regarding their movements in polymers in specific environments.

Our mathematical model abstracts from what current physics and chemistry propose. Beyond exposing an interesting mathematical object to investigate, our model puts a challenge to research in physics and chemistry: To determine the extent to which the postulates meet reality, and what solitons and their physical relatives may afford to build very small computers.

6. Multiple Soliton Waves Make a Difference

We now turn to modelling the situation, when more than one soliton travels through a soliton graph. We refer to this as the multi-soliton model. The main problem to be addressed is that of multiple solitons converging towards the same node. After defining inputs in the new model, we provide a set of characteristic examples of problems encountered with the original definition of a soliton path. These examples are used to derive a new definition of how solitons traverse a graph in Section 7 below.

In the single-soliton model the elementary input symbols are pairs of exterior nodes. As mentioned, an alternative, not explored in detail, would be to consider just the exterior nodes as input symbols. For the multi-soliton model we define the input symbols as bursts of exterior nodes or pairs of exterior nodes as follows.

Definition 9 Bursts of Inputs. Let S be a finite non-empty set not containing the symbols $\|$ and $\perp$. Moreover, let $S \cap \mathbb{N}_0 = \emptyset$.

A *burst over* S is a word of the form

$$s_1\|_{k_1}s_2\|_{k_2}\cdots s_{m-1}\|_{k_{m-1}}s_m\perp$$

with the following properties:

(i) $m \in \mathbb{N}$;

(ii) $s_1, s_2, \ldots, s_m \in S$;

(iii) $k_1, k_2, \ldots, k_{m-1} \in \mathbb{N}_0$;

The *length* of such a burst is m.

For $m \in \mathbb{N}$, let $\mathcal{B}_m(S)$ be the set of all bursts of length m over S. Let

$$\mathcal{B}_{\leq m}(S) = \bigcup_{i=1}^{m} \mathcal{B}_i(S) \quad \text{and} \quad \mathcal{B}(S) = \bigcup_{i\geq 1} \mathcal{B}_i(S).$$

When there is no risk of confusion we omit the reference to the set S, that is, we write $\mathcal{B}$ instead of $\mathcal{B}(S)$ etc.

With the definition above we have two specific applications in mind. Consider a soliton graph with X as its set of exterior nodes. As explained further below, the cases of $S = X \times X$ and $S = X$ are of particular interest.

A burst over S is the basic input symbol to the automata under consideration. It is to be interpreted as follows. If the burst is initiated at time t, the symbol s_1 is input at time t; s_2 is input at time $t + k_1$; and, in general, s_j is input at time $t + \sum_{i=1}^{j-1} k_i$. Here the empty sum is defined to be 0. The symbol $\perp$ indicates that the input process pauses until the system has stabilized.

Let G be a soliton graph with set X of exterior nodes. A burst as input has two interpretations:

(i) The set S could be the set X with the implied meaning that $x \in X$ indicates the node where the soliton is injected.

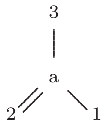
(ii) The set S could be the set $X \times X$ with the implied meaning that $(x, x') \in X \times X$ indicates the nodes where the soliton is injected and received, respectively.

As in the single-soliton model, we only consider the case of $S = X \times X$.

The definition of a burst does not exclude that two distinct solitons enter the graph at the same node or try to travel on the same edge. These situations will be excluded as consequences of our definition of configurations and their trails.

We consider a few simple examples which show that changes to Definition 2 are required for the multi-soliton model and that the multi-soliton model allows for state transitions which do not exist in the single-soliton model. We indicate the position of the solitons in the graphs by symbols: $\bullet$ for the first one, $\circ$ for the second one, and continuing with $\diamond$ and further symbols as may be needed. In each example we first describe the properties of the soliton graph under consideration and then show special situations occurring when selected bursts are input. For the movements of the solitons we compare the effect of the rules of Definition 2 and of Proposition 5.

Example 10. The *3-tree* graph (*soliton valve* [16], *soliton junction* [39]):



(I) Single soliton: The automaton is strongly deterministic and has three states. The basic transitions are

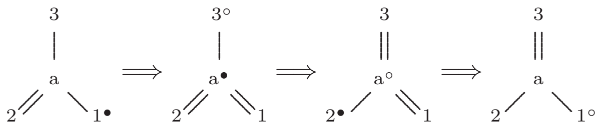
$$\tau_{1,2} = \tau_{2,1},\ \tau_{1,3} = \tau_{3,1},\ \tau_{2,3} = \tau_{3,2},\ \text{and}\ \tau_{1,1} = \tau_{2,2} = \tau_{3,3} = \iota.$$

These satisfy the following relations:

$$\tau_{1,2}^2 = \tau_{1,3}^2 = \tau_{2,3}^2 = \iota,\ \tau_{1,3}\tau_{1,2} = \tau_{1,2}\tau_{2,3} = \tau_{2,3}\tau_{1,3},\ \tau_{1,3}\tau_{2,3} = \tau_{2,3}\tau_{1,2} = \tau_{1,2}\tau_{1,3}.$$

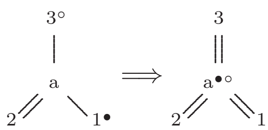
The transition monoid is the symmetric group $\mathfrak{S}_3$.

(II) Input $(1,2)\|_1(3,1)\perp$:



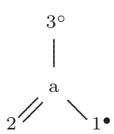
There is nothing unusual and the behaviour is equivalent to $\tau_{2,3}$.

(III) Input $(1,2)\|_0(3,2)\perp$:



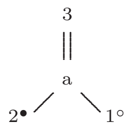
What happens now? The solitons have the same target. Can one decide in advance when such a situation arises? Both solitons would leave at the same time on the same edge and it is not clear what happens to the weight of the edge from a to 2. Regardless of what happens to the weight, the resulting graph is not a soliton graph.

(IV) Input $(1,2)\|_0(3,1)\perp$:



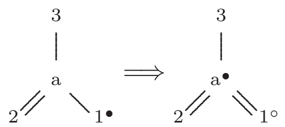
This looks similar to the previous case. However, the targets of the solitons are different. By Definition 2, the soliton $\bullet$ can move while $\circ$ cannot.

Following the construction in Proposition 5, both can leave leading to:

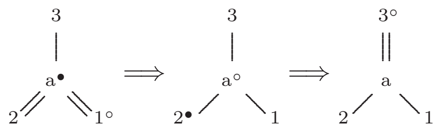


In this case the input would be equivalent to $(2,3)\perp$. This shows that Proposition 5 does not hold for the case of multiple solitons. However, its construction leads to an intuitively more convincing result than the original definition.

(v) Input $(1,2)\|_1(1,2)\perp$: The first step would lead to the following situation.

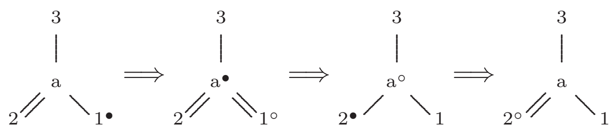


According to Definition 2 the first soliton can move; the second one is stuck. If one insists that a soliton moves in every step, this could be treated as an impossible input, resulting in the identity transformation. Can one decide whether such a situation will arise? If one removes the targets from the input, that is, one inputs $1 \|_1 1$, then one can continue



and this is even deterministic.

Using the construction in Proposition 5 instead, both solitons can move



resulting in the identity transformation.

Example 10 shows that the definitions of soliton paths in Definition 2 and Proposition 5 are not equivalent in the case of multiple solitons, not even when the solitons do not meet on the same node. Moreover, in certain situations it is not clear how the weights of edges would change even when the soliton move itself is possible.

Example 11. Consider the graph G shown in Figure 5. There are several general observations to be made about such a graph. A careful analysis of several cases that may occur when one or two solitons enter this graph leads to the following observations.

(I) A single soliton: The path from h to k is impervious. The automaton has four states corresponding to the four arrangements of alternating weights on the two cycles. The basic transitions are $\tau_{1,1}$, $\tau_{1,2} = \tau_{2,1} = \iota$, and $\tau_{2,2}$ satisfying the relations $\tau_{1,1}^2 = \tau_{2,2}^2 = \iota$ and $\tau_{1,1}\tau_{2,2} = \tau_{2,2}\tau_{1,1}$. Hence, the transition monoid is the group $\mathfrak{S}_2 \times \mathfrak{S}_2$.

(II) Two solitons entering at different exterior nodes: The two cases of the first soliton entering at nodes 1 or 2 are analogous. Hence, we examine only the former. This leads to four cases depending on the exit nodes of the two solitons.

In the sequel, by 'left cyle' we mean the cycle containing nodes $a, b, \ldots, f$, and by 'right cycle' we mean the cycle with nodes $m, n, \ldots, r$, viewing the graph from the reader's perspective. From the perspective of solitons entering at nodes 1 or 2, 'left' and 'right' would be interchanged.

(A) Input $(1,1)\|_j(2,1)\bot$: Regardless of the value of j, the first soliton $\bullet$ moves in the direction of the left cycle.

(1) Let $j \leq 11$: The soliton $\bullet$ is somewhere on the path

$$1, h, g, a, b, \ldots, f, a, g, h,$$

when the second soliton $\circ$ is about to enter the graph. After the next step, $\circ$ is at node k and cannot move towards node h as the path from k to h is impervious. It will have to move towards the right cycle. Then $\bullet$ will reach node h no later than $\circ$ returns to node k. Hence $\bullet$ must leave the graph by node 1 and does so. The soliton $\circ$ could leave by node 2, but is not permitted to do so according to the specific input burst.

(2) Let $j \geq 12$: The soliton $\bullet$ is at node 1 or has already left the graph via node 1 while $\circ$ is at node 2 entering the graph. The soliton $\circ$ cannot leave at 1. The situation is similar to the previous one.

There are two interpretations of the situation in these two cases. They depend on what one considers the action of a burst on a soliton graph: Do all solitons in the burst have to traverse the graph successfullly? Or does one ignore those solitons in the burst which cannot do so and only consider the other ones? With the former interpretation, the burst $(1,1)\|_j(2,1)\bot$ causes the transition ι. With the latter, it causes the transition $\tau_{1,1}$.

(B) Input $(1,1)\|_j(2,2)\bot$: The transition is $\tau_{1,1}\tau_{2,2}$ for all $j \geq 0$.

(C) Input $(1,2)\|_j(2,1)\bot$: The transition is ι for all $j \geq 0$.

(D) Input $(1,2)\|_j(2,2)\bot$: A case distinction similar to that for the burst $(1,1)\|_j(2,1)\bot$ is needed. The resulting transition is either $\tau_{2,2}$ or ι.

These four types of inputs together with the four types where $\bullet$ enters at node 2 do not lead to new soliton graphs beyond those obtained for the single-soliton model.

(iii) Two solitons entering at the same exterior node: Because of symmetry, it suffices to consider the case of 1 being the entry node. Again there are four cases depending on the exit nodes, triggered by bursts

$$(1,1)\|_j(1,1)\perp,\ (1,1)\|_j(1,2)\perp,\ (1,2)\|_j(1,1)\perp,\ \text{and } (1,2)\|_j(1,2)\perp,$$

respectively. The parameter j plays a crucial rôle. A detailed study of the cases reveals the following:

The parity of the occurrence of the nodes in the burst influences what is going to happen. If, in a burst an exterior node occurs an even number of times then its weight will be unchanged after the burst has completely left the graph; if it occurs an odd number of times, its weight will have changed. Moreover, once every soliton has left the graph, the weights in the cycles may have changed, but the weights of (a,g) and (l,m) are 1 and those of (g,h) and (l,k) are 2. This observation is based on the fact that an even number of traversals is needed for a soliton to exit. Thus, if there were any additional states, these would differ from the ones considered so far regarding the weights on the path from h to k and possibly of the edges $(h,1)$ and $(k,2)$. But, for bursts of length 2, these weights remain unchanged. Hence, all edges except the ones in the cycles have the same weights as in G. In other words, bursts of at most length 2 do not increase the number of states.

In summary, there are new paths, but no new states in the case of bursts of length 2. Longer bursts seem not to exhibit new phenomena. ■

The two examples lead to the following observations:

(i) The constructions of soliton paths according to Definition 2 and Proposition 5 are not equivalent when multiple solitons are concerned. The latter is more convincing.

(ii) Some soliton in a burst may not be able to complete the traversal. What is the transition?

(iii) Two solitons may have to move, and be able to do so, on the same edge at the same time. What is the weight of the edge going to be?

(iv) An impervious path may become pervious.

(v) Non-determinism may arise when more than one soliton is present.

The postulates listed in Section 5 will serve as guidance in unclear situations.

Rather than continuing with further detailed examples, some of them rather intriguing, we now just list the special situations to be found in the multi-soliton model some of which require a reconsideration of the definitions. We assume that G is a given soliton graph. The following observations and the previous examples provide the intuitive basis for the formal definitions in the next section of this paper.

Situation 12 Solitons Following. Two solitons are going in the same direction, right-to-left say.

$$\text{---}\ a\ =\ b^{\bullet}\ \text{---}\ c^{\circ}\ =$$

With the standard rules they just move along. There is, potentially, a physical problem as waves tend to stretch over several atoms.

Using Observation 8 one could argue that this problem could be avoided by using longer paths. However, this still leaves the problem of how to prevent such situations from arising to begin with. ♢

Situation 13 Direct Collision. There are two solitons travelling in opposite directions, about to arrive at the same node in the next step:

$$- \; a^{\bullet} \; - \; b \; = \; c^{\circ} \; =$$

Here • travels from left to right and ∘ travels from right to left. The weight to the left of a was 2, that to the right of c was 1. Using the rules provided so far, both solitons can move to b. According to the model one arrives at the situation

$$- \; a \; = \; b^{\bullet\circ} \; - \; c \; =$$

from which one cannot continue with the existing rules. • arrived on an edge of weight 1 and needs an edge of weight 2, but cannot turn around. The situation for ∘ is analogous.

Whether this makes physical sense may depend on the actual physical environment, not just the molecule in isolation. ♢

Situation 14 Blockage. There are two solitons travelling in opposite directions, about to arrive at two nodes just one edge apart:

$$a^{\bullet} \; - \; b \; = \; c \; - \; d^{\circ}$$

Again • travels from left to right and ∘ travels from right to left. After one step one gets the following configuration.

$$a \; = \; b^{\bullet} \; = \; c^{\circ} \; = \; d$$

Neither • nor ∘ can move anymore.

A burst which inevitably leads to such a *blockage* should be avoided. In keeping with the analogous situation in the single-soliton model, that is, when there is no soliton path for the given input, the transition should be defined to be the identity mapping. ♢

Situation 15 Direct Same-Weight Merge. There are two solitons approaching a node of degree 3, both entering through an edge of weight 1.

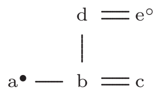
$$\begin{array}{cccccc} & & d^{\circ} & & & \\ & & | & & & \\ a^{\bullet} & - & b & = & c & - \end{array}$$

Some edges leading into nodes a and d have weight 1. Both solitons move to node b.

$$\begin{array}{cccccc} & & d & & & \\ & & \| & & & \\ a & = & b^{\bullet\circ} & = & c & - \end{array}$$

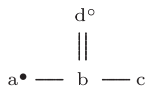
Now • could move to c or d, and ∘ could move to c or a according to the existing rules. But not both can move to node c. ♢

Situation 16 Delayed Same-Weight Merge. There are two solitons approaching a node of degree 3, both from an edge of weight 1, but with one time step different.

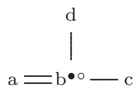


There is no problem with the existing rules: • goes on to c while ∘ goes on to a. This is consistent with the intuitive wave model. ♢

Situation 17 Direct Different-Weight Merge. There are two solitons approaching a node of degree 3, • on an edge of weight 1, ∘ on an edge of weight 2.

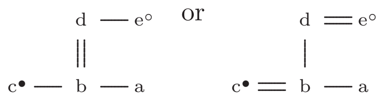


After one step on has:

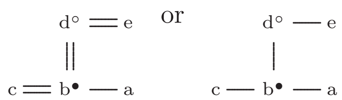


Here ∘ can move on to node c, but • can go nowhere. ♢

Situation 18 Delayed Different-Weight Merge. There are two solitons approaching the same node of degree 3, separated by one step in time:

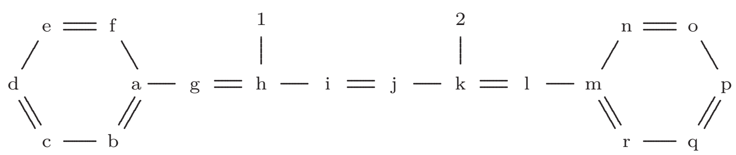


The next step leads to one of the following two cases, respectively:



In the first case, each soliton would move along the edge (b, d), but could not do so at the same time. In the second case, ∘ moves to b; • can move to a, but not to d. ♢

Situation 19 Impervious Paths. Two or more solitons can open up an impervious path. Consider the soliton graph



shown in Figure 5. Using the burst $(1,1)\|_1(1,1)\perp$ the path from h to k is open to the second soliton. ♢

7. How Multiple Solitons Travel

For the single-soliton model it is sufficient to consider the paths a soliton might travel through. In the multi-soliton model one needs to consider multiple paths and their interaction. This idea is captured in the following definitions. It is important to avoid an intuitive trap: When modelling the movement of multiple solitons, there is no order among the movements of each of them. The most adequate view, albeit a quite severe abstraction, is to have a timewise indistinguishable movement. Thus, we treat such systems as self-clocked, where events which are close in time are treated as simultaneous. Given that a soliton wave may be rather long compared to the virtual clock times, this does not seem to imply an undue restriction.

For the sequel, we assume that $G = (N, E, w)$ is a soliton graph and that the nodes appearing in bursts are exterior nodes of G.

Definition 20 Position Map. For $m \in \mathbb{N}$, let $\mathfrak{m} = \{1, 2, \ldots, m\}$. Further, let $G = (N, E, w)$ be a soliton graph such that $N \cap \mathbb{N}_0 = \emptyset$. A *position map* for m is a mapping of $\mathfrak{m}$ into $N \cup \mathbb{N}_0$.

If π is a position map for m, then $\pi(i)$ indicates at which node the ith soliton is or how many steps are still required until it will enter the graph. Thus $\pi(i) = 1$ means that the ith soliton will enter the graph in the next step. $\pi(i) = n$ with $n \in N$ means that the soliton is at node n. $\pi(i) = 0$ means, by definition, that the i-th soliton has left the graph.

Definition 21 Initial Position Map for a Burst. Let

$$b = (n_1, n'_1)\|_{k_1}(n_2, n'_2)\|_{k_2} \cdots (n_m, n'_m)\perp$$

be a burst of length m. The *initial position map* π_b *for* b is defined as follows: Let r be minimal such that $k_1 = k_2 = \cdots k_r = 0$ and $k_{r+1} > 0$ or $r = m - 1$. Then

$$\pi_b(i) = \begin{cases} n_i, & \text{if } 1 \le i \le r+1, \\ k_{r+1}, & \text{if } i = r+2, \\ \pi_b(i-1) + k_{i-1}, & \text{if } i > r+2. \end{cases}$$

For example, let

$$b = (n_1, n'_1)\|_0(n_2, n'_2)\|_2(n_3, n'_3)\|_0(n_4, n'_4)\|_1(n_5, n'_5)\perp$$

be a burst. Then π_b is given by the following table:

soliton i	1	2	3	4	5
position $\pi_b(i)$	n_1	n_2	2	2	3

This indicates that the first and second solitons are at nodes n_1 and n_2, respectively, and that the remaining ones are waiting for 2 or 3 steps before entering the graph. It may sometimes be convenient to illustrate a position map as shown in Figure 7. The connections to exterior nodes are extended as needed by dotted lines with additional node positions which indicate the *waiting* positions.

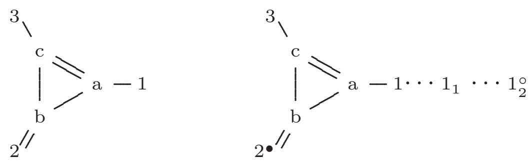


Figure 7: A soliton graph and the drawing for the initial position map π_b of the burst $b = (2,1)\|_2(1,3)\perp$.

Definition 22 Final Position Map. A position map π for m is said to be *final* if $\pi(i) = 0$ for all $i \in \mathfrak{m}$.

The processing of a burst starts with its initial position map and ends with a final position map corresponding in terms of the number of solitons. Small intermediate steps occur leading from the initial position map to the final position map. The graph undergoes a sequence of changes until a (stable) soliton graph is reached again. The duration of the sequence as well as the actual changes can be non-deterministic. We refer to the (stable) soliton graphs as states and to the other graphs as intermediate states.

In general, for a soliton graph $G = (N, E, w)$ one considers the underlying graph $\hat{G} = (N, E)$ without weights. We need to consider arbitrary weighted graphs based on $\hat{G}$ (or G) where the weight does not need to satisfy the condition of soliton graphs. We still restrict the weights of edges to be either one or two. However, the weight of a node of degree 2 could be 2, 3, or 4 and the weight of a node of degree 3 could be between 3 and 6. Such weighted graphs serve to define the state transitions of a soliton automaton.

Definition 23 Potential Successor Map. Let G be a soliton graph. Let $m \in \mathbb{N}$, and let π and π' be position maps for m. Let

$$b = (n_1, n'_1)\|_{k_1}(n_2, n'_2)\|_{k_2} \cdots (n_m, n'_m)\perp$$

be a burst of length m.

The map π' is a *potential (direct) successor* of π (with respect to b), if and only if

$$\pi'(i) = \begin{cases} \pi(i) - 1, & \text{if } \pi(i) \in \mathbb{N}_0 \text{ and } \pi(i) > 1, \\ n_i, & \text{if } \pi(i) \in \mathbb{N}_0 \text{ and } \pi(i) = 1, \\ n, & \text{if } \pi(i) \in N,\ \pi(i) \neq n'_i,\ n \in N, \text{ and } \big(\pi(i), n\big) \in E, \\ 0, & \text{if } \pi(i) = n'_i \text{ or if } \pi(i) = 0. \end{cases}$$

for $i = 1, 2, \ldots, m$.

In general, a position map π can have several potential successor maps π'; for the computation of the latter, the weights of edges are ignored etc. On the other hand, the initial position map π_b of a burst b has at most two potential successor maps.

Lemma 24. *Let G be a soliton graph, let b be a burst of length m with $m \in \mathbb{N}$, and let π_b be the initial position map for b. Then there are only one or two potential successor maps π'_b for π_b.*

Proof. The value of $\pi_b(i)$ with $i \in \mathfrak{m}$ is either in $\mathbb{N}$ or equal to n_i. In the former case, there are two mutually exclusive possibilities: if $\pi_b(i) > 1$ then $\pi'_b(i) = \pi_b(i) - 1$; if $\pi_b(i) = 1$ then $\pi'_b(i) = n_i$. In the latter case, there is a unique node $n \in N$ such that $(n_i, n) \in E$, hence $\pi'_b(i) = n$ is one possibility. The other one is $\pi'_b(i) = 0$ if $n_i = n'_i$. $\square$

We can now define configurations and configuration trails for bursts. Such a trail consists of a finite sequence of pairs (G_j, π_j) with $j = 0, 1, \ldots, k$ for some $k \in \mathbb{N}_0$, each called a configuration, where each G_j is a weighted graph with $\hat{G}$ as the underlying unweighted graph and each π_j is a position map. For each j with $0 \leq j < k$, π_{j+1} is a potential successor of π_j, G_j must meet certain weight conditions, and the weights in G_{j+1} are computed according to certain rules similar to the ones for the single-soliton model. The details are as follows:

Definition 25 Configuration and Configuration Trail. Let $G = (N, E, w)$ be a soliton graph. Let $m \in \mathbb{N}$, and let π and π' be position maps for m. Let

$$b = (n_1, n'_1)\|_{k_1}(n_2, n'_2)\|_{k_2} \cdots (n_m, n'_m)\bot$$

be a burst of length m.

(I) A *configuration* (for b) is a pair (G', π) such that $G' = (N, E, w')$ is a weighted graph with weights in $\{1, 2\}$ and π is a position map for m.

(II) A *configuration trail* for G and b is a finite sequence

$$(G_0, \pi_0), (G_1, \pi_1), \ldots$$

of configurations for b with the following properties.

(A) $G_0 = G$, and π_0 is the initial position map for b.

(B) π_1 is a potential successor of π_0 such that $\pi_0(i) \in N$ implies $\pi_1(i) \in N$ for all $i \in \mathfrak{m}$. $G_1 = (N, E, w_1)$ is obtained from $G_0 = (N, E, w_0)$ by changing the weights of some edges as follows: If $\pi_0(i) \in N$, then

$$w_1\big(\pi_0(i), \pi_1(i)\big) = w_1\big(\pi_1(i), \pi_0(i)\big) = 3 - w_0\big(\pi_0(i), \pi_1(i)\big).$$

For all other edges the weights remain unchanged.

(C) Let $j > 1$. The sequence

$$(G_0, \pi_0), (G_1, \pi_1), \ldots, (G_j, \pi_j)$$

is a configuration trail, if and only if

$$(G_0, \pi_0), (G_1, \pi_1), \ldots, (G_{j-1}, \pi_{j-1})$$

is a configuration trail such that π_{j-1} is not final, and $G_j(N, E, w_j)$, π_j and the sequence satisfy the following conditions (for all $i \in \mathfrak{m}$):

(1) π_j is a potential successor of π_{j-1}.

(2) If $\pi_{j-1}(i) \in N$ is exterior and $\pi_{j-2}(i) = 1$, then $\pi_j(i) \in N$.

(3) If $\pi_{j-1}(i) \in N$ is exterior and equal to n'_i, and if $\pi_{j-2}(i) \in N$, then $\pi_j(i) = 0$.

(4) If $\pi_{j-1}(i) \in N$ is interior and $\pi_{j-2}(i) \in N$, then

$$w_{j-2}\big(\pi_{j-2}(i), \pi_{j-1}(i)\big) \neq w_{j-1}\big(\pi_{j-1}(i), \pi_j(i)\big).$$

(5) If $\pi_j(i) \neq 0$, then $\pi_j(i) \neq \pi_{j-1}(i)$ and $\pi_j(i) \neq \pi_{j-2}(i)$.

(6) G_j is obtained from G_{j-1} by changing the weights of some edges as follows: If $\big(\pi_{j-1}(i), \pi_j(i)\big) \in E$, then

$$w_j\big(\pi_{j-1}(i), \pi_j(i)\big) = w_j\big(\pi_j(i), \pi_{j-1}(i)\big) = 3 - w_{j-1}\big(\pi_{j-1}(i), \pi_j(i)\big).$$

All other weights remain unchanged.

(iii) A configuration trail is *legal*, if it satisfies the following conditions for all $j \geq 1$:

(a) If $\pi_{j-1}(i)$ and $\pi_{j-1}(i')$ are nodes and $\pi_{j-1}(i) = \pi_{j-1}(i')$ for some distinct i and i', then $\pi_j(i) \neq \pi_j(i')$.

(b) If $\pi_{j-1}(i)$ and $\pi_{j-1}(i')$ are nodes with $\big(\pi_{j-1}(i), \pi_{j-1}(i')\big) \in E$, then $\pi_j(i) \neq \pi_{j-1}(i')$ or $\pi_j(i') \neq \pi_{j-1}(i)$.

(iv) A configuration trail

$$(G_0, \pi_0), (G_1, \pi_1), \ldots, (G_j, \pi_j)$$

is *partial* if π_j is not final. Otherwise it is *total*.

We explain some of the subtle points of this definition.

(i) Note that the graph in a configuration need not be a soliton graph. It represents the situation when all solitons have reached the “next” nodes on their ways. The position map defines where they are.

(ii) Condition ii.b guarantees that the possibility of $\pi_1(i) = 0$ according to Definition 23 is excluded.

(iii) When $j > 1$, $\pi_{j-1}(i) = n_i$ is ambiguous as n_i could be equal to n'_i. Therefore, we consider $\pi_{j-2}(i)$ in Conditions ii.c.2 and ii.c.3 to distinguish how the node has been reached, from the exterior or from the interior.

(iv) As stated, Parts ii.b and ii.c may be undefined without the legality conditions. Integrating these might have made things harder to read. We chose this slightly inconsistent presentation to make things easier to comprehend.

(v) The legality conditions state that no two solitons can traverse the same edge at the same time regardless of their mutual directions. As a consequence, no two solitons can enter the same exterior node at the same time; this holds true both for exterior nodes used as entry points and those used as exit points. Two can be at an interior node simultaneously, but must leave it on different edges. Moreover, two solitons cannot simply swap places. Typical cases which are excluded by the legality condition are shown in Example 10(iii) and in Situation 14.

The next proposition claims that, for any graph in a configuration of a legal configuration trail, the number of solitons at any interior node n is less than the degree of n.

Proposition 26. *Let $G = (N, E, w)$ be a soliton graph and let b be a burst of length m. Let*

$$(G_0, \pi_0), (G_1, \pi_1), \ldots, (G_j, \pi_j)$$

be any legal configuration trail for G and b. Then

$$|\{ \, i \mid i \in \mathfrak{m}, \pi_h(i) = n \, \}| < d(n)$$

for $h = 0, 1, \ldots, j-1$ and all interior nodes $n \in N$.

Proof. Consider (G_h, π_h) with $0 \leq h < j$ and an interior node n. Because of the legality condition, no more than $d(n)$ solitons can arrive at the node n simultaneously. We show that $d(n)$ solitons cannot arrive at n simultaneously when there is another legal step in the trail.

We distinguish several cases according to the degree of n and to the number of solitons at n prior to the step.

First consider $d(n) = 2$. We show that at most one soliton can move onto node n when $h < j$.

(i) Suppose there is no soliton at node n and that two solitons are about to move to that node. The situation is as follows or symmetrical to it:

$$\mathrm{a}^{\bullet} = \mathrm{n} - \mathrm{b}^{\circ}$$

Both solitons move to n resulting in the following situation:

$$\mathrm{a} - \mathrm{n}^{\bullet\circ} = \mathrm{b}$$

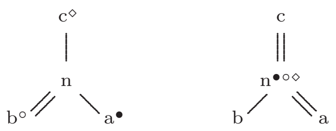
Then $\bullet$ needs a single bond to leave to the right, and $\circ$ needs a double bond to leave to the left. Therefore, step $h+1$ does not exist. Thus two solitons cannot enter n in this case.

(ii) Suppose there are solitons present at n, and let h be smallest with this property. This implies, by (1), that there is only one soliton, say $\diamond$, at n. This soliton has to leave on one of the two edges. Any soliton entering node n in the same step can only use the other one of the edges. Thus, by the legality condition there is at most one soliton at n after this step.

This completes the proof for $d(n) = 2$.

Second consider $d(n) = 3$. The proof is similar.

(i) Suppose there is no soliton at node n and that three solitons are about to move to n. The situations before and after the step are as follows:



The soliton $\circ$ cannot leave as it would need an edge of weight 1. Therefore, step $h+1$ does not exist. Thus three solitons cannot enter a node in this case.

(ii) Suppose there are k solitions at n, and let h be smallest with this property. As before this implies that $1 \leq k \leq 2$. In the next step these solitons must leave n on k different edges. By the legality condition any soliton entering node n must use one of the remaining $3-k$ edges. Hence at most $3-k$ solitons can do so. This shows, that there are at most 2 solitons at n after this step.

This completes the proof for $d(n) = 3$. □

Using the assumptions of Proposition 26, the statement does not hold in general for $h = j$. In that case

$$|\{\, i \mid i \in \mathfrak{m}, \pi_h(i) = n \,\}| = d(n)$$

is possible. However not all solitons can leave node n because of the legality conditions.

Corollary 27. *Let $G = (N, E, w)$ be a soliton graph and let b be a burst of length m. Let*

$$(G_0, \pi_0), (G_1, \pi_1), \ldots, (G_j, \pi_j)$$

be any total legal configuration trail for G and b. Then

$$|\{\, i \mid i \in \mathfrak{m}, \pi_h(i) = n \,\}| < d(n).$$

for $h = 0, 1, \ldots, j$ and all interior nodes $n \in N$.

Definition 28 Result of a Burst. Let G be a soliton graph and let b be a burst. The *result of burst b on G* is the set $\mathsf{Result}(G, b)$ of weighted graphs G' such that there is a total legal configuration trail for G and b transforming G into G'.

The set $\mathsf{Result}(G, b)$ should be considered as analogous, in the multi-soliton model, to the set $S(G, n, n')$ in the single-soliton model. We show below that every element of $\mathsf{Result}(G, b)$ is again a soliton graph.

We extend the operator Result to sets of graphs and bursts and then define its closure under iteration: Let $\mathcal{G}$ be the set of soliton graphs with the same underlying graph. Let X be the set of exterior nodes of these graphs. Let $B \subseteq \mathcal{B}(X \times X)$ be a set of bursts. Define

$$\mathsf{Result}(\mathcal{G}, B) = \bigcup_{G \in \mathcal{G}} \bigcup_{b \in B} \mathsf{Result}(G, b).$$

For $i \in \mathbb{N}_0$ let

$$\mathsf{Result}^i(\mathcal{G}, B) = \begin{cases} \mathcal{G}, & \text{if } i = 0, \text{ and} \\ \mathsf{Result}\big(\mathsf{Result}^{i-1}(\mathcal{G}, B), B\big), & \text{if } i > 0. \end{cases}$$

Finally, let

$$\mathsf{Result}^*(\mathcal{G}, B) = \bigcup_{i \geq 0} \mathsf{Result}^i(\mathcal{G}, B).$$

For a given graph G, the set of soliton graphs with G as underlying graph is finite. Therefore, the set $\mathcal{G}$ is finite. Hence also $\mathsf{Result}^*(\mathcal{G}, B)$ is finite and there is a finite subset B' of B such that $\mathsf{Result}^*(\mathcal{G}, B)$ is equal to $\mathsf{Result}^*(\mathcal{G}, B')$ and $\mathsf{Result}^*(\mathcal{G}, B')$ can be computed in finitely many steps.

Proposition 26 establishes that no interior node n can have more than $d(n) - 1$ solitons occupying it. The following more precise statement clarifies the connection between the degree of an interior node, its weight, and the number of solitons at the node.

Proposition 29 Interior Nodes without Solitons. *Let $G = (N, E, w)$ be a soliton graph and let*

$$b = (n_1, n_1')\|_{k_1}(n_2, n_2')\|_{k_2} \cdots (n_m, n_m')\bot$$

be a burst. Let

$$(G_0, \pi_0), (G_1, \pi_1), \ldots, (G_j, \pi_j)$$

be any legal configuration trail for G and b with $j > 1$. Then, for $h = 0, 1, \ldots, j$ and all interior nodes $n \in N$, $w_h(n) = d(n) + 1$ whenever $\pi_h^{-1}(n) = \emptyset$.

Proof. As the trail is legal, at most $d(n) - 1$ solitons can be at n at any step $h < j$. For $h = 0$ the statement holds true. Consider the smallest h such that solitons arrive at n for the first time. Let h' be smallest such that $h < h' \leq j$ such that no solitons are present at node n at step h'. If no such h and h' exists, the statement is trivially true.

Hence, suppose h and h' exist. We show that the statement holds true at step h'. By induction, this implies the claim.

We distinguish two main cases and several sub-cases:

Case 1: Let $d(n) = 2$. At step h one has one of the following two situations:

$$\mathrm{a} \;-\; \mathrm{n}^\bullet \;-\; \mathrm{b} \qquad \text{or} \qquad \mathrm{a} = \mathrm{n}^\bullet = \mathrm{b}$$

Without loss of generality, the soliton moves from left to right. In step $h+1$ it moves to node b. If no further soliton moves to node n in that step, one has $h' = h+1$ and $w_{h+1}(n) = 3$ as claimed. On the other hand, if another soliton $\circ$ moves to node n in that step, it must also move from left to right because of the legality condition. Hence we get the respective other one of the situations above with $\bullet$ replaced by $\circ$. By induction the property as claimed follows.

Case 2: Let $d(n) = 3$. In step h one or two solitons can enter. Without loss of generality, we assume the situation in step $h-1$ is as follows:

$$\begin{array}{ccccc} & & \mathrm{b} & & \\ & & \| & & \\ \mathrm{a} & - & \mathrm{n} & - & \mathrm{c} \end{array}$$

Case 2.1: Assume that only a single soliton $\bullet$ enters node n at step h: this could be from any one of the nodes a, b and c. The cases of a and of c are analogous. Thus it suffices to consider the first two, which result in the following situations:

$$\begin{array}{ccccc} & & \mathrm{b} & & \\ & & \| & & \\ \mathrm{a} & = & \mathrm{n}^{\bullet} & - & \mathrm{c} \end{array} \qquad \text{or} \qquad \begin{array}{ccccc} & & \mathrm{b} & & \\ & & | & & \\ \mathrm{a} & - & \mathrm{n}^{\bullet} & - & \mathrm{c} \end{array}$$

In step $h+1$ the soliton will have to leave by node b in the first case and by one of nodes a or c in the second case; without loss of generality we assume the former. If no new solitons arrive, one has $h' = h+1$, and the weight condition holds as claimed.

If a single new soliton $\circ$ arrives, it must come from a or c in the first case, resulting in one of the two situations above with node names permuted; in the second case $\circ$ can come from b or c resulting in situations similar to the first one above. If, on the other hand, two solitons $\circ$ and $\diamond$ arrive, they must come from a and c in the first case resulting in

$$\begin{array}{ccccc} & & \mathrm{b} & & \\ & & | & & \\ \mathrm{a} & - & \mathrm{n}^{\circ\diamond} & = & \mathrm{c} \end{array}$$

In this situation, the soliton arriving from c cannot leave legally, hence h' does not exist and the claim follows. In the second case they must come from b and c, leading to

$$\begin{array}{ccccc} & & \mathrm{b} & & \\ & & \| & & \\ \mathrm{a} & = & \mathrm{n}^{\circ\diamond} & = & \mathrm{c} \end{array}$$

Before we continue looking at the latter new situation, we investigate, what happens, when already at step h two solitons enter node n.

Case 2.2: Assume that two solitons $\circ$ and $\diamond$ enter node n at step h. There are two non-equivalent cases. They can come from a and b or, symmetrically, from c and b resulting in an illegal situation, or they come from a and c resulting in a situation similar to the one above with the weight of node n equal to 6.

From here we combine the two subcases, considering only the situation

$$\begin{array}{ccc} & \mathrm{b} & \\ & \| & \\ \mathrm{a} = & \mathrm{n}^{\circ\diamond} & = \mathrm{c} \end{array}$$

Both solitons must leave in the next step. If no new soliton arrives then that is step h', and the claim follows. Otherwise at most one new soliton can arrive at node n because of the legality condition. The resulting situation is equivalent the one considered above in Case 2.1 with the weight of node n being 3.

The claim follows by induction. □

Proposition 30 Preservation of Soliton Graphs under Bursts. *Let G be a soliton graph and let b a burst. Every $G' \in \mathsf{Result}(G, b)$ is a soliton graph.*

Proof. Every $G' \in \mathsf{Result}(G, b)$ is obtained by a total legal configuration trail. As the trail is total, there is no soliton on any node in the end. Hence, by Proposition 29, G' is a soliton graph. □

Proposition 31 Model Consistency. *Let G be a soliton graph. Let n and n' be exterior nodes of G and let $b = (n, n')\bot$. Then $S(G, n, n') = \mathsf{Result}(G, b)$. Moreover, there is a one-to-one correspondence between soliton paths from n to n' and total legal configuration trails for b.*

Proof. This is a direct consequence of the equivalence of the constructions in Proposition 5 and in Definition 2 and, thus, with Definition 25, for the special case of bursts of length 1. □

Definition 32 Multi-Soliton Automaton. Let G be a soliton graph with set X of exterior nodes. Let $B \subseteq \mathcal{B}(X \times X)$ be a set of bursts. Let

$$\mathsf{States}(G, B) = \mathsf{Result}^*(G, B).$$

The *B-soliton automaton* of G is the finite automaton $\mathcal{A}_B(G)$ with inputs $b \in B$, state set $\mathsf{States}(G, B)$ and non-deterministic transition function

$$\tau(G', b) = \begin{cases} \mathsf{Result}(G', b), & \text{if } \mathsf{Result}(G', b) \neq \emptyset, \\ \{G'\}, & \text{otherwise,} \end{cases}$$

for $G' \in \mathsf{States}(G, B)$ and $b \in B$.

Note that $\mathsf{States}(G, B)$ is bounded. Therefore, there is finite set B of bursts such that $\mathsf{States}(G, B) = \mathsf{States}(G, B')$ for all sets B' of bursts with $B \subseteq B'$.

Proposition 33 Basic Properties of a Soliton Automaton. *Let G be a soliton graph with set X of exterior nodes. Let $B \subseteq \mathcal{B}(X \times X)$, $m \in \mathbb{N}$, and let B_m and $B_{\leq m}$ be the sets of bursts from B with lengths m and at most m, respectively.*

(i) *$\mathcal{A}_B(G)$ is connected (as automaton) for every B. Every state can be reached from G.*

(ii) *$\mathcal{A}_{B_{\leq m}}(G)$ is a subautomaton of $\mathcal{A}_{B_{\leq m+1}}(G)$.*

(iii) *There is a soliton graph G such that $\mathcal{A}_{\mathcal{B}_1}(G)$ is a proper subautomaton of $\mathcal{A}_{\mathcal{B}_{\leq 2}}(G)$.*

(iv) *There is a $k \in \mathbb{N}$, depending on G, such that*

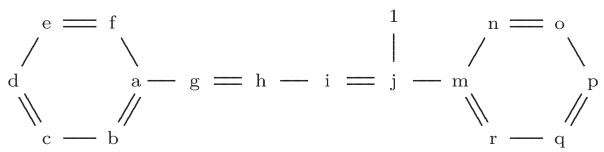
$$\mathsf{States}(G, B_{\leq k}) = \mathsf{States}(G, B_{\leq k+j})$$

for all $j \in \mathbb{N}$.

(v) *There is a $k \in \mathbb{N}$, depending on G, such that $\mathcal{A}_{B_{\leq k}}(G) = \mathcal{A}_{B_{\leq k+j}}(G)$ for all $j \in \mathbb{N}$.*

(vi) *Observation 8 does not hold in general for bursts of lengths greater than 1.*

Proof. The first statement is a direct consequence of the definition of the set $\mathsf{States}(G, B)$. The second statement is a consequence of the inclusion $B_{\leq m} \subseteq B_{\leq m+1}$. For the third statement we provide an example: Let G be the following soliton graph.



The path going to the right at node j is impervious for single solitons. However, it is used by the burst $(1, 1)\|_1(1, 1)\perp$, and this changes the weights on both cycles. The automaton $\mathcal{A}_{\mathcal{B}_1}(G)$ has two states while $\mathcal{A}_{\mathcal{B}_{\leq 2}}(G)$ has four states. The transition monoid of the former is $\mathfrak{S}_2$, that of the latter is $\mathfrak{S}_2 \times \mathfrak{S}_2$ or by isomorphism $\mathfrak{V}_4$. The fourth statement is a consequence of the fact that the set of soliton graphs with the same underlying graph is bounded. The fifth statement follows from the fourth by finiteness. For the sixth statement one considers different values of k in the burst $(1, 1)\|_k(1, 1)\perp$ for the example above. $\square$

In the single-soliton model all inputs cause involutorial transformations; hence the soliton automaton is strongly connected and, moreover, the transition monoid is a group. We believe that this might be true also for the multi-soliton model, but expect that some kind of reversal on bursts may be needed. In the fifth statement of Proposition 33 we only assert that the state set will stabilize when a certain length of bursts has been reached. The sixth statement says that at some stage, the automata are the same. We don't know, whether this happens at the same stages.

The example used for the fourth statement enables an impervious path leading to a part of the graph which would be unaccessible otherwise. The example suggests that we should expect a direct product of transition monoids arising from the single-soliton model. We do not think that this is the whole picture.

8. From Here, Where?

Modelling the effect of more than a single soliton turned out to be significantly more complicated than expected. We believe that our model captures most of the essential facts; whether it does, should be answered by physics. One can, however, also treat our model, while originally motivated by physical or chemical processes, as a complicated network traffic model, for instance that of a railway system, in which many entities move around nearly independently, only controlled by local signals. In that sense our model turns into that of parallel asynchronous processes, regardless of its original motivation.

The reader should keep in mind that much of this paper and our ideas is based on physical phenomena known, but not completely explored. Taking our model and its consequences as a hypothesis, physical research could reveal how much of it is realistic and where future considerations of molecular computing should go.

Many natural mathematical questions remain unanswered and are left for a successor to this paper: One needs to clarify the distinction between determinism and strong determinism. What is the time or length bound for bursts, such that adding bursts exceeding these bounds will not change the transition monoid of the automaton? Are the transformations induced by bursts involutorial? [9] Can resets be caused by bursts? [10] Can matching theory help?

To some of these and further natural questions we have partial answers. It has become evident, however, that there are fundamental differences between the single-soliton and the multi-soliton models. Even some of the most elementary properties of multi-soliton behaviour, taken as defined mathematically above, still need to be investigated.

Our work, speculative for computer science, raises concrete questions for physics: (a) how do multiple solitons interact, if at all, at the molecular level? (b) can behaviours postulated by this paper be confirmed by experiments?

It is not clear whether the two notions of determinism considered for soliton automata so far suffice. It is not clear either how these should be distinguished in a physically meaningful sense.

In the multi-wave scenario the length of the soliton wave may be important. Can it really be ignored as in our model? If the answer is no, the length of chains through which a soliton travels could matter even at the logical level.

Is the length of a burst relevant? Most likely it is in some way. The relevance might depend on the size of the number of exterior nodes and on the structure of the graph.

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[9] While the paper was under review, this question has been answered in the negative by Tore Koß in [50, Proposition 1]. That paper is contained in the same special issue, pages 179–186.

[10] This question was answered affirmatively by Tore Koß in the same paper, [50, Theorems 3 and 5].

But what is it?

Considering the bursts as input symbols to a finite automaton, which kinds of transition semigroups arise? Which bursts need to be considered such that all possible transitions can be achieved? What is the precise relation between burst length and stabilization time?

In the case of single-soliton automata the transition monoid is known to be a group of some restricted kind. Is this true also in the case of multi-soliton automata?

This list of questions can be continued quite easily. In this paper we set the stage for automata based on multi-soliton waves in molecules. The questions raised above are left for further studies. At this point we have only rudimentary answers.

Acknowledgements

This research was partially supported by the Natural Sciences and Engineering Research Council of Canada. The authors acknowledge the helpful comments provided by one of the reviewers that led to an improvement of Proposition 33.

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(Received: September 10, 2021; revised: February 15, 2022)