Stochastic mechanics of graph rewriting

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Abstract

We propose an algebraic approach to stochastic graph-rewriting which extends the classical construction of the Heisenberg-Weyl algebra and its canonical representation on the Fock space. Rules are seen as particular elements of an algebra of 'diagrams' (the diagram algebra $\mathscr{D}$). Diagrams can be thought of as formal computational traces represented in partial time. They span a vector space which carries a natural filtered Hopf algebra structure. Diagrams can be evaluated to normal diagrams (each corresponding to a rule) and generate an associative unital (non-commutative) $*$-algebra of rules (the rule algebra $\mathscr{R}$). Evaluation becomes a morphism of unital associative algebras which maps general diagrams in $\mathscr{D}$ to normal ones in $\mathscr{R}$. In this algebraic reformulation, usual distinctions between graph observables (real-valued maps on the set of graphs defined by counting subgraphs), and rules disappear. Instead, natural algebraic substructures of $\mathscr{R}$ arise: formal observables are seen as rules with equal left and right hand sides and form a commutative subalgebra, the ones counting subgraphs forming a sub-subalgebra of identity rules. Actual graph-rewriting (of the DPO type) is recovered as a canonical *representation* of the rule algebra as linear operators over the vector field generated by (isomorphism classes of) finite graphs. The construction of the representation is in close analogy and subsumes the classical (multi-type bosonic) Fock space representation of the Heisenberg-Weyl algebra.

This subtle shift of point of view (away from its canonical representation to the rule algebra itself) has far-reaching and unexpected consequences. We find that natural variants of the evaluation morphism map give rise to concepts of graph transformations hitherto not considered (these will be described in a separate paper, as in this extended abstract we limit ourselves to the simplest concept namely that of DPO-rewriting). We prove very simply a DPO version of the jump-closure theorem, namely that the sub-space of representations of formal graph observables closed under the action of any rule set. From this new jump-closure result follows that for any set of rules $\mathcal{R}$, one can derive a formal and self-consistent Kolmogorov backward equation for (representations) of formal observables.

1. Introduction

Graphs and derivatives (colored graphs, nested graphs, site graphs etc.) are basic components in the modern toolkit of modeling. They appear in varied situations such as the study of epidemics, social dynamics of opinions, ad hoc networks, spin glasses (Gleeson 2013), and also combinatorial chemical reaction networks (Danos et al. 2007). Oftentimes, one has competing rewiring operations or *rules* which locally remodel the graph and, thus, naturally define a Markovian process on the discrete set of graphs. This is the situation we are interested in this paper. Our specific goal is to establish a new route to the study of these models. Traditionally one uses graph transformation systems (Heindel 2009) and the notion of rule and rule application. Here we posit as our primary object a notion of rule diagram. Such diagrams can be seen as formal composition of rules in 'true concurrency' style. Operationally, diagrams can also be understood as neighbourhoods of realizations of processes of interest (and might be seen as specific closed sets in the Skorokod topologies used in Ref. (Gupta et al. 2004)). We put together a formalism to represent such diagrams and their evaluations. With this algebraification of rule composition, the world of rules becomes autonomous - rules can be formally composed using the diagram algebra and then evaluated to (linear combination of) rules by means of a specific evaluation mechanism. Four different variants of evaluation appear and we restrict here to the simplest form (but see below). The net result is that rules form a unital associative algebra $\mathscr{R}$, while (formal) graph observables are just special rules which form a commutative subalgebra of $\mathscr{R}$. The vector space of finite graphs comes back in the picture as the carrier of a natural representation of the rule algebra. Actual graph rewriting is now seen as the induced action and we recover DPO-type rewriting (no implicit edge-deletion is allowed when deleting a node). Other evaluation strategies allow to recover the SPO-type and two new types appear (by time-symmetry). There is no reason in our analysis to prefer DPO-rewriting other than that it allows for shortcuts in the construction of $\mathscr{R}$. Other variants are perfectly workable and we will work them out in another paper.

Ideas presented here are somewhat anticipated in Lowe's 1993 paper on the concept of rule composition (Lowe 1993) for SPO-rewriting. Diagrams themselves are implicit in Hayman's recent construction on traces. But, it is only by decoupling the algebra of rule from its representations that we can operationalise these ideas and develop an efficient and versatile combinatorial framework for quantitative graph-rewriting. Indeed, our construction embodies a combinatorial engine for accurate handling of the many counting situations which arise in the manipulation of graph rewriting systems. In particular, a special case of this construction is that of discrete typed graphs (no edges): $\mathscr{R}$ then boils down to the Heisenberg-Weyl algebra, and $\mathscr{R}$'s representation to the traditional interpretation on this algebra as acting on the multi-type Fock space. Our combinatorial engine thus subsumes analytic combinatorics on the Fock space (Blasiak et al. 2007). Another type of combinatorial work we can put our engine to use is the derivation of the formal forward equation for graph observables. These equations are widely used in the study of stochastic graph models and often use ad hoc counting arguments. A recent example can be found in Ref. (Basak et al. 2015, p21). The derivation relies on a re-derivation of the jump-closure theorem (Danos et al. 2014). Not only do we find a much cleaner derivation but it also generalises in a straightforward manner to obtain a compact formula for the case of correlators of observables (aka multivariate moments). Besides, and this is a more subtle difference, as said, we derive jump-closure for DPO-rewriting which is more intricate than the SPO-version obtained earlier.

2. Preliminaries

Relations. We will work with relations over finite sets. The set of relations between the sets A and B will be denoted by $Rel(A, B)$. The set of one-to-one relations between A and B (aka partial maps from A to B) will be denoted by either $Rel_{11}(A, B)$ or $A \rightharpoonup B$ depending on the context. The domain and codomain of a relation r are defined as $dom(r) = \{a \mid (a, b) \in r\}$ and $cod(r) = \{b \mid (a, b) \in r\}$. $r \in Rel(A, B)$ induces a function $r[\_] : \wp(A) \to \wp(B)$ where $r[U] \triangleq \{b \mid \exists u \in U.(u, b) \in r\}$ for $U \subseteq A$. The identity relation over A will be noted $id_A \in Rel(A, A)$. Sequential composition of relations $r \in Rel(A, B)$ and $s \in Rel(B, C)$ will be denoted by $r; s \in Rel(A, C)$. The Kleene closure of $r \in Rel(A, A)$ will be denoted by $r^* \in Rel(A, A)$. We use r^+ as a notation for $r; r^*$. If $r \in Rel(A, B)$, we denote by $r^{-1} \in Rel(B, A)$ the inverse relation. The equivalence relation generated by $r \in Rel(A, A)$ will be noted $cl_\sim(r)$.

Graphs. We will use exclusively directed multigraphs, however we insist on the fact that all these developments hold in the setting of colored or undirected graphs (Behr et al. 2016). Graphs will be represented as tuples $G = (V, E, s, t)$ where V and E are finite sets of respectively vertices and edges, and $s, t : E \to V$ are the maps associating edges to their source and target vertices. When we allow s and t to be partial maps, we call the graph *partial*. An edge e such that $s(e)$ or $t(e)$ is undefined is *dangling*. If G is a partial graph, we denote by $total(G)$ the largest total subgraph of G, i.e. the graph where all dangling edges of G are removed. The connected component relation $\mathbf{cc}(G) \subseteq V \times V$ is the equivalence relation generated by $\{(s(e), t(e)) \mid e \in E\}$. Given a pair of equivalence relations $\sim_V, \sim_E$ on respectively V and E, A *partial injective morphism of graphs* from (V, E, s, t) to (V', E', s', t') is a pair of one-to-one relations $(f_V : Rel_{11}(V, V'), f_E : Rel_{11}(E, E')$ such that $f_E; s' = s; f_V$ $f_V \circ s = s' \circ f_E$ whenever s and $s' \circ f_E$ are defined (and similarly for t). isomorphisms (f_V, f_E) is an *isomorphism* whenever f_V and f_E are bijections. The set of isomorphism classes of finite graphs will be denoted $G_{\cong}$.

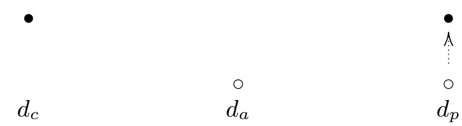
3. The rule diagram & rule algebra

We introduce *rule diagrams*, a syntax for truly concurrent traces of graph rewriting systems. Moreover, these diagrams admit a notion of composition which encompasses the usual notion of matching together with a notion of normalization which implements rewriting. These diagrams and their normal forms span *algebras* which, in the next sections, will be the basis for an interpretation of stochastic graph rewriting systems as *representations*.

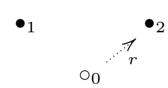
Polarized discrete diagrams. Rule diagrams and their reduction semantics are defined in terms of simpler *polarized discrete diagrams* (pdds), that correspond to traces of set rewriting ((Heindel 2009), Sec. 2) processes. We will denote the set of discrete diagrams, defined below, by D_0.

Definition 1 (Polarized discrete diagram). *A pdd is a tuple $d = (i, o, r, m)$ where i, o are finite, disjoint* input *and* output *sets and $r \in Rel_{11}(i, o), m \in Rel_{11}(o, i)$ will be respectively called the* rule *and the* match *relations. We require the pdd to be* acyclic*; formally, this corresponds to requiring that $id_i \cap (r; m)^+ = \emptyset$ and symmetrically, $id_o \cap (m; r)^+ = \emptyset$. A pdd is* normal *whenever $m = \emptyset$.*

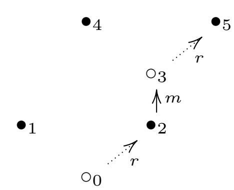
The input and output sets should be thought of as vertices on which some finite set of rules operate. These rules (grouped in the rule relation) are themselves strung together along the match relation. Pdds admit a simple graphical syntax that we now illustrate on small examples. In the pictures to follow, elements of i will be depicted as $\circ$, elements of o as $\bullet$, the rule relation as dotted arrows and the match relation as full arrows. The acyclicity of pdds induces a partial order on elements that we will interpret as the global arrow of time; the diagrams will be displayed vertically with the time going upwards. Besides the empty pdd $d_{\{\}} = (\emptyset, \emptyset, \emptyset, \emptyset)$, the simplest examples correspond to the *creation*, *annihilation* and *preservation* of a vertex, corresponding respectively to normal pdds d_c, d_a, d_p:


(1)

concretely given by $d_c = (\emptyset, \{\bullet\}, \emptyset, \emptyset)$, $d_a = (\{\circ\}, \emptyset, \emptyset, \emptyset)$ and $d_p = (\{\circ\}, \{\bullet\}, \{(\circ, \bullet)\}, \emptyset)$. A rule that matches a vertex and creates another one can be presented as the pdd $d_1 = (\{\circ_0\}, \{\bullet_1, \bullet_2\}, \{(\circ_0, \bullet_2)\}, \emptyset)$, displayed here:


(2)

As an illustration of a non-normal pdd, we can compose (as will be made precise in Prop. 5) two instances of the previous pdd, for example *matching* the top instance's input to $\bullet_2$:


(3)

This last pdd corresponds concretely to:

$$d_2 = (\{\circ_0, \circ_3\}, \{\bullet_1, \bullet_2, \bullet_4, \bullet_5\}, \{(\circ_0, \bullet_2), (\circ_3, \bullet_5)\}, \{(\bullet_2, \circ_3)\})$$

These examples hint at the fact that pdds are composed of an union of alternating sequences of elements of i and o (as the sequence $(\circ_0, \bullet_2, \circ_3, \bullet_5)$ in Fig. 3), corresponding to the history (that we call *worldline*) of some element during the rewriting process. This trivial consequence of the choice of one-to-one relations for the rule and match relations together with acyclicity of pdds is pivotal in the definition (to follow) of rule diagrams.

Definition 2 (Worldlines). *Let $d = (i, o, r, m)$ be a pdd. We define the worldline relation*

$$\begin{array}{rcl} \omega(d) & \subseteq & (i \cup o) \times (i \cup o) \\ \omega(d) & = & cl_\sim(r \cup m) \end{array}$$

Informally, $\omega(d)[\{x\}]$ is the connected component of x in d seen as a bipartite graph. However, the one-to-oneness and acyclicity conditions place some constraints:

Lemma 3. *Let $d = (i, o, r, m)$ be a pdd and $x, y \in i \cup o$ such that $(x, y) \in \omega(d)$. Then:*

$$\begin{array}{lcl} x, y \in i & \Rightarrow & (x, y) \in (r; m)^* \cup (r; m)^{*-1} \\ x, y \in o & \Rightarrow & (x, y) \in (m; r)^* \cup (m; r)^{*-1} \\ x \in i, y \in o & \Rightarrow & (x, y) \in r; (m; r)^* \cup r; (m; r)^{*-1} \\ x \in o, y \in i & \Rightarrow & (x, y) \in m; (r; m)^* \cup m; (r; m)^{*-1} \end{array}$$

Proof. This is a trivial consequence of acyclicity and the fact that r, m are one-to-one. □

A pdd also has a natural notion of interface, corresponding to those parts of i and o that are not matched:

Definition 4 (Interface of a pdd, diagram matches)**.** *Let $d = (i, o, r, m)$ be a pdd. We define its* input interface *by $\mathcal{I}(d) \triangleq i \backslash cod(m)$ and its* output interface *by $\mathcal{O}(d) \triangleq o \backslash dom(m)$. The set of* diagram matches *from $d \in D_0$ to $d' \in D_0$ is defined by $\mathcal{M}_0(d, d') \triangleq Rel_{11}(\mathcal{O}(d), \mathcal{I}(d'))$.*

Using the diagram d_2 of Fig. 3 as an example, we have $\mathcal{I}(d_2) = \{\circ_0\}$ while $\mathcal{O}(d_2) = \{\bullet_1, \bullet_4, \bullet_5\}$. Pdds admit a straightforward notion of composition by concatenation along a match relation on their interfaces.

Proposition 5 (Associative composition)**.** *Consider two disjoint pdds $d = (i, o, r, m)$, $d' = (i', o', r', m')$ and a diagram match $n \in \mathcal{M}_0(d, d')$. Let us denote by $d \rhd_n d'$ (or equivalently $d' \lhd_n d$) the tuple*

$$(i \cup i', o \cup o', r \cup r', m \cup m' \cup n)$$

We have that (i) $d \rhd_n d'$ is a pdd and (ii) the resulting notion of composition is associative: there is a bijection $\alpha_{d,d',d''}$ from the set $\{(n, n') \mid n \in \mathcal{M}_0(d, d'), n' \in \mathcal{M}_0(d \rhd_n d', d'')\}$ to the set $\{(w, w') \mid w' \in \mathcal{M}_0(d', d''), w \in \mathcal{M}_0(d, d' \rhd_{w'} d'')\}$ that verifies, for all $(w, w') = \alpha_{d,d',d''}(n, n')$,

$$(d \rhd_n d') \rhd_{n'} d'' = d \rhd_w (d' \rhd_{w''} d'')$$

Proof. (i) By disjointness of d and d', $r \cup r'$ is one-to-one. Observe that by definition of interfaces, $m \cup m'$ and n have disjoint support and are by assumption one-to-one, therefore $m \cup m' \cup n$ is one-to-one. *(ii)* Let $(d \rhd_n d') \rhd_{n'} d''$ be a composite. By definition, $\mathcal{O}(d \rhd_n d') = \mathcal{O}(d') \uplus (\mathcal{O}(d) \backslash dom(n))$, therefore n' uniquely decomposes as $n' = n'_0 \uplus n'_1$ where $n'_0 \in Rel_{11}(\mathcal{O}(d) \backslash dom(n), \mathcal{I}(d''))$ and $n'_1 \in Rel_{11}(\mathcal{O}(d'), \mathcal{I}(d''))$. One then obtains the sought identity by setting $w = n \cup n'_0$ and $w' = n'_1$. The converse computation yields the claimed bijection. □

The diagram d_2 in Fig. 3 corresponds to the composition of d_1 with $d'_1 = (\{\circ_3\}, \{\bullet_4, \bullet_5\}, \{(\circ_3, \bullet_5)\}, \emptyset)$ along the match relation $m = \{(\bullet_2, \circ_3)\}$.

Observe that acyclicity and one-to-oneness of the relations r and m imply trivially that worldline equivalence classes have at most a singleton intersection with either the input or output interface of a pdd. This motivates the definition of the *boundary relations*, which relate elements of a pdd with the interfaces through the worldline relation:

Definition 6 (Boundary relations)**.** *Let $d = (i, o, r, m)$ be given. We define the* input boundary relation *$\mathcal{I}_\omega(d)$ and the* output boundary relation *$\mathcal{O}_\omega d)$:*

$$\begin{array}{lcl} \mathcal{I}_\omega(d) & \in & Rel_{11}(i \cup o, \mathcal{I}(d)) \\ \mathcal{I}_\omega(d) & = & \omega(d); id_{\mathcal{I}(d)} \\ \mathcal{O}_\omega(d) & \in & Rel_{11}(i \cup o, \mathcal{O}(d)) \\ \mathcal{O}_\omega(d) & = & \omega(d); id_{\mathcal{O}(d)} \end{array}$$

The notion of normalization that we apply to pdds corresponds to taking the trace of the worldline relation against the interface of a diagram.

Definition 7 (Normalization)**.** *We define the normalization map $\partial_0 : D_0 \to D_0$ by*

$$\partial_0(d) = (\mathcal{I}(d), \mathcal{O}(d), \mathcal{I}_\omega(d)^{-1}; \mathcal{O}_\omega(d), \emptyset)$$

Clearly, for d normal one has $\partial_0(d) = d$. The following lemma lists some properties of normalization:

Lemma 8. *Let d and $\partial_0(d)$ be as in Def. 7. One has that (i) $\mathcal{I}(d) = \mathcal{I}(\partial_0(d))$ and $\mathcal{O}(d) = \mathcal{O}(\partial_0(d))$, and (ii) $\mathcal{I}_\omega(d)^{-1}; \mathcal{O}_\omega(d) = \mathcal{I}_\omega(\partial_0(d))^{-1}; \mathcal{O}_\omega(\partial_0(d))$.*

Proof. (i) is a trivial consequence of having an empty match relation in $\partial_0(d)$. As for *(ii)*, we clearly have the inclusion

$$\mathcal{I}_\omega(d)^{-1}; \mathcal{O}_\omega(d) \supseteq \mathcal{I}_\omega(\partial_0(d))^{-1}; \mathcal{O}_\omega(\partial_0(d))$$

The converse inclusion proceeds easily by using the first point and unfolding Def. 2, 6 and 7. □

Normalization is compatible with composition:

Proposition 9. *Let $d, d' \in D_0$. (i) $\mathcal{M}_0(d, d') = \mathcal{M}_0(\partial(d), \partial(d')))$ and (ii) $\forall n \in \mathcal{M}_0(d, d'), \partial_0(d \rhd_n d') = \partial_0(\partial_0(d) \rhd_n \partial_0(d'))$.*

Proof. (i) By Lemma 8, interfaces are preserved by reduction therefore $\mathcal{M}_0(d, d') = \mathcal{M}_0(\partial_0(d), \partial_0(d'))$. *(ii)* It is sufficient to check equality of the reduced rule relation. Observe that $\mathcal{I}(d \rhd_n d') = \mathcal{I}(d) \uplus \mathcal{I}(d') \backslash cod(n)$ and $\mathcal{O}(d \rhd_n d') = \mathcal{O}(d') \uplus \mathcal{O}(d) \backslash dom(n)$. For the left hand side, we obtain

$$\begin{array}{lcl} A & = & \mathcal{I}_\omega(d \rhd_n d')^{-1}; \mathcal{O}_\omega(d \rhd_n d') \\ & = & id_{\mathcal{I}(d \rhd_n d')}; \omega(d \rhd_n d'); id_{\mathcal{O}(d \rhd_n d')} \end{array}$$

Splitting the input interfaces according to n and simplifying using Lemma 3:

$$\begin{array}{lcl} A & = & id_{\mathcal{I}(d)}; \omega(d \rhd_n d'); id_{\mathcal{O}(d \rhd_n d')} \\ & \uplus & id_{\mathcal{I}(d') \backslash cod(n)}; \omega(d \rhd_n d'); id_{\mathcal{O}(d \rhd_n d')} \\ & = & id_{\mathcal{I}(d)}; \omega(d \rhd_n d'); id_{\mathcal{O}(d \rhd_n d')} \\ & \uplus & id_{\mathcal{I}(d') \backslash cod(n)}; r'; (m'; r')^*; id_{\mathcal{O}(d')} \end{array}$$

Splitting the output interfaces according to n and simplifying:

$$\begin{array}{lcl} A = & & id_{\mathcal{I}(d)}; \omega(d \rhd_n d'); id_{\mathcal{O}(d')} \\ & \uplus & id_{\mathcal{I}(d)}; \omega(d \rhd_n d'); id_{\mathcal{O}(d) \backslash dom(n)} \\ & \uplus & id_{\mathcal{I}(d') \backslash cod(n)}; r'; (m'; r')^*; id_{\mathcal{O}(d')} \\ & = & id_{\mathcal{I}(d)}; r; (m; r)^*; n; r'; (m'; r')^*; id_{\mathcal{O}(d')} \\ & \uplus & id_{\mathcal{I}(d)}; r; (m; r)^*; id_{\mathcal{O}(d) \backslash dom(n)} \\ & \uplus & id_{\mathcal{I}(d') \backslash cod(n)}; r'; (m'; r')^*; id_{\mathcal{O}(d')} \end{array}$$

For the right hand side, letting $\mathbf{d} = \partial_0(d) \rhd_n \partial_0(d')$, we have:

$$B = \mathcal{I}_\omega(\mathbf{d})^{-1}; \mathcal{O}_\omega(\mathbf{d})$$

Unfolding and using that interfaces are preserved, we derive:

$$\begin{array}{lcl} B & = & id_{\mathcal{I}(\mathbf{d})}; \omega(\mathbf{d}); id_{\mathcal{O}(\mathbf{d})} \\ & = & id_{\mathcal{I}(\partial_0(d) \rhd_n \partial_0(d'))}; \omega(\mathbf{d}); id_{\mathcal{O}(\partial_0(d) \rhd_n \partial_0(d'))} \\ & = & id_{\mathcal{I}(d \rhd_n d')}; \omega(\mathbf{d}); id_{\mathcal{O}(d \rhd_n d')} \end{array}$$

Splitting the input and output interfaces according to n and simplifying,

$$\begin{array}{lcl} B & = & id_{\mathcal{I}(d)}; \omega(\mathbf{d}); id_{\mathcal{O}(d')} \\ & \uplus & id_{\mathcal{I}(d)}; \omega(\mathbf{d}); id_{\mathcal{O}(d) \backslash dom(n)} \\ & \uplus & id_{\mathcal{I}(d') \backslash cod(n)}; \omega(\mathbf{d}); id_{\mathcal{O}(d')} \end{array}$$

Let us denote by resp. $\partial_0(r) \triangleq \mathcal{I}_\omega(d)^{-1}; \mathcal{O}_\omega(d)$ and $\partial_0(r') \triangleq \mathcal{I}_\omega(d)^{-1}; \mathcal{O}_\omega(d)$ the rule relations of resp. $\partial_0(d)$ and $\partial_0(d')$. By definition,

$$\omega(\mathbf{d}) = cl_\sim(\partial_0(r) \cup \partial_0(r') \cup n)$$

and we have by further simplifications:

$$\begin{array}{lclcl} \partial_0(r) & = & \mathcal{I}_\omega(d)^{-1}; \mathcal{O}_\omega(d) & = & id_{\mathcal{I}(d)}; \omega(d); id_{\mathcal{O}(d)} \\ & & & = & r; (m; r)^* \\ \partial_0(r') & = & \mathcal{I}_\omega(d')^{-1}; \mathcal{O}_\omega(d') & = & id_{\mathcal{I}(d')}; \omega(d'); id_{\mathcal{O}(d')} \\ & & & = & r'; (m'; r')^* \end{array}$$

Substituting these equations and performing some more trivial simplifications, one obtains the equality. □

During the construction of the rule and rule diagram algebras, diagrams will only be considered up to isomorphisms, defined as follows:

Definition 10 (Isomorphism of pdds)**.** *Let $d, d' \in D_0$ be such that $d = (i, o, r, m)$ and $d' = (i', o', r', m')$. An isomorphism from d to d' is a pair of bijections $f = (f_i : i \to i', f_o : o \to o')$ such that $(\circ_1, \bullet_2) \in r \Leftrightarrow (f_i(\circ_1), f_o(\bullet_2)) \in r'$ and $(\bullet_2, \circ_1) \in m \Leftrightarrow (f_o(\bullet_2), f_i(\circ_1)) \in m'$. This will be denoted by $f : d \cong d'$.*

Rule diagrams. A *rule diagram* is a suitable coupling of a pair of pdds supported by respectively a set of vertices and a set of edges. The set of rule diagrams will be denoted by D.

Definition 11 (Rule diagram)**.** *A* rule diagram *is a tuple*

$$d = (d_V, d_E, s_i, t_i, s_o, t_o)$$

where $d_V = (i_V, o_V, r_V, m_V)$ and $d_E = (i_E, o_E, r_E, m_E)$ are pdds verifying conditions 1 to 5 below.

1. *$G_i(d) \triangleq (i_V, i_E, s_i, t_i)$ and $G_o(d) \triangleq (o_V, o_E, s_o, t_o)$ are graphs;*
2. *(r_V, r_E) is a partial graph morphism from $G_i(d)$ to $G_o(d)$;*

1. and 2. are summarized in the following diagram, where the horizontal components are graphs and the vertical ones pdds:

$$\begin{tikzcd}
i_V \arrow[r, bend left, "r_V"] & o_V \arrow[l, bend left, "m_V"] \\
i_E \arrow[u, shift left, "s_i"] \arrow[u, shift right, "t_i"'] \arrow[r, bend left, "r_E"] & o_E \arrow[u, shift left, "s_o"] \arrow[u, shift right, "t_o"'] \arrow[l, bend left, "m_E"]
\end{tikzcd}$$

Further, we require the following.

3. *d must fulfill the* delayed morphism *condition: letting $s = s_i \cup s_o$, one has*
$$(e, e') \in \omega(d_E) \Rightarrow (s(e), s(e')) \in \omega(d_V)$$
and similarly for $t = t_i \cup t_o$.
4. *We ask the diagrams to be* globally acyclic. *Let*
$$r'_V \quad \triangleq \quad \mathbf{cc}(G_i(d)); r_V; \mathbf{cc}(G_o(d))$$
be the rule relation up to **cc**. *We require:*
$$id_{o_V} \cap (m_V; r'_V)^+ = \emptyset$$
For the scope of this paper, we add the following:
5. *d verifies the* totality *condition:*
$$id_{\mathcal{I}(d_E)}; s_i; \mathcal{I}_\omega(d_V) \text{ and } id_{\mathcal{O}(d_E)}; s_o; \mathcal{O}_\omega(d_V)$$
are total functions from resp. $\mathcal{I}(d_E)$ to $\mathcal{I}(d_V)$ and $\mathcal{O}(d_E)$ to $\mathcal{O}(d_V)$; and similarly for t_i, t_o.

A rule diagram is normal *whenever d_V and d_E are normal pdds. The set of normal rule diagrams will be denoted $\mathcal{N}(D)$.*

Observe that a normal diagram is isomorphic to a *rule* in the graph rewriting sense (Heindel 2009).

Definition 12 (Rule associated to a normal diagram)**.** *Let $d \in \mathcal{N}(D)$. By definition, $r = (r_V, r_E)$ is a partial injective graph morphism from $G_i(d)$ to $G_o(d)$. The* rule *associated to d will be denoted by $G_o(d) \overset{r}{\Leftarrow} G_i(d)$. Conversely, any rule $g' \overset{r}{\Leftarrow} g$ induces trivially a normal diagram.*

Let us discuss the conditions listed in Def. 11. The *delayed morphism* condition ensures that reduction can be properly defined on rule diagrams. Global acyclicity allows to have a sequential interpretation of rule diagrams as stackings of rules: in this sense, it is a "correctness" criterion. However, it is not required for having a well-defined reduction. Finally, the *totality* condition is a simplifying assumption we make for the scope of this paper: it enforces that the source and target maps in any normalized diagram are total functions (i.e. that the corresponding notion of graph rewriting is DPO (Heindel 2009)). An account of more general types of rewriting is available in a preprint (Behr et al. 2016). Examples of diagrams that do not verify totality and global acyclicity are available in Sec. A of the appendix. As a first example, we consider a normal diagram corresponding to a rule which acts identically on an edge. We use the same pictural conventions as for pdds for vertices and we use $\blacklozenge$ to denote input edges and $\lozenge$ for output edges.

$$\begin{tikzcd}
\bullet_2 & \blacklozenge_b \arrow[l, "s_o"'] \arrow[r, "t_o"] & \bullet_3 \\
\circ_0 \arrow[u, dotted, "r_V"] & \lozenge_a \arrow[l, "s_i"] \arrow[r, "t_i"'] \arrow[u, dotted, "r_E"'] & \circ_1 \arrow[u, dotted, "r_V"']
\end{tikzcd} \tag{4}$$

The concrete representation for this diagram is $d = (d_V, d_E, s_i, t_i, s_o, t_o)$ with $d_V = (\{\circ_0, \circ_1\}, \{\bullet_2, \bullet_3\}, \{(\circ_0, \bullet_2), (\circ_1, \bullet_3)\}, \emptyset)$ for vertices, $d_E = (\{\lozenge_a\}, \{\blacklozenge_b\}, \{(\lozenge_a, \blacklozenge_b)\}, \emptyset)$ for edges and the obvious maps for s_i, t_i, s_o, t_o. This type of diagram, made up of only one identity rule for some arbitrary graph, will be called in the following an *observable* (here, the graph is reduced to a single edge, we therefore call the corresponding diagram an *edge observable*). Rule diagrams have a straightforward notion of isomorphism:

Definition 13 (Isomorphism of rule diagrams)**.** *Let $d = (d_V, d_E, s_i, t_i, s_o, t_o)$ and $d' = (d'_V, d'_E, s'_i, t'_i, s'_o, t'_o)$ be rule diagrams. An isomorphism from d to d' is a pair of discrete diagram isomorphisms (Def. 10)*

$$\begin{array}{lcllcl} f_V & : & d_V \cong d'_V & f_E & : & d_E \cong d'_E \\ f_V & = & (f_{V,i}, f_{V,o}) & f_E & = & (f_{E,i}, f_{E,o}) \end{array}$$

such that $(f_{V,i}, f_{E,i})$ is a graph isomorphism from $G_i(d)$ to $G_i(d')$ and $(f_{V,o}, f_{E,o})$ is a graph isomorphism from $G_o(d)$ to $G_o(d')$. The set of isomorphism classes of rule diagrams will be noted $D_{\cong}$. Isomorphism classes of normal rule diagrams will be noted $\mathcal{N}(D_{\cong})$.

Normalization of rule diagrams is defined as the componentwise normalization of the vertices and edges pdds.

Definition 14 (Normalization of rule diagrams)**.** *Let us consider a rule diagram $d = (d_V, d_E, s_i, t_i, s_o, t_o)$. We define its normal form as $\partial(d) \triangleq (\partial_0(d_V), \partial_0(d_E), \bar{s}_i, \bar{t}_i, \bar{s}_o, \bar{t}_o)$ where*

$$\bar{s}_i \triangleq id_{\mathcal{I}(d_E)}; s_i; \mathcal{I}_\omega(d_V) \quad \bar{s}_o \triangleq id_{\mathcal{O}(d_E)}; s_o; \mathcal{O}_\omega(d_V)$$

and similarly for $\bar{t}_i, \bar{t}_o$.

The following proposition states that normalization preserves the structure of rule diagrams.

Proposition 15. *(i) Normalization is a function $\partial : D \to \mathcal{N}(D)$ and (ii) $\partial \circ \partial = \partial$.*

Proof. (i) Let us show that the conditions listed in Def. 11 are verified by $\partial(d)$.

1. Totality directly implies $G_i(\partial(d))$ and $G_o(\partial(d))$ are graphs.
2. Injectivity is trivial. Let $(e_i, e_o) \in \mathcal{I}(d_E) \times \mathcal{O}(d_E)$, then by the delayed morphism condition, $(s_i(e_i), s_o(e_o)) \in \omega(d_V)$ therefore $(\bar{s}_i(e_i), \bar{s}_o(e_o)) \in \omega(d_V)$. By Def. 7, this pair of vertices is trivially in the reduced rule relation. The same argument goes for t_i, t_o.
3. By the previous point and using that the match relation is empty, the delayed morphism condition is trivially verified.

4. Trivial by emptyness of the match relation of $\partial(d)$.
5. Totality is by construction.

Normality of $\partial(d)$ as well as *(ii)* are trivial. ☐

As for pdds, rule diagrams admit a notion of binary composition along a match:

Definition 16 (Composition)**.** *Consider two disjoint rule diagrams*

$$\begin{array}{rcl} d & = & (d_V, d_E, s_i, t_i, s_o, t_o); \\ d' & = & (d'_V, d'_E, s'_i, t'_i, s'_o, t'_o) \end{array}$$

and a pair of matches on respectively vertices and edges

$$n = (n_V, n_E) \in \mathcal{M}_0(d_V, d'_V) \times \mathcal{M}_0(d_E, d'_E)$$

Whenever the object defined by

$$d \rhd_n d' = (d_V \rhd_{n_V} d'_V, d_E \rhd_{n_E} d'_E, s_i \cup s'_i, t_i \cup t'_i, s_o \cup s'_o, t_o \cup t'_o)$$

is a valid rule diagram (i.e. $d \rhd_n d' \in D$), we call it the composition of d and d' along n. This object might equivalently be denoted by $d' \lhd_n d$.

The reader might be unsatisfied seeing that we need to refer to the definition of rule diagrams to carve out the set of allowed composites of such diagrams. Before adressing this problem, let us give a few examples of composites. The diagram to the left of Fig. 11 provides an example of composition of an edge observable with a "vertex annihilation" diagram d_a. The following example corresponds to a vertex observable precomposed and postcomposed with edge observables.

$$\begin{tikzcd}
\bullet_8 & \blacklozenge_d \arrow[l] \arrow[r] & \bullet_9 \\
\circ_6 \arrow[u, dotted] & \lozenge_c \arrow[l] \arrow[u, dotted] \arrow[r, "t_i"'] & \circ_7 \arrow[u, dotted] \\
 & & \bullet_5 \arrow[u] \\
 & & \circ_4 \arrow[u, dotted] \\
\bullet_2 \arrow[uuu] & \blacklozenge_b \arrow[l] \arrow[uuu] \arrow[r, "t_o"] & \bullet_3 \arrow[u] \\
\circ_0 \arrow[u, dotted] & \lozenge_a \arrow[l] \arrow[u, dotted] \arrow[r] & \circ_1 \arrow[u, dotted]
\end{tikzcd} \tag{5}$$

This example highlights in a striking way the "delayed morphism" condition: here, $(\blacklozenge_b, \lozenge_c)$ are in the match relation but $(t_o(\blacklozenge_b), t_i(\lozenge_c))$ are *not*. This makes the following proposition, which characterizes the admissible matches, not totally trivial. As a side note, the totality condition only appears here as a simplifying assumption.

Proposition 17 (Admissible matches)**.** *Let d, d', n be as in Def. 16. $d \rhd_n d'$ is a rule diagram if and only if (i) n is a partial injective morphism of graphs from $G_o(\partial(d))$ to $G_i(\partial(d'))$ and (ii) $d \rhd_n d'$ verifies the totality condition. Such a n will be called* admissible*. We denote the set of admissible matches from d to d' by $\mathcal{M}(d, d')$.*

Proof. Assume $d \rhd_n d' \in D$ with $n = (n_V, n_E)$. First, observe that this implies trivially that $d \rhd_n d' \in D$ verifies the totality condition. Now observe that by construction, $n_V \in Rel_{11}(\mathcal{O}(d_V), \mathcal{I}(d'_V))$ and $n_E \in Rel_{11}(\mathcal{O}(d_E), \mathcal{I}(d'_E))$. Consider e, e' such that $e' = n_E(e)$. We have to prove that n is a partial injective morphism of graphs from $G_o(\partial(d))$ to $G_i(\partial(d'))$ (see Prop. 15 for their definitions), i.e. that $n_V(\bar{s}_o(e)) = \bar{s'}_i(e')$.

By definition of reduction, $(s_o(e), \bar{s}_o(e)) \in \omega(d_V)$ and symmetrically, $(s'_i(e'), \bar{s'}_i(e')) \in \omega(d'_V)$; while the delayed morphism property (dmp) ensures that $(s_o(e), s'_i(e')) \in \omega(d_V \rhd_{n_V} d'_V)$. Since d and d' are disjoint and n is by assumption one-to-one, this is only possible if $n_V(\bar{s}_o(e)) = \bar{s'}_i(e')$ is verified. Mirroring this argument for t, t' yields the result that n is a partial injective morphism of graphs.

Conversely, assume n is as stated. We only prove that $d \rhd_n d'$ verifies the dmp (the other defining properties of rule diagrams are easily verified). It is enough to exhibit the dmp for a pair of edges (e, e') with e in d and $e' \in d'$, as otherwise it is satisfied by assumption. Assume that $(e, e') \in \omega(d_E \rhd_{n_E} d'_E)$. Using one-to-oneness and acyclicity of pdds, we obtain that $(e, e') \in \omega(d_E); n_E; \omega(d'_E)$. Therefore, there exists $e_o \in \mathcal{O}(d_E), e'_i \in \mathcal{I}(d'_E)$ such that $(e, e_o) \in \omega(d_E)$, $(e'_i, e') \in \omega(d'_E)$ and $e'_i = n_E(e_O)$; and one can apply the dmp on (e, e_o) and (e'_i, e'), by assumption. The goal is reduced to proving that $(s_o(e_o), s'_i(e'_i)) \in \omega(d_V \rhd_{n_V} d'_V)$. Since d and d' are disjoint, this can only be if the vertices related by $\omega(d_V)$ in the interface are related through n_V, i.e. it is enough to prove that

$$(s_o; \omega(d_V); id_{\mathcal{O}(d_V)}; n_V)(e_o) = (s_i; \omega(d'_V); id_{\mathcal{I}(d'_V)})(e'_i)$$

which by definition of $\bar{s}$ and $\bar{s'}$ corresponds to having $n_V(\bar{s}_o(e_o)) = \bar{s'}_i(e'_i)$. Since e_o is an edge of $G_o(\partial(d))$ and e'_i is an edge of $total(G_i(\partial(d')))$, $n_V(\bar{s}_o(e_o)) = \bar{s'}_i(e'_i)$. The exact same argument for the target maps t_o, t'_i concludes the proof. ☐

The associativity of composition of pdds lifts to rule diagrams:

Proposition 18. *Let $d, d', d'' \in D$. There exists a bijection $\alpha_{d,d',d''}$ from the set $\{(n, n') \mid n \in \mathcal{M}(d, d'), n' \in \mathcal{M}(d \rhd_n d', d'')\}$ to the set $\{(w, w') \mid w' \in \mathcal{M}(d', d''), w \in \mathcal{M}(d, d' \rhd_{w'} d'')\}$ that verifies, for all $(w, w') = \alpha_{d,d',d''}(n, n')$,*

$$(d \rhd_n d') \rhd_{n'} d'' = d \rhd_w (d' \rhd_{w''} d'')$$

Proof. The source and target maps s_i, t_i, s_o, t_o of a triple composite are given by the union of the corresponding data from each component, independently of the chosen matches. Therefore, it is enough to apply Prop. 5 to conclude. ☐

Remark 19. *The rule diagram $d_\emptyset = (d_{\{\}}, d_{\{\}}, \emptyset, \emptyset, \emptyset, \emptyset)$ acts as a neutral element for the composition: $d_\emptyset \rhd_\emptyset d' = d' \rhd_\emptyset d_\emptyset = d'$.*

Moreover, normalization respects composition:

Proposition 20. *Let $d, d' \in D$ and $n \in \mathcal{M}(d, d')$. One has (i) $n \in \mathcal{M}(\partial(d), \partial(d'))$ and (ii) $\partial(d \rhd_n d') = \partial(\partial(d) \rhd_n \partial(d'))$.*

Proof. (i) Using the assumption $n \in \mathcal{M}(d, d')$, by Prop. 17, n is an injective morphism of graphs from $G_o(\partial(d))$ to $G_i(\partial(d'))$ and therefore $n \in \mathcal{M}(\partial(d), \partial(d'))$. The proof of *(ii)* follows the same pattern as the proof of Prop. 9. ☐

The rule diagram & rule algebra. $Pdds$ and rule diagrams span vector spaces that admit, thanks to the composition operation, the structure of *algebras* In the following, we denote by $(span(X), +, \cdot)$ the formal vector space of finite linear combinations with real coefficients over a set X where $v + v'$ is the pointwise addition and $\lambda \cdot v$ is the scalar multiplication. We let $\delta : X \to span(X)$ be the map associating $x \in X$ to the basis vector $\delta(x)$. However, where the context allows it, we will drop δ and denote a basis element by its index in X. In the remainder of this paper, we will only deal explicitly with isomorphism classes of combinatorial structures where required.

Definition 21 (Vector space of rule diagrams and normal rule diagrams)**.** *We denote the $\mathbb{R}$-vector space spanned by $D_\cong$ by $\mathscr{D} = (span(D_\cong), +, \cdot)$. Since $\mathcal{N}(D_\cong) \subseteq D_\cong$, there exists a subvector space of $\mathscr{D}$ spanned by (isomorphism classes of) normal diagrams which will be denoted by $\mathscr{R}$, together with a canonical inclusion $\psi : \mathscr{R} \hookrightarrow \mathscr{D} = id_{\mathscr{R}}$.*

$\mathscr{D}$ admits an algebra structure induced by diagram composition. Let us define the product.

Definition 22 (Product in $\mathscr{D}$)**.** *Let $\delta(d), \delta(d') \in \mathscr{D}$ be two basis vectors for $d, d' \in D_{\cong}$. We define their product as:*

$$\delta(d') *_{\mathscr{D}} \delta(d) \triangleq \sum_{n \in \mathcal{M}(d,d')} \delta(d' \underset{n}{\lhd} d)$$

This extends to arbitrary elements of $\mathscr{D}$ by linearity:

$$\left(\sum_{d'} \beta_{d'} \delta(d')\right) *_{\mathscr{D}} \left(\sum_{d} \alpha_d \delta(d)\right) \triangleq \sum_{d,d'} \alpha_d \beta_{d'} \delta(d') *_{\mathscr{D}} \delta(d)$$

Theorem 23. *$*_{\mathscr{D}}$ makes $\mathscr{D}$ into an associative algebra with unit $\mathbf{1}_{\mathscr{D}} = 1 \cdot \delta(d_{\emptyset})$. We call $(\mathscr{D}, *_{\mathscr{D}}, \mathbf{1}_{\mathscr{D}})$ the* rule diagram algebra*.*

Proof. Bilinearity of $*_{\mathscr{D}}$ is straightforward. Let us prove associativity. Clearly it is enough to consider basis vectors. We have:

$$\begin{array}{rl} & (\delta(d'') *_{\mathscr{D}} \delta(d')) *_{\mathscr{D}} \delta(d) \\ = & \displaystyle\sum_{n' \in \mathcal{M}(d',d'')} \delta(d'' \underset{n'}{\lhd} d') *_{\mathscr{D}} d \\ = & \displaystyle\sum_{n' \in \mathcal{M}(d',d'')} \sum_{n \in \mathcal{M}(d, d'' \lhd_{n'} d')} \delta((d'' \underset{n'}{\lhd} d') \underset{n}{\lhd} d) \end{array}$$

Applying Prop. 18, we can rewrite the last equation as

$$\sum_{w \in \mathcal{M}(d,d')} \sum_{w' \in \mathcal{M}(d' \lhd_w d, d')} \delta(d'' \underset{w'}{\lhd} (d' \underset{w}{\lhd} d))$$

Let us check the unit law. Observe that for all $d \in D$, $\emptyset$ is the only element in $\mathcal{M}(d_{\emptyset}, d)$ and in $\mathcal{M}(d, d_{\emptyset})$, therefore

$$\delta(d_{\emptyset}) *_{\mathscr{D}} \delta(d) = d_{\emptyset} \underset{\emptyset}{\rhd} d = d = d \underset{\emptyset}{\rhd} d_{\emptyset} = \delta(d) *_{\mathscr{D}} \delta(d_{\emptyset})$$

This lifts trivially to arbitrary vectors. □

The normalization map extends by linearity to a linear map from $\mathscr{D}$ to $\mathscr{R}$ that we call the *reduction map*.

Definition 24 (Reduction map)**.** *The function $\bar{\varphi}$ defined on basis vectors as*

$$\begin{array}{rcll} \bar{\varphi}(\delta(d)) & = & \delta(\partial(d)) & \textit{if } \partial(d) \in \mathcal{N}(D), \\ & = & 0 \cdot \delta(d_{\emptyset}) & \textit{otherwise} \end{array}$$

extends straightforwardly to a linear map $\bar{\varphi} : \mathscr{D} \to \mathscr{R}$.

The unital associative algebra structure on $\mathscr{D}$ can be pushed forward to $\mathscr{R}$ by composing normal diagrams and normalizing back their composition.

Definition 25 (Product in $\mathscr{R}$)**.** *Let $v, v' \in \mathscr{R}$ be given. We define their product as:*

$$v' *_{\mathscr{R}} v \triangleq \bar{\varphi}\left(\psi(v') *_{\mathscr{D}} \psi(v)\right)$$

Theorem 26. *(i) $\bar{\varphi}$ is a homomorphism of algebras from $(\mathscr{D}, *_{\mathscr{D}})$ to $(\mathscr{R}, *_{\mathscr{R}})$; (ii) $*_{\mathscr{R}}$ makes $\mathscr{R}$ into an associative algebra with unit $\mathbf{1}_{\mathscr{R}} = 1 \cdot d_{\emptyset}$ and $\bar{\varphi}$ is a homomorphism of associative unital algebras. We call $(\mathscr{R}, *_{\mathscr{R}}, \mathbf{1}_{\mathscr{R}})$ the* rule algebra*.*

Proof. (i) By bilinearity of $*_{\mathscr{R}}$ and $*_{\mathscr{D}}$, it is enough to consider basis vectors. We have to prove $\bar{\varphi}(\delta(d') *_{\mathscr{D}} \delta(d)) = \bar{\varphi}(\delta(d')) *_{\mathscr{R}} \bar{\varphi}(\delta(d))$. Unfolding the definition of $*_{\mathscr{R}}$, we get:

$$\bar{\varphi}(\delta(d')) *_{\mathscr{R}} \bar{\varphi}(\delta(d)) = \bar{\varphi}\left(\psi(\bar{\varphi}(\delta(d'))) *_{\mathscr{D}} \psi(\bar{\varphi}(\delta(d)))\right)$$

therefore, the goal reduces to proving

$$\bar{\varphi}(\delta(d') *_{\mathscr{D}} \delta(d)) = \bar{\varphi}\left(\psi(\bar{\varphi}(\delta(d'))) *_{\mathscr{D}} \psi(\bar{\varphi}(\delta(d)))\right)$$

Let us proceed by case analysis. Assume $\partial(d) \notin \mathcal{N}(D)$ or $\partial(d') \notin \mathcal{N}(D)$. Then point 2. of Prop. 20 imply that both sides reduce to $0 \cdot \delta_{\emptyset}$ and the equality holds. Now, assume that $\partial(d), \partial(d') \in \mathcal{N}(D)$. Then $\psi(\bar{\varphi}(\delta(d))) = \delta(\partial(d))$ and $\psi(\bar{\varphi}(\delta(d))) = \delta(\partial(d'))$, and it is sufficient to prove that $\bar{\varphi}(\delta(d') *_{\mathscr{D}} \delta(d)) = \bar{\varphi}\left(\delta(\partial(d')) *_{\mathscr{D}} \delta(\partial(d))\right)$, which boils down to point 1. of Prop. 20. *(ii)* The unit part is trivial. As for associativity, it suffices to apply the homomorphism property to $\bar{\varphi}(\psi(x) *_{\mathscr{D}} \psi(y) *_{\mathscr{D}} \psi(z))$ in the two possible ways to obtain the sought equality. □

An important subalgebra of $\mathscr{R}$ is that of *observables*, which will be denoted by $\mathscr{O}$. Its elements are (linear combinations of) normal diagrams $g' \overset{r}{\Leftarrow} g$ where g and g' are isomorphic. In a slight abuse of notation, we will note this $g \overset{r}{\Leftarrow} g$. The particular case where r is an isomorphism from g to g' will be denoted $g \overset{\cong}{\Leftarrow} g$ - as we will see these correspond (via the representation to be defined below) to function on graphs counting the number of matches for a given graph. If r is not an iso, but simply a injective morphism, then we are only counting such matches where nodes deleted by r (and recreated subsequently) are sent to nodes of same degree in the target graph. To stress the difference between true identities and general obervables we will sometimes explicitly call the latter ones 'thin' identities.

In the following, we will work directly with representatives, without loss of generality.

Proposition 27. *The family $\mathscr{O} \triangleq \{g \overset{r}{\Leftarrow} g\}_{g \in G_{\cong}}$ is a commutative subalgebra of $\mathscr{R}$.*

Proof. Commutativity of $\mathscr{O}$ is easy. Let $d = g \overset{r}{\Leftarrow} g$, $d' = g' \overset{r'}{\Leftarrow} g'$ and $n = (n_V, n_E) \in \mathcal{M}(d, d')$ be given as in Def. 16. By Prop. 17, n is an partial graph morphism from g to g'. Let us write $\mathbf{d} = d \rhd_n d'$. We prove that there is a graph isomorphism from $\mathcal{I}(\mathbf{d}) = G_i(\partial(\mathbf{d}))$ to $\mathcal{O}(\mathbf{d}) = G_o(\partial(\mathbf{d}))$. Let e be an edge of $\mathcal{I}(d)$. By assumption, e has an image e' in $\mathcal{O}(d)$ through a graph isomorphism σ_d.

1. Assume $e' \in \mathit{dom}(n_E)$, then $s_o(e')$ and $t_o(e')$ are in $\mathcal{I}(d')$ (since n is a graph morphism) and we conclude easily to.
2. Assume $e' \notin \mathit{dom}(n_E)$. Then $e' \in \mathcal{O}(\mathbf{d})$. The only nontrivial case is whenever $s_o(e')$ or $t_o(e')$ overlaps $\mathit{dom}(n_V)$, in which case we use the totality hypothesis to rule out the possibility of $s_o(e')$, $t_o(e')$ being deleted in d': $s_o(e')$, $t_o(e')$ are related through the match relation of d' to $\mathcal{O}(d')$.

The case of isolated vertices is treated similarly. All in all, this prove that $\mathcal{I}(\mathbf{d})$ injects in $\mathcal{O}(\mathbf{d})$. Reversing the same argument concludes to the existence of an isomorphism. Therefore, thin observables form a subalgebra. □

4. Representation

Let $\mathcal{G} \triangleq \mathit{span}(G_{\cong})$ be the vector space spanned by isomorphism classes of graphs. We construct a *representation* (that is, a homomorphism of unital associative algebras) of the algebra $\mathscr{R}$ to the algebra $\mathit{End}(\mathcal{G})$ of endomorphisms over the vector space $\mathcal{G}$. In Sec. 5, we will show how this representation implements mass-action stochastic graph rewriting. In this section, we proceed by *(i)* constructing a linear map $\rho : \mathscr{R} \to \mathit{End}(\mathcal{G})$ and *(ii)* proving that ρ is indeed a homomorphism. The whole construction is in close analogy to the representation theory of the Heisenberg-Weyl algebra. We will therefore use notations drawn from quantum mechanics: elements of $\mathcal{G}$ will be denoted by $|v\rangle$ for $v \in \mathcal{G}$. $\mathcal{G}$ admits (by definition of span) a Hamel basis constituted of linear combinations of the form $1 \cdot \delta(g)$ for each $g \in G_{\cong}$. We will denote these by $|g\rangle$. Among all elements of $\mathcal{G}$, we distinguish the vector corresponding to the (trivial isomorphism class of the) empty graph: $|\emptyset\rangle$; it is is the counterpart of the *vacuum vector* in the construction of the bosonic Fock space representation for the Heisenberg-Weyl algebra (Blasiak et al. 2007) and it will play a similar role here.

Constructing the representation. The representation map $\rho : \mathscr{R} \to End(\mathcal{G})$ must satisfy *(i)* linearity and *(ii)* for all $v, v' \in \rho$, the equation $\rho(v' *_{\mathscr{R}} v) = \rho(v')\rho(v)$. It is sufficient to define ρ on a basis of $\mathscr{R}$ and then extend it by linearity; similarly, an operator in $End(\mathcal{G})$ is entirely characterized by its action on basis vectors $|g\rangle$. In the following, we will use the notation $g' \overset{r}{\Leftarrow} g$ for normal diagrams seen as rules, as in Def. 12. We will omit δ and simply write $\rho(g' \overset{r}{\Leftarrow} g)$ where unambiguous.

Definition 28 (Representation map)**.**

$$\begin{array}{rcl} \rho(g' \overset{r}{\Leftarrow} g)\,|\emptyset\rangle & \triangleq & \begin{cases} |g'\rangle & \textit{if } g = \emptyset \\ 0 \cdot |\emptyset\rangle & \textit{else} \end{cases} \\ \rho(g' \overset{r}{\Leftarrow} g)\,|g'' \neq \emptyset\rangle & \triangleq & \rho(g' \overset{r}{\Leftarrow} g *_{\mathscr{R}} g'' \Leftarrow \emptyset)\,|\emptyset\rangle \end{array}$$

This extends to a linear operator $\rho : \mathscr{R} \to End(\mathcal{G})$. Note that the first definition implies the equation $|g\rangle = \rho(g \Leftarrow \emptyset)\,|\emptyset\rangle$ for all $g \in G_{\cong}$. We have:

Theorem 29. *ρ is a homomorphism of unital algebras.*

Proof. Let $d, d' \in \mathcal{N}(D_{\cong})$ be given. By linearity, it suffices to prove $\rho(d' *_{\mathscr{R}} d) = \rho(d')\rho(d)$ and $\rho(\mathbb{1}_{\mathscr{R}}) = \mathbb{1}_{End(\mathcal{G})}$. It is enough to test these equalities on basis vectors of $\mathcal{G}$. By definition of ρ, we trivially have

$$\rho(\mathbb{1}_{\mathscr{R}})\,|\emptyset\rangle = \rho(d_{\emptyset})\,|\emptyset\rangle = \rho(\emptyset \Leftarrow \emptyset)\,|\emptyset\rangle = |\emptyset\rangle$$

Let us test the homomorphism property on $|\emptyset\rangle$: if d is not of the form $d = g \Leftarrow \emptyset$ then $\rho(d')\rho(d)\,|\emptyset\rangle = 0 \cdot |\emptyset\rangle$. Since $\forall n, \mathcal{I}(d) \subseteq \mathcal{I}(d \rhd_n d')$, one also has $\rho(d' *_{\mathscr{R}} d)\,|\emptyset\rangle = 0 \cdot |\emptyset\rangle$ and the equality holds. Assume now that d is of the form $g \Leftarrow \emptyset$. Then by definition, $\rho(d')\rho(g \Leftarrow \emptyset)\,|\emptyset\rangle = \rho(d')\,|g\rangle = \rho(d' *_{\mathscr{R}} g \Leftarrow \emptyset)\,|\emptyset\rangle$. Let us proceed to the case of a basis vector $|g \neq \emptyset\rangle$. We have thanks to the previous result $\rho(\mathbb{1}_{\mathscr{R}})\,|g\rangle = \rho(\mathbb{1}_{\mathscr{R}} * g \Leftarrow \emptyset)\,|\emptyset\rangle = |g\rangle$. Finally, using the previous results together with the associativity of $*_{\mathscr{R}}$,

$$\begin{array}{rcl} \rho(d' *_{\mathscr{R}} d)\,|g\rangle & = & \rho(d' *_{\mathscr{R}} d *_{\mathscr{R}} g \Leftarrow \emptyset)\,|\emptyset\rangle \\ & = & \rho(d')\rho(d *_{\mathscr{R}} g \Leftarrow \emptyset)\,|\emptyset\rangle \\ & = & \rho(d')\rho(d)\,|g\rangle \end{array}$$

□

The following result will be useful in constructing a stochastic dynamics.

Lemma 30. *ρ ranges in row-finite operators.*

Proof. It is enough to consider $d = f' \overset{r}{\Leftarrow} f$. We have to prove that for all h, there are finitely many $|g\rangle$ such that $(\rho(d)\,|g\rangle)_h$ is nonzero, i.e. such that

$$\rho(f' \overset{r}{\Leftarrow} f *_{\mathscr{R}} g \Leftarrow \emptyset)\,|\emptyset\rangle$$

has a strictly positive component in $|h\rangle$. But since h is a finite graph, there are only finitely many g and n such that

$$\partial(f' \overset{r}{\Leftarrow} f \lhd_n g \Leftarrow \emptyset) = h \Leftarrow \emptyset$$

□

5. Stochastic mechanics of graph rewriting

Stochastic mechanics in a nutshell. We are interested in describing the time evolution of a probability distribution supported by $G_{\cong}$. As these are not necessarily finitely supported, they do not fit in $\mathcal{G} = span(G_{\cong})$. Therefore, we define our space of *states* to be the real Fréchet space $\hat{\mathcal{G}} \triangleq (\mathbb{R}^{G_{\cong}}, \{\|\text{-}\|_k\}_{k\in\mathbb{N}})$ of all real sequences indexed by $G_{\cong}$ with seminorms $\|f\|_k \triangleq |f(g_k)|$. $\mathcal{G}$ is a subspace of $G_{\cong}$. The convex subset of subprobability states $Prob \subset \hat{\mathcal{G}}$ contains all states $\psi \in \hat{\mathcal{G}}$ that are i) *positive*, i.e. $\forall x \in X, \psi(x) \geqslant 0$ and ii) *subnormalized*, i.e. $\sum_x \psi(x) \leqslant 1$. Substochastic operators, denoted by $Stoch$, are those operators $A \in End(V)$ which verify $A(Prob) \subseteq Prob$.

A stochastic dynamics in our setting will be a continuous-time Markov chain that will be given by an *Hamiltonian* $H \in End(\mathcal{G})$. We require this operator to be *infinitesimal stochastic*, which means that $H = (h_{xy})_{x,y\in X}$ verifies i) $h_{xx} \leqslant 0$ for all x, ii) $h_{xy} \geqslant 0$ for all $x \neq y$ and iii) $\sum_x h_{xy} = 0$ for all y. The stochastic dynamics induced by a Hamiltonian is a semigroup $P : [0, \infty) \to Stoch(G_{\cong})$ of substochastic operators (i.e. $P(s)P(t) = P(s+t)$ for all $s, t \geqslant 0$) which is the pointwise minimal non-negative solution of the (backwards) *master equation*:

$$\frac{dP}{dt} = HP \tag{6}$$

Given an initial state ψ, the corresponding trajectory is given by $t \mapsto P(t)\psi$. See Norris (Norris 1998) for a thorough treatment of the subject. Note that the above only makes formal sense whenever $H \in End(\mathcal{G})$ can be interpreted as an element of $End(\hat{\mathcal{G}})$. In this paper, as a consequence of Lemma 30, it will be by construction always the case:

Lemma 31. *For all $H \in End(\mathcal{G})$ if H is row-finite then $H \in End(\hat{\mathcal{G}})$.*

Proof. Operators in $End(\mathcal{G})$ must map finite linear combinations to finite linear combinations, therefore they must be column-finite. If such an operator is moreover row-finite, its application is trivially well-defined on all elements of $\hat{\mathcal{G}}$. □

The projection. It will be useful to integrate elements of $\hat{\mathcal{G}}$ against the counting measure. In analogy with the notations of quantum mechanics, we call this the *projection* and denote this linear (partial) operation by

$$\begin{array}{rcl} \langle| & : & \hat{\mathcal{G}} \rightharpoonup \mathbb{R} \\ \langle| & = & v \in \hat{\mathcal{G}} \mapsto \sum_g v(g) \end{array}$$

Hamiltonians verify the following special property:

Lemma 32. *If $H \in End(\mathcal{G})$ is infinitesimal stochastic, $\langle|\,H = 0$.*

Proof. By condition *(iii)* of the definition of infinitesimal stochastic operators, columns vectors $H\,|g\rangle$ of H sum to zero. □

Operators for graph observables. The quantities of interest in stochastic graph rewriting-based models are "graph-counting observables". They correspond to the number of occurrences of some subgraph isomorphic to a pattern h in the graph being rewritten, say g – in other words, the number of injections from h to g, denoted by $[h; g]$. In our setting, these quantities are computed by graph-counting operators. A *graph observable* for a pattern $h \in G_{\cong}$ is an operator $O_h \in End(\mathcal{G})$ which verifies

$$O_h\,|g\rangle = [h; g]\,|g\rangle \tag{7}$$

i.e. every basis vector $|g\rangle$ is an eigenvector with eigenvalue $[h; g]$. Note that one could take this as a definition. However, it will be useful to express these operators in terms of the representations of the elements of the subalgebra of thin graph observables $\mathscr{O}$ (see Prop. 27):

$$O_h \triangleq \rho(h \overset{r_h}{\Longleftarrow} h) \text{ for some } r_h$$

Let us verify that this matches Eq. 7:

$$\begin{array}{rcl} \rho(h \overset{r_h}{\Longleftarrow} h)\,|g\rangle & = & \rho(h \overset{r_h}{\Longleftarrow} h)\rho(g \Leftarrow \emptyset)\,|\emptyset\rangle \\ & = & \rho(h \overset{r_h}{\Longleftarrow} h *_{\mathscr{R}} g \Leftarrow \emptyset)\,|\emptyset\rangle \end{array} \tag{8}$$

Consider an arbitrary composite $(g \Leftarrow \emptyset) \rhd_n (h \overset{r_h}{\Longleftarrow} h)$ for some admissible match $n \in \mathcal{M}(g \Leftarrow \emptyset, h \overset{r_h}{\Longleftarrow} h))$. By Prop. 17, n must be an injective graph morphism from g to h. Assume that n is not surjective: then

$$\rho(\bar{\varphi}((h \overset{r_h}{\Longleftarrow} h) \lhd_n (g \Leftarrow \emptyset))) \,|\emptyset\rangle = 0 \,|\emptyset\rangle$$

in other words, the only contributions to Eq. 8 are those where n is an injective and surjective partial map from g to h, i.e. an embedding of h in g. It follows that

$$\langle|\, \rho(h \overset{r_h}{\Longleftarrow} h) \,|g\rangle = [h; g]_{r_h}$$

where $[h; g]_{r_h} \subseteq [h; g]$ for the subset of matches of h in g that are compatible with r_h deletions - meaning each node deleted by r_h (and then recreated) is matched to a node of same degree.

Hamiltonians for stochastic graph rewriting. We have now all the ingredients required to produce the Hamiltonian corresponding to a stochastic graph rewriting system.

Proposition 33. *Let $\left\{g_i' \overset{r_i}{\Longleftarrow} g_i \in \mathcal{N}\right\}_{i \in I}$ be a finite family of normal diagrams seen as rules and $\{\kappa_i \in [0, +\infty)\}_{i \in I}$ their associated rates. Define*

$$H = \sum_{i \in I} \kappa_i (\rho(g_i' \overset{r_i}{\Longleftarrow} g_i) - \rho(g_i \overset{r_i}{\Longleftarrow} g_i))$$

where $g_i \overset{r_i}{\Longleftarrow} g_i$ is the thin observable obtained from $g_i' \overset{r_i}{\Longleftarrow} g_i$. We have that (i) H is infinitesimal stochastic, (ii) $H \in End(\mathcal{G})$ is row-finite.

We will need the following lemma.

Lemma 34. *For all $g_1 \overset{r_1}{\Longleftarrow} g \in \mathcal{N}$, $g_2 \overset{r_2}{\Longleftarrow} g \in \mathcal{N}$,*

$$\langle|\, \rho(g_1 \overset{r_1}{\Longleftarrow} g) = \langle|\, \rho(g_2 \overset{r_2}{\Longleftarrow} g)$$

Proof. We start with $|h = \emptyset\rangle$. If $g \neq \emptyset$ then the claim is trivially verified. Let us then assume $g = \emptyset$ (implying $r_1, r_2 = \emptyset$):

$$\begin{aligned} \langle|\, \rho(g_1 \overset{r_1}{\Longleftarrow} \emptyset) \,|\emptyset\rangle &= \langle|\, |g_1\rangle = 1 \\ &= \langle|\, |g_2\rangle \\ &= \langle|\, \rho(g_2 \overset{r_2}{\Longleftarrow} \emptyset) \,|\emptyset\rangle \end{aligned}$$

For $|h \neq \emptyset\rangle$, we have by definition of ρ:

$$\begin{aligned} \langle|\, \rho(g_1 \overset{r_1}{\Longleftarrow} g) \,|h\rangle &= \langle|\, \rho(g_1 \overset{r_1}{\Longleftarrow} g *_{\mathscr{R}} h \Leftarrow \emptyset) \,|\emptyset\rangle \\ &= \textstyle\sum_n \langle|\, \rho(g_1 \overset{r_1}{\Longleftarrow} g \lhd_n \bar{\varphi}(h \Leftarrow \emptyset)) \,|\emptyset\rangle \end{aligned}$$

Only admissible matches n which are surjective graph morphisms from h to g contribute to this sum. Also, $\mathcal{M}(h \Leftarrow \emptyset, g_1 \overset{r_1}{\Longleftarrow} g) = \mathcal{M}(h \Leftarrow \emptyset, g_2 \overset{r_2}{\Longleftarrow} g)$. Applying reduction we may write:

$$\begin{aligned} \textstyle\sum_n \langle|\, \rho(\bar{\varphi}(g_1 \overset{r_1}{\Longleftarrow} g \lhd_n h \Leftarrow \emptyset)) \,|\emptyset\rangle &= \textstyle\sum_n \langle|\, \rho(g_1 \Leftarrow \emptyset) \,|\emptyset\rangle \\ &= \textstyle\sum_n \langle|\, \rho(g_2 \Leftarrow \emptyset) \,|\emptyset\rangle \end{aligned}$$

where the last line follows by the first case of our analysis. Applying the same reasoning in reverse yields the claim. ☐

We can now prove Prop. 33:

Proof. It suffices to consider the case of one rule $g' \overset{r}{\Leftarrow} g$. It is enough to prove that for all $|g\rangle$,

$$\langle|\, (\rho(g' \overset{r}{\Leftarrow} g) - \rho(g \overset{r}{\Leftarrow} g)) \,|g\rangle = 0$$

where $g \overset{r}{\Leftarrow} g$ is the thin observable obtained from $g \overset{r}{\Leftarrow} g$. This is a straightforward consequence of Lemma 34. Row-finiteness is a direct consequence of Lemma 30. ☐

Jump-closure for observables. As presented at the beginning of this section, any Hamiltonian (as obtained from Prop. 33) induces a stochastic dynamics, from which one can – in principle – derive all quantities of interest. However, one is typically not interested in the full dynamical system, but only in the *expected value of some graph observable* (or higher moments thereof). The remainder of this section re-proves in our algebraic setting a series of results (Danos et al. 2014) which allow to derive from a Hamiltonian a formal (in the sense that solutions do not always exist) system of ordinary differential equations (ODEs) which describes the time evolution of the expected value of graph observables. The key result is *jump-closure* of observables under the action of a Hamiltonian. In words, this result implies that the time evolution of the expected value of a graph observable O_g is a function of the time evolution of the expected value of a finite family of other observables. This induces a coupled system of ODEs which, in good cases, closes on a finite set of variables. Even when that is not the case, this presentation of the dynamics has the quality of being amenable to approximations (Danos et al. 2014). Let us prove jump-closure:

Theorem 35 (Jump-closure for observables)**.** *For all Hamiltonian H as produced in Prop. 33 and all $g \in G_{\cong}$, there exists a finite family $\mathcal{F} \subseteq G_{\cong}$ such that*

$$\langle|\, O_g H = \sum_{h \in \mathcal{F}} \alpha_{g,h,H} \langle|\, O_h$$

for some constants $\{\alpha_{g,h,H}\}_{h \in \mathcal{F}}$.

Proof. By linearity, it is sufficient to consider the case where H is generated by a single rule $d = f' \overset{r}{\Leftarrow} f$ with rate κ, yielding

$$H = \kappa(\rho(f' \overset{r}{\Leftarrow} f) - O_f)$$

where $O_f = f \overset{r}{\Leftarrow} f$. The goal is reduced to exhibiting $\mathcal{F}$ s.t.

$$\langle|\, (O_g \rho(f' \overset{r}{\Leftarrow} f) - O_g O_f) = \sum_{h \in \mathcal{F}} \alpha_{g,h,H} \langle|\, O_h$$

Since observables $\mathscr{O}$ form a subalgebra of $\mathscr{R}$ (Prop. 27), $O_g O_f$ is trivially a finite linear combination of observables. Let us consider the term $\langle|\, O_g \rho(f' \overset{r}{\Leftarrow} f)$:

$$\begin{aligned} \langle|\, O_g \rho(f' \overset{r}{\Leftarrow} f) &= \langle|\, \rho(g \overset{r_g}{\Longleftarrow} g *_{\mathscr{R}} f' \overset{r}{\Leftarrow} f) \\ &= \textstyle\sum_n \alpha_{g,H,h_n} \langle|\, \rho(h_n' \overset{r_n}{\Longleftarrow} h_n) \end{aligned}$$

where $n \in \mathcal{M}(f' \overset{r}{\Leftarrow} f, g \overset{r_g}{\Longleftarrow} g)$. Lemma 34 allows us to write:

$$\begin{aligned} \textstyle\sum_n \alpha_{g,h_n,H} \langle|\, \rho(h_n' \overset{r_n}{\Longleftarrow} h_n) &= \textstyle\sum_n \alpha_{g,h_n,H} \langle|\, \rho(h_n \overset{r_n}{\Longleftarrow} h_n) \\ &= \textstyle\sum_n \alpha_{g,h_n,H} O_{h_n} \end{aligned}$$

which concludes the proof. ☐

Jump-closure for products of observables. As we will show, jump-closure for observables corresponds to the data of a system of ODEs describing the time evolution of the expected value (the first "moment") of an observable. The same procedure can be extended to yield ODEs describing the time evolution of higher moments, i.e. expected values of *products* of observables. The action of a Hamiltonian on a product of observables will be expressed in term of the *commutator* of these operators. Let us recall the definition of the commutator.

Definition 36 (Commutator)**.** *The* commutator $[A, B]$ *of two operators $A, B \in End(\mathcal{G})$ is defined by*

$$[A, B] \triangleq AB - BA$$

It is trivially bilinear.

The commutator of two operators quantifies their lack of commutativity – in this respect, it is a quantitative account of the independence of the processes represented by these operators. In particular, we have:

Lemma 37. *For all observables $O_h, O_g \in \mathscr{O}$, $[O_h, O_g] = 0$.*

Proof. Trivial consequence of Prop. 27. ☐

We will need the following lemma when dealing with nested commutators.

Lemma 38. *Let $\mathcal{O} = \{O_i\}_{1 \leqslant i \leqslant n}$ be a finite family of commuting operators (i.e. $[O_i, O_j] = 0$ for all i, j), B an operator and $\sigma \in S_n$ a permutation of $\{1, \ldots, n\}$. Let us define the notation*

$$\mathbf{C}^{\sigma}(\mathcal{O}, B) \triangleq [O_{\sigma(1)}, [O_{\sigma(2)}, \ldots [O_{\sigma(n)}, B] \ldots]]$$

Then for all $\sigma \in S_n$, $\mathbf{C}^{\sigma}(\mathcal{O}, B) = \mathbf{C}^{id}(\mathcal{O}, B) \triangleq \mathbf{C}(\mathcal{O}, B)$.

Proof. We proceed by induction. Let us start wit h $n = 2$ and with $\mathcal{O}_2 = \{O_1, O_2\}$. Using the fact that observables commute,

$$\begin{array}{rcl} [O_1, [O_2, B]] & = & [O_1, O_2 B - B O_2] \\ & = & [O_1, O_2 B] - [O_1, B O_2] \\ & = & O_1 O_2 B + B O_2 O_1 - O_2 B O_1 - O_1 B O_2 \\ & = & O_2 O_1 B + B O_1 O_2 - O_2 B O_1 - O_1 B O_2 \\ & = & [O_2, O_1 B] - [O_2, B O_1] = [O_2, [O_1, B]] \end{array}$$

For $n = k + 1$, the result follows by setting $B = C^{\sigma}(\mathcal{A}_n \backslash \{O_1\})$ and applying the induction hypothesis. ☐

The following proposition asserts that the expected value of observables under the action of a Hamiltonian can be reordered in an useful form.

Proposition 39 (Jump-closure for products of observables)**.** *For all Hamiltonian H as produced in Prop. 33, for all $n \geqslant 2$ and all finite family of observables $\mathcal{O} = \{O_i\}_{1 \leqslant i \leqslant n}$, noting $\mathcal{O}_m^{\sigma} = \{O_{\sigma(i)}\}_{1 \leqslant \sigma(i) \leqslant m}$,*

$$\langle | \, O_1 \ldots O_n H = \sum_{\sigma \in S_n} \sum_{m=1}^{n} \langle | \, \frac{\mathbf{C}(\mathcal{O}_m^{\sigma}, H) \prod_{i > m} O_{\sigma(i)}}{m!(n-m)!} \tag{9}$$

where S_n is the symmetric group over n elements.

Proof. We proceed by induction on n, starting from $n = 2$. We have:

$$\begin{array}{rcl} \langle | \, O_1 O_2 H & = & \langle | \, (O_1 [O_2, H] + O_1 H O_2) \\ & = & \langle | \, (O_1 [O_2, H] + ([O_1, H] + H O_1) O_2) \\ & = & \langle | \, (O_1 [O_2, H] + [O_1, H] O_2 + H O_1 O_2) \end{array}$$

The term $\langle | \, H O_1 O_2$ vanishes per Lemma 32. Observe also that $O_1 [O_2, H] = [O_1, [O_2, H]] + [O_2, H] O_1$. We obtain:

$$\begin{array}{rcl} \langle | \, O_1 O_2 H = & \langle | \, ([O_1, [O_2, H]] + [O_2, H] O_1 + [O_1, H] O_2) \\ = & \langle | \, \left(\mathbf{C}(\mathcal{O}_2^{id}, H) + \sum_{\sigma \in S_2} \mathbf{C}(\mathcal{O}_1^{\sigma}, H) O_{\sigma(2)} \right) \end{array}$$

Applying Lemma 38, one obtains the sought formula. Let us treat the inductive case $n = k + 1$. Given a family $\mathcal{O}_n = \{O_i\}_{1 \leqslant i \leqslant n}$ and writing $O'_i = O_i$ for all $i < k$ and $O'_k = O_k O_n$, we get a family of operators $\mathcal{O}'_k$. The result follows easily by applying the induction hypothesis on this family. ☐

Eq. 9 shows that in order to compute higher moments, it is required to compute the full nested commutators $\mathbf{C}(\mathcal{O}_m^{\sigma}, H)$. This computation can be simplified slightly with the following observation. Any element of $v \in \mathscr{R}$ can be decomposed uniquely as $v = \hat{v} + \mathring{v}$ with $\hat{v} \in \mathscr{R} \backslash \mathscr{O}$ and $\mathring{v} \in \mathscr{O}$. This decomposition lifts to Hamiltonians by linearity of the representation.

Definition 40 (Non-observable part of a Hamiltonian)**.** *Let H be constructed as in Prop. 33. H admits a unique decomposition*

$$H = \hat{H} + \mathring{H}$$

where $\hat{H} = \rho(\hat{v})$ for $\hat{v} \in \mathscr{R} \backslash \mathscr{O}$ and $\mathring{H} = \rho(\mathring{v})$ for $\mathring{v} \in \mathscr{O}$.

The following Lemma takes advantage of this decomposition to simplify commutators:

Lemma 41 (Commutator simplification for Hamiltonians)**.** *For all graph observable operator O_h and all Hamiltonian H as defined in Prop. 33, $[O_h, H] = [O_h, \hat{H}]$.*

Proof. Direct consequence of linearity of the commutator and of Lemma 37. ☐

This allows for the following refined version of Proposition 39:

Corollary 42 (Refined jump-closure for products of observables)**.** *Let H and $\mathcal{O}$ be as in Prop. 39. With the same notations, it holds that*

$$\langle | \, O_1 \ldots O_n H = \sum_{\sigma \in S_n} \sum_{m=1}^{n} \langle | \, \frac{\mathbf{C}(\mathcal{O}_m^{\sigma}, \hat{H}) \prod_{i > m} O_{\sigma(i)}}{m!(n-m)!} \tag{10}$$

Proof. Straightforward using Lemma 41 and Lemma 38. ☐

Existence of solutions: what we know. As introduced at the beginning of this section, jump-closure provides a method for producing coupled systems of ODEs that describe the expected value of observables (or product thereof). We conclude this section by *(i)* exposing when and how these differential systems are obtained and *(ii)* discussing the relevance of the solutions, if any, with respect to the underlying system.

Let H be an Hamiltonian and let $P : [0, \infty) \to Stoch$ be the semigroup induced by the semigroup associated to H. Let us denote the time-evolving subprobability by $|\psi(t)\rangle = P(t)\psi$, for $\psi \in Prob$ some initial condition. The expression $\langle | \, O_g p(t)$ describes formally the time evolution of the expected value of O_g. By definition of the master equation (Eq. 6), we have:

$$\frac{d}{dt} \langle | \, O_g \, |\psi(t)\rangle = \langle | \, O_g H \, |\psi(t)\rangle$$

and by Thm. 35, there must exists a finite family $\mathcal{F} \subset G_{\cong}$ s.t.

$$\frac{d}{dt} \langle | \, O_g \, |\psi(t)\rangle = \sum_{h \in \mathcal{F}} \alpha_{g,h,H} \langle | \, O_h \, |\psi(t)\rangle$$

In the exact same way, one can derive a formal system of ODEs for the expected value of finite products of observables (sometimes called *correlators*), thus giving access to all moments of $p(t)$. Starting from Eq. 10 (and reusing the same notations), one obtains:

$$\frac{d}{dt} \langle | \, O_1 \ldots O_n H = \sum_{\sigma \in S_n} \sum_{m=1}^{n} \langle | \, \frac{\mathbf{C}(\mathcal{O}_m^{\sigma}, \hat{H}) \prod_{i > m} O_{\sigma(i)}}{m!(n-m)!} \, |\psi(t)\rangle$$

whence, in both cases, we have produced a (potentially infinite) formal system of differential equations – *formal* in the sense that the following problems might arise:

1. it might have no unique solution;
2. it might be explosive (Norris 1998): p might not be defined at all times and might range in subprobabilities, in which case the relation of the "solution" with the actual expected value of the observable is subject to caution.

In general, for finite systems (meaning that only finitely many states are accessible from a given reference initial state x_0) all the above objects make sense, have unique solutions and the meaning of their solution is indeed, as expected, the time-dependent mean value of the associated observable (starting at x_0). This is also easily seen to be true if the observables are finitely supported. To quote (Spieksma 2012), "Other cases are not quite as clear".

It remains to be seen whether the few available sufficient conditions on H and and on observables for the derived system of ODEs to have solutions can be exploited to guarantee existence of solutions for a substantial class of dynamics studied in this paper. An adaption of energy-based graph-rewriting systems (as studied in (Danos et al. 2013)) can be a good guess for obtaining a substantial such class. Indeed, in the discrete case (see eg (Danos and Oury 2013)), we know that energy-driven dynamics converges to a multidimensional Poisson distribution and the dynamics is non-explosive, which is a first indication that the extended FE has solutions for a wide class of observables.

6. Outlook

We have introduced in this paper an algebra of graph-rewriting rules. Rules are seen as normal forms of a combinatorial algebra of diagrams. The diagram algebra is a syntax which we believe has independent interest as it describes what one might call abstract computational traces, or neighbourhoods of such traces. This is reminiscent of structures introduced for trace compression (Danos et al. 2012) used in causal analysis and diagnosis methods and developed for the specific case of site-graph rewriting (specifically, the Kappa language) (Danos et al. 2007). It would be a worthwhile effort to investigate rather this formalism lends itself better to trace compression. (Incidentally, there is a more relaxed version of diagrams where one does not ask for global acyclicity. Not every diagram can now be built inductively from rules but the evaluation of diagrams works as before.)

With the algebraic part of the paper in place, we turn to actual rewriting which is now seen as a *representation* of the rule algebra on the vector space spanned by graphs. In the discrete case (no edges), this construction boils down to the Heisenberg-Weyl (HW) algebra and its canonical representation on the Fock space (see references in (Blasiak et al. 2010)), so we are on familiar territory. The fundamental property of this representation is the property of *jump-closure*, that is to say, we show that observables are closed under (the representation of) rules. This development compares advantageously to Ref. (Danos et al. 2014) where one obtains jump-closure in a rather ad hoc way and in the easiest setting of SPO rewriting (our method can do both with equal ease). The actual combinatorial expression of jump-closure reduces in our new framework to a straightforward evaluation in the diagram algebra. Besides the conceptual clarification which the new technique provides, it also marks an improvement as a practical computational tool. It can also be said that the former approach can handle the case of correlators only in an indirect way by using the algebra structure of observables. The direct derivation we propose here is compellingly simple in comparison.

From jump closure, one can immediately derive the so-called rate equations for graph observables and arbitrary moments thereof. These equations are ubiquitous in the physics and applied mathematical literature. A recent example is Ref. (Basak et al. 2015, p21) where the authors derive the forward equation for a voter model with rewiring (up to order 3). This is still doable by hand, but would become extremely difficult at higher orders or for more complex models. Evidently, it would be interesting to find non trivial classes of rules and observables for which one can have guarantees on the existence and meaning of solutions to these equations, but, further than the case of finitely supported observables, little seems to be known. In Ref. (Spieksma 2012), one finds hard-earned conditions which could allow one some progress, but this remains to be seen. Ergodicity conditions which one can derive from assuming potentials driving the dynamics (perhaps by adapting the work done in Ref. (Danos et al. 2013) for site-graphs) offers an interesting and complementary option.

Another interesting avenue is the search for combinatorial applications which parallel those obtained via the HW algebra in the discrete case. Some discrete dynamics, such as multi-type birth-death processes, admit closed forms that one can derive in a systematic way by means of standard analytical combinatorics techniques (umbral calculus (Blasiak et al. 2010)). Preliminary results show that we can extend these ideas to graph-based dynamics.

Returning to purely algebraic part of the paper, other types of rewriting follow naturally form the approach. Relaxing condition 5) on diagrams (Section 3) gives rise to a Hopf algebra of diagrams for which one can define four different evaluation morphisms. Each corresponds to a different way to handle worldlines of edges which outlast or predate that of their ends. The simplest evaluation is the only one considered here and corresponds to DPO-rewriting. Other types induce different canonical representations and lead to other types of graph rewriting (among which SPO-rewriting and a hitherto unconsidered dual variant). We will pursue this interesting classification in further work and build this variant stochastic mechanical frameworks for each obtained notion of graph-rewriting.

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A. Rule diagrams, untamed

An example of diagram not satisfying the totality condition. The reader might wonder which are the "pathological" diagrams that give rise to partial graphs after normalization. Let us give such an example. The following diagram is an edge observable attached to a rule that deletes a vertex (notice there is no output vertex on top of $\circ_4$). We invite the reader to check that the right hand side of the diagram is indeed the outcome after normalization.

$$\begin{tikzcd}
 & & \circ_4 & & & & & \\
\bullet_2 & \blacklozenge_b \arrow[l] \arrow[r] & \bullet_3 \arrow[u] & {} \arrow[r, mapsto, "\partial"] & {} & \bullet_2 & \blacklozenge_b \arrow[l] & \\
\circ_0 \arrow[u, dotted] & \lozenge_a \arrow[l] \arrow[r] \arrow[u, dotted] & \circ_1 \arrow[u, dotted] & & & \circ_0 \arrow[u, dotted] & \lozenge_a \arrow[l] \arrow[r] \arrow[u, dotted] & \circ_1
\end{tikzcd} \tag{11}$$

Observe that the output graph is partial. As has already been investigated by the authors (Behr et al. 2016), these partial normal forms have a rich theory which is related to particular types of graph rewriting techniques.

An example of diagram not satisfying the global acyclicity condition. The following is an example of diagram that does not satisfy global acyclicity.

$$\begin{tikzcd}
\bullet_2 \arrow[drr, bend left] & \blacklozenge_b \arrow[l] \arrow[r] & \bullet_3 \\
\circ_0 \arrow[u, dotted] & \lozenge_a \arrow[l] \arrow[r] \arrow[u, dotted] & \circ_1 \arrow[u, dotted]
\end{tikzcd} \tag{12}$$

One easily checks that the (unique) vertex pdd here is indeed acyclic. The outcome of normalisation will be a loop observable.