Rule Algebras for Adhesive Categories

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Abstract

We show that every adhesive category gives rise to an associative algebra of rewriting rules induced by the notion of double-pushout (DPO) rewriting and the associated notion of concurrent production. In contrast to the original formulation of rule algebras in terms of relations between (a concrete notion of) graphs, here we work in an abstract categorical setting. Doing this, we extend the classical concurrency theorem of DPO rewriting and show that the composition of DPO rules along abstract dependency relations is, in a natural sense, an associative operation. If in addition the adhesive category possesses a strict initial object, the resulting rule algebra is also unital. We demonstrate that in this setting the canonical representation of the rule algebras is obtainable, which opens the possibility of applying the concept to define and compute the evolution of statistical moments of observables in stochastic DPO rewriting systems.

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1 Introduction

Double pushout graph (DPO) rewriting [9] is the most well-known approach to algebraic graph transformation. The underlying rewriting mechanics are specified in terms of the universal properties of pushouts – for this reason, the approach is domain-independent and instantiates across a number of concrete notions of graphs and graph-like structures. Moreover, the introduction of adhesive and quasi-adhesive categories [11, 10] (which, roughly speaking, ensure that the pushouts involved are "well-behaved", i.e. they satisfy similar exactness properties as pushouts in the category of sets and functions) entailed that a standard corpus of theorems [14] that ensures the "good behavior" of DPO rewriting holds if the underlying ambient category is (quasi-)adhesive.

An important classical theorem of DPO rewriting is the *concurrency theorem*, which involves an analysis of *two* DPO productions applied in series. Given a *dependency relation* (which, intuitively, determines how the right-hand side of the first rule overlaps with the left-hand side of the second), a purely category-theoretic construction results in a *composite* rule which applies the two rules simultaneously. The concurrency theorem then states that in any graph, the two rules can be applied in series in a way consistent with the relevant dependency relation if and only if the composite rule can be applied, yielding the same result.

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The operation that takes two rules together with a dependency relation and produces a composite rule can be considered as an algebraic operation on the set of DPO productions for a given category. From this viewpoint, it is natural to ask whether this operation is associative. It is remarkable that this appears to have been open until now. Our main contribution is an elementary proof of associativity of this type of composition.

Associativity is advantageous for a number of reasons. In [2, 4], the first author and his team developed the *rule algebra* framework for a concrete notion of multigraphs. Inspired by a standard construction in mathematical physics, the operation of rule composition along a common interface yields an associative algebra: given a free vector space with basis the set of DPO rules, the product of the associative algebra takes two basis elements to a formal sum, over all possible dependency relations, of their compositions. This associative algebra is useful in applications, being the formal carrier of combinatorial information that underlies *stochastic* interpretations of rewriting. The most famous example in mathematical physics is the Heisenberg-Weyl algebra [6, 7], which served as the starting point for [2]. Indeed, [2, 4] generalized the Heisenberg-Weyl construction from mere set rewriting to multigraph rewriting. Our work, since it is expressed abstractly in terms of adhesive categories, entails that the Heisenberg-Weyl and the DPO graph rewriting rule algebra can *both* be seen as two instances of the same construction, expressed in abstract categorical terms.

Structure of the paper. Following the preliminaries in Section 2, we prove our main result in Section 3. Next, in Section 4 we give the abstract definition of rule algebra, and demonstrate that it captures the well-known Heisenberg-Weyl algebra in Section 5. We conclude with applications to combinatorics and stochastic mechanics in Sections 6 and 7.

2 Adhesive categories and Double-Pushout rewriting

We briefly review standard material, following mostly [11] (see [8, 14] for further references).

▶ **Definition 2.1** ([11], Def. 3.1)**.** A category $\mathbf{C}$ is said to be *adhesive* if

(i) $\mathbf{C}$ has pushouts along *monomorphisms*,
(ii) $\mathbf{C}$ has pullbacks, and if
(iii) pushouts along monomorphisms are *van Kampen (VK)squares*.

Examples include **Set** (the category of sets and set functions), **Graph** (the category of directed multigraphs and graph homomorphisms), any presheaf topos, and any elementary topos [12]. One might further generalize by considering *quasi-adhesive categories* (see [11, 10]). We now recall *Double-Pushout (DPO) rewriting* in an adhesive category.

▶ **Definition 2.2** ([11], Def. 7.1)**.** A span p of morphisms

$$L \xleftarrow{l} K \xrightarrow{r} R \tag{1}$$

is called a *production*. p is said to be *left linear* if l is a monomorphism, and *linear* if both l and r are monomorphisms. We denote the set of linear productions by $Lin(\mathbf{C})$. We will also frequently make use of the alternative notation $L \overset{p}{\rightharpoonup} R$ where $p = (L \xleftarrow{l} K \xrightarrow{r} R) \in Lin(\mathbf{C})$.

A homomorphism of productions $p \to p'$ consists of arrows, $L \to L'$, $K \to K'$ and $R \to R'$, such that the obvious diagram commutes. A homomorphism is an isomorphism when all of its components are isomorphisms. We do not distinguish between isomorphic productions.

▶ **Definition 2.3** ([11], Def. 7.2)**.** Given a production p as in (1), a *match* of p in an object $C \in ob(\mathbf{C})$ is a morphism $m : L \to C$. A match is said to satisfy the *gluing condition* if there exists an object E and morphisms $g : K \to E$ and $v : E \to C$ such that (2) is a pushout.

$$\begin{array}{ccc} L & \xleftarrow{\;l\;} & K \\ {\scriptstyle m}\downarrow & \lrcorner & \downarrow{\scriptstyle g} \\ C & \xleftarrow{\;v\;} & E \end{array} \tag{2}$$

More concisely, the *gluing condition* holds if there is a *pushout complement* of $C \xleftarrow{m} L \xleftarrow{l} K$.

To proceed, we need to recall a number of properties of pushouts and pushout complements in adhesive categories. We start with some basic pasting properties that hold in any category.

▶ **Lemma 2.4.** *Given a commutative diagram as below,*

$$\begin{array}{ccccc} A & \longrightarrow & B & \longrightarrow & E \\ \downarrow & & \downarrow & & \downarrow \\ C & \longrightarrow & D & \longrightarrow & F \end{array}$$

- *(pullback version) if the right square is a pullback then the left square is a pullback if and only if the entire exterior rectangle is a pullback.*
- *(pushout version) If the left square is a pushout then the right square is a pushout if and only if the entire exterior rectangle is a pushout.*

▶ **Lemma 2.5** ([11], Lemmas 4.2, 4.3 and 4.5)**.** *In any adhesive category:*
(i) *Monomorphisms are stable under pushout.*
(ii) *Pushouts along monomorphisms are also pullbacks.*
(iii) *Pushout complements of monomorphisms (if they exist) are unique up to isomorphism.*

From here on, we will focus solely on *linear productions*, which entails due to the above statements a number of practical simplifications.

▶ **Definition 2.6** (compare [11], Def. 7.3)**.** Let $\mathbf{C}$ be an adhesive category, and denote by $Lin(\mathbf{C})$ the set of linear productions on $\mathbf{C}$. Given an object $C \in \mathbf{C}$ and a linear production $p \in Lin(\mathbf{C})$, we denote the *set of admissible matches* $\mathcal{M}_p(C)$ as the set of monomorphisms $m : L \hookrightarrow C$ for which m satisfies the *gluing condition*. As a consequence, there exists objects and morphisms such that in the diagram below both squares are pushouts:

$$\begin{array}{ccccc} L & \xleftarrow{\;l\;} & K & \xrightarrow{\;r\;} & R \\ {\scriptstyle m}\downarrow & & \downarrow{\scriptstyle k} & & \downarrow{\scriptstyle m'} \\ C & \xleftarrow{\;l'\;} & K' & \xrightarrow{\;r'\;} & D \end{array} \tag{3}$$

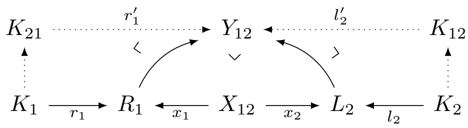
We write $p_m(C) := D$ for the object "produced" by the above diagram. The process is called *derivation* of C along production p and admissible match m, and denoted $C \underset{p,m}{\Longrightarrow} p_m(C)$.

Note that by virtue of Lemma 2.5, the object $p_m(C)$ produced via a given derivation of an object C along a linear production p and an admissible match m is *unique up to isomorphism.* From here on, we will refer to linear productions as *linear (rewriting) rules.* Next, we recall the concept of *(concurrent) composition* of linear rules.

3 Concurrent composition and associativity

Convention. unless mentioned otherwise, all arrows are assumed to be monomorphisms.

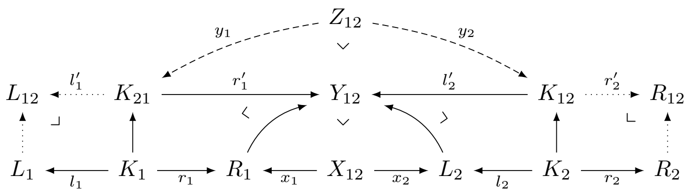
For rules $p_1, p_2 \in Lin(\mathbf{C})$, a *dependency relation* consists of an object X_{12} and a span of monomorphisms $\mathbf{m} : R_1 \xleftarrow{x_1} X_{12} \xrightarrow{x_2} L_2$, s.t. K_{12}, K_{21} and morphisms illustrated below exist, where the cospan $R_1 \to Y_{12} \leftarrow L_2$ is the pushout of $\mathbf{m}$, and the two indicated regions are also pushouts; i.e. there exist pushouts complements of $K_1 \xrightarrow{r_1} R_1 \to Y_{12}$ and $K_2 \xrightarrow{l_2} L_2 \to Y_{12}$.



(4)

Intuitively, the existence of the left and right pushout diagrams amounts to the two rules agreeing on the overlap specified by X_{12}, and amenable to being executed concurrently. We refer to such $\mathbf{m}$ as an *admissible match* of p_2 in p_1 and denote the set of these by $p_2 \Vdash p_1$.

Algebraically speaking, given p_1, p_2 and $\mathbf{m} \in p_2 \Vdash p_1$, we can consider "concurrent execution" to be an operation that composes p_1 and p_2 "along" $\mathbf{m}$ to obtain a rule $p_2 \overset{\mathbf{m}}{\blacktriangleleft} p_1$. To obtain $p_2 \overset{\mathbf{m}}{\blacktriangleleft} p_1$, we extend (4) by taking two further pushouts (marked with dotted arrows) and take a pullback (marked with dashed arrows):



(5)

Now we define the *composite of* p_1 *with* p_2 *along* m as

$$p_2 \overset{\mathbf{m}}{\blacktriangleleft} p_1 := (L_{12} \xleftarrow{z_1} Z_{12} \xrightarrow{z_2} R_{12})\,,\ z_1 := l_1' \circ y_1\,,\ z_2 := r_2' \circ y_2\,. \tag{6}$$

The following well-known result shows that composition is compatible with application.

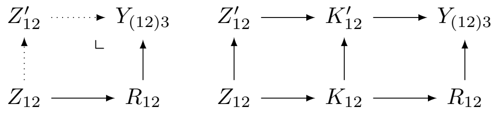
▶ **Theorem 3.1** (Concurrency Theorem; [11], Thm. 7.11). *Let $p, q \in Lin(\mathbf{C})$ be two linear rules and $C \in ob(\mathbf{C})$ an object.*

- *Given a two-step sequence of derivations $C \underset{p,m}{\Longrightarrow} p_m(C) \underset{q,n}{\Longrightarrow} q_n(p_m(C))$, there exists a composite rule $r = p_2 \overset{\mathbf{d}}{\blacktriangleleft} p_1$ for unique $\mathbf{d} \in q \Vdash p$, and a unique admissible match $e \in \mathcal{M}_r(C)$, such that $C \underset{r,e}{\Longrightarrow} r_e(C)$ and $r_e(C) \cong q_n(p_m(C))$.*
- *Given a dependency relation $\mathbf{d} \in q \Vdash p$, $r = p_2 \overset{\mathbf{d}}{\blacktriangleleft} p_1$ and an admissible match $e \in \mathcal{M}_r(C)$, there exists a unique pair of admissible matches $m \in \mathcal{M}_p(C)$ and $n \in \mathcal{M}_q(p_m(C))$ such that $C \underset{p,m}{\Longrightarrow} p_m(C) \underset{q,n}{\Longrightarrow} q_n(p_m(C))$ with $q_n(p_m(C)) \cong r_e(C)$.*

The following technical lemma will be of use when proving our main result.

▶ **Lemma 3.2** (Admissibility is compatible with composition). *Suppose that $p_1, p_2 \in Lin(\mathbf{C})$ and suppose that $m_{(12)3} \in p_3 \Vdash \left(p_2 \overset{m_{12}}{\blacktriangleleft} p_1\right)$. Let $p_2 \overset{m_{12}}{\blacktriangleleft} p_1$ be as shown in (6), computed as in (5). Let $p_2' = Y_{12} \xleftarrow{l_2'} K_{12} \xrightarrow{r_2'} R_{12}$. Then $m_{(12)3} \in p_2' \Vdash p_3$.*

Proof. By the assumption $m_{(12)3} \in p_3 \Vdash \left(p_2 \overset{m_{12}}{\blacktriangleleft} p_1\right)$, there exists the pushout below left.



By construction (see (5)), the arrow $Z_{12} \to R_{12}$ factors through K_{12}. Taking the pushout of the span $Z'_{12} \leftarrow Z_{12} \to K_{12}$ results in the diagram drawn above right. Since the whole region and the left square are pushouts, the right square is a pushout (Lemma 2.4). ◀

We now show that *concurrent composition of linear rules* is, in a natural sense, associative.

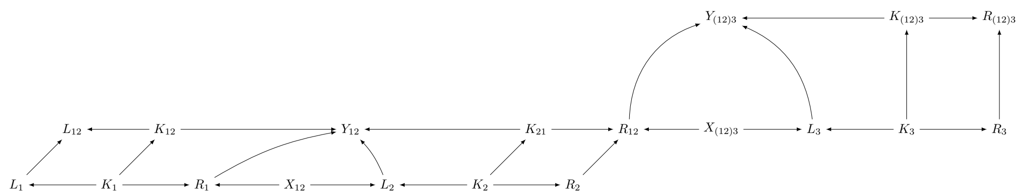
▶ **Theorem 3.3** (Associativity Theorem). *The composition operation* $.\overset{\cdot}{\blacktriangleleft}.$ *is* associative *in the following sense: given linear rules* $p_1, p_2, p_3 \in Lin(\mathbf{C})$*, there exists a bijective correspondence between pairs of admissible matches* $m_{21} \in p_2 \Vdash p_1$ *and* $m_{3(21)} \in p_3 \Vdash \left(p_2 \overset{m_{12}}{\blacktriangleleft} p_1\right)$*, and pairs of admissible matches* $m_{32} \in p_3 \Vdash p_2$ *and* $m_{(32)1} \in \left(p_3 \overset{m_{23}}{\blacktriangleleft} p_2\right) \Vdash p_1$ *such that*

$$p_3 \overset{m_{3(21)}}{\blacktriangleleft} \left(p_2 \overset{m_{21}}{\blacktriangleleft} p_1\right) = \left(p_3 \overset{m_{32}}{\blacktriangleleft} p_2\right) \overset{m_{(32)1}}{\blacktriangleleft} p_1 \,. \tag{7}$$

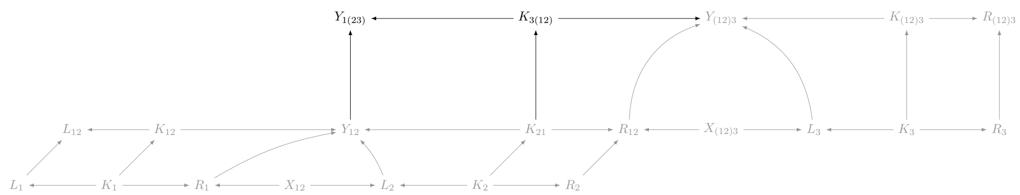
Proof. Since DPO derivations are symmetric, it suffices to show one side of the correspondence. Our proof is constructive, demonstrating how, given a pair of admissible matches

$$\left(m_{21} \in p_2 \Vdash p_1 \text{ and } m_{3(21)} \in p_3 \Vdash \left(p_2 \overset{m_{12}}{\blacktriangleleft} p_1\right)\right),$$

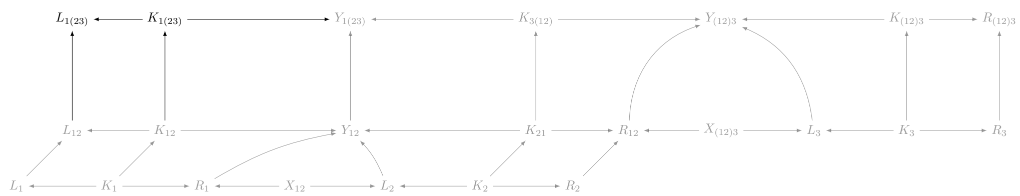
one obtains $m_{32} \in p_3 \Vdash p_2$ and $m_{(32)1} \in (p_3 \overset{m_{32}}{\blacktriangleleft} p_2) \Vdash p_1$ satisfying (7). We begin with $p_2 \overset{m_{21}}{\blacktriangleleft} p_1$, p_3 and the dependency relation $m_{3(21)}$, illustrated below.



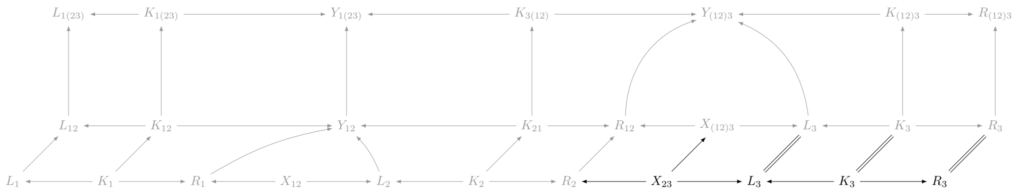
By Lemma 3.2, since the match $m_{3(21)}$ is by assumption admissible, we can find a pushout complement and pushout to extend the above diagram as follows,



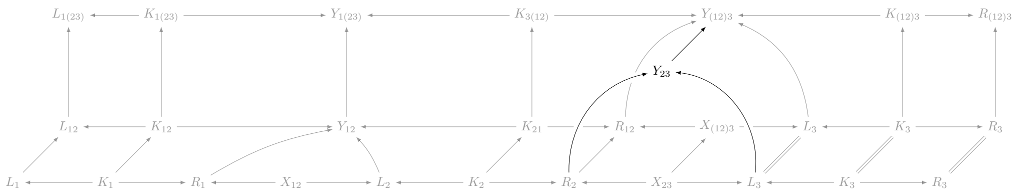
and again as below.



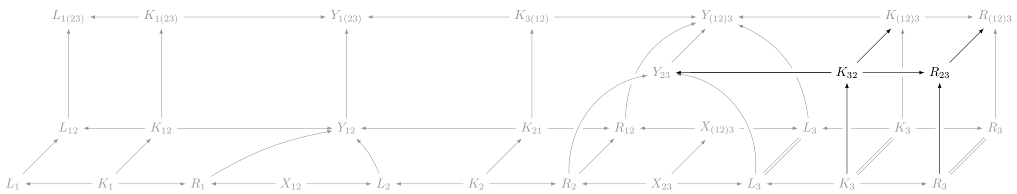
In the next step, we compute X_{23} as the evident pullback. Then we further extend the diagram via repeating the components of rule p_3.



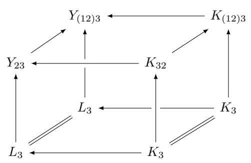
Now we push out R_2 and L_3 along X_{23}, obtaining $Y_{23} \to Y_{(12)3}$ from the universal property.



Next, we compute K_{32} by pulling back Y_{23} and $K_{1(23)}$ along $Y_{(12)3}$. We obtain $K_3 \to K_{32}$ from the universal property. To obtain the other morphisms, push out K_{32} and R_3 along K_3.

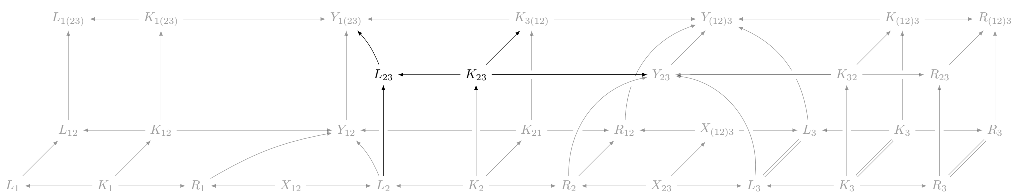


We need to establish that the newly constructed front face on the left is a pushout. To do so, let us consider the cube on the left in isolation.

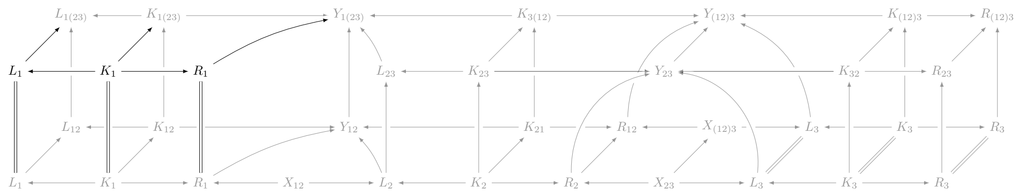


The rear face is a pushout, and therefore also a pullback. The bottom face is trivially both a pushout and a pullback. Pasting these two pushouts together yields a pushout, and since the top face – by construction – is a pullback, the front face is a pushout by Lemma 2.4: hence all faces of the cube, apart from the left and the right, are both pushouts and pullbacks.

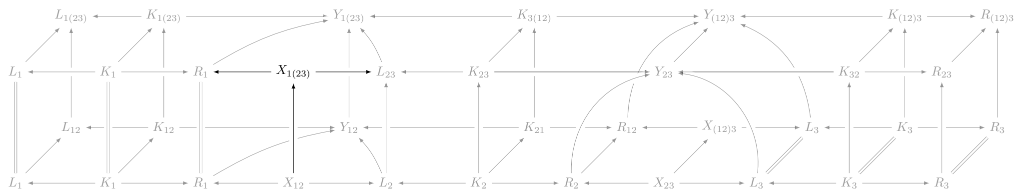
We take advantage of the symmetry involved, and obtain two further pushouts as front faces in the following. Moreover, the two new upper faces are pushouts also.



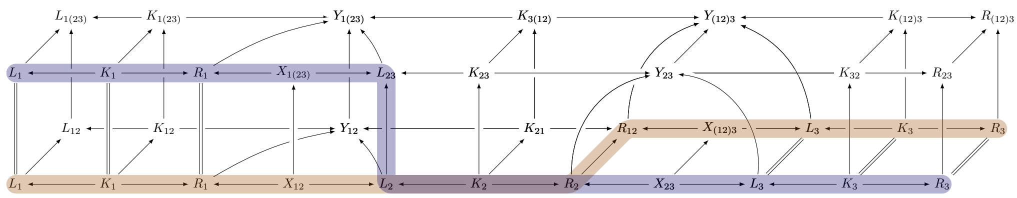
The next step is a trivial repetition of rule p_1: the new upper faces are both pushouts since they both arise as two pushouts pasted together.



We now obtain $X_{(12)3}$ by pulling back R_1 and L_{23} along $Y_{1(23)}$, the remaining monomorphism $X_{12} \to X_{(12)3}$ follows from the universal property.



The final step consists in proving that the cospan $R_1 \to Y_{1(23)} \leftarrow L_{23}$ is the pushout of the span $R_1 \leftarrow X_{1(23)} \to L_{23}$. Since the proof requires a somewhat lengthy diagram chase, we relegate this part of the proof to Appendix A.1. To conclude, the associativity property manifests itself in the following form, whereby the data provided along the path highlighted in orange below permits to uniquely compute the data provided along the path highlighted in blue (with both sets of overlaps computing the same "triple composite" production):



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4 From associativity of concurrent derivations to rule algebras

In DPO rewriting, each linear rewriting rule has a non-deterministic effect when acting on a given object, in the sense that there generically exist multiple possible choices of admissible match of the rule into the object. One interesting way of incorporating this non-determinism into a mathematical rewriting framework is motivated by the physics literature:

- Each linear rule is lifted to an element of an abstract *vector space*.
- Concurrent composition of linear rules is lifted to a *bilinear multiplication operation* on this abstract vector space, endowing it with the structure of an *algebra*.
- The action of rules on objects is implemented by mapping each linear rule (seen as an element of the abstract algebra) to an endomorphism on an abstract vector space whose basis vectors are in bijection with the objects of the adhesive category.

While this recipe might seem somewhat ad hoc, we will demonstrate in Section 5 that it recovers in fact one of the key constructions of quantum physics and enumerative combinatorics, namely we recover the well-known Heisenberg-Weyl algebra and its canonical representation.

▶ **Definition 4.1.** Let $\delta : Lin(\mathbf{C}) \to \mathcal{R}_{\mathbf{C}}$ be defined as a morphism which maps each linear rule $p = (I \overset{r}{\rightharpoonup} O) \in Lin(\mathbf{C})$ to a basis vector $\delta(p)$ of a free $\mathbb{R}$-vector space $\mathcal{R}_{\mathbf{C}} \equiv (\mathcal{R}_{\mathbf{C}}, +, \cdot)$. In order to distinguish between elements of $Lin(\mathbf{C})$ and $\mathcal{R}_{\mathbf{C}}$, we introduce the notation

$$(O \overset{r}{\Leftarrow} I) := \delta\left(I \overset{r}{\rightharpoonup} O\right) . \tag{8}$$

We will later refer to $\mathcal{R}_{\mathbf{C}}$ as the $\mathbb{R}$-vector space of *rule algebra elements*.

▶ **Definition 4.2.** Define the *rule algebra product* $*_{\mathcal{R}_{\mathbf{C}}}$ as the binary operation

$$*_{\mathcal{R}_{\mathbf{C}}} : \mathcal{R}_{\mathbf{C}} \times \mathcal{R}_{\mathbf{C}} \to \mathcal{R}_{\mathbf{C}} : (R_1, R_2) \mapsto R_1 *_{\mathcal{R}_{\mathbf{C}}} R_2 , \tag{9}$$

where for two basis vectors $R_i = \delta(p_i)$ encoding the linear rules $p_i \in Lin(\mathbf{C})$ $(i = 1, 2)$,

$$R_1 *_{\mathcal{R}_{\mathbf{C}}} R_2 := \sum_{\mathbf{m}_{12} \in p_1 \Vdash p_2} \delta\left(p_1 \overset{\mathbf{m}_{12}}{\blacktriangleleft} p_2\right) . \tag{10}$$

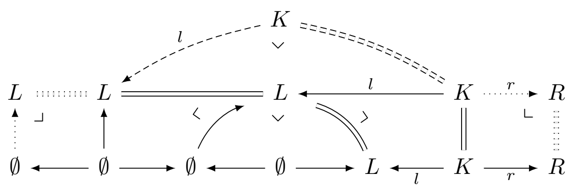
The definition is extended to arbitrary (finite) linear combinations of basis vectors by bilinearity, whence for $p_i, p_j \in Lin(\mathbf{C})$ and $\alpha_i, \beta_j \in \mathbb{R}$,

$$\left(\sum_i \alpha_i \cdot \delta(p_i)\right) *_{\mathcal{R}_{\mathbf{C}}} \left(\sum_j \beta_j \cdot \delta(p_j)\right) := \sum_{i,j} (\alpha_i \cdot \beta_j) \cdot \left(\delta(p_i) *_{\mathcal{R}_{\mathbf{C}}} \delta(p_j)\right) . \tag{11}$$

We refer to $\mathcal{R}_{\mathbf{C}} \equiv (\mathcal{R}_{\mathbf{C}}, *_{\mathcal{R}_{\mathbf{C}}})$ as the ***rule algebra*** (of linear DPO-type rewriting rules over the adhesive category $\mathbf{C}$).

▶ **Theorem 4.3.** *For every adhesive category $\mathbf{C}$, the associated rule algebra $\mathcal{R}_{\mathbf{C}} \equiv (\mathcal{R}_{\mathbf{C}}, *_{\mathcal{R}_{\mathbf{C}}})$ is an* associative algebra*. If $\mathbf{C}$ in addition possesses a* strict initial object *$c_\emptyset \in ob(\mathbf{C})$, $\mathcal{R}_{\mathbf{C}}$ is in addition a* unital algebra*, with unit element $R_\emptyset := (c_\emptyset \overset{\emptyset}{\Leftarrow} c_\emptyset)$.*

Proof. Associativity follows immediately from the associativity of the operation $.\overset{\cdot}{\blacktriangleleft}.$ proved in Theorem 3.3. The claim that $R_\emptyset$ is the unit element of the rule algebra $\mathcal{R}_{\mathbf{C}}$ of an adhesive category $\mathbf{C}$ with strict initial object follows directly from the definition of the rule algebra product for $R_\emptyset *_{\mathcal{R}_{\mathbf{C}}} R$ and $R *_{\mathcal{R}_{\mathbf{C}}} R_\emptyset$ for $R \in \mathcal{R}_{\mathbf{C}}$. For clarity, we present below the category-theoretic composition calculation that underlies the equation $R_\emptyset *_{\mathcal{R}_{\mathbf{C}}} R = R$:



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The property of a rule algebra being unital and associative has the important consequence that one can provide *representations* for it. The following definition, given at the level of adhesive categories with strict initial objects, captures several of the concrete notions of canonical representations in the physics literature; in particular, it generalizes the concept of canonical representation of the Heisenberg-Weyl algebra as explained in Section 5.

▶ **Definition 4.4.** Let $\mathbf{C}$ be an adhesive category with a strict initial object $c_\emptyset \in ob(\mathbf{C})$, and let $\mathcal{R}_\mathbf{C}$ be its associated rule algebra of DPO type. Denote by $\hat{\mathbf{C}}$ the $\mathbb{R}$-*vector space of objects of* $\mathbf{C}$, whence (with $|C\rangle$ denoting the basis vector of $\hat{\mathbf{C}}$ associated to an element $C \in ob(\mathbf{C})$)

$$\hat{\mathbf{C}} := span_\mathbb{R}\left(\{|C\rangle | C \in ob(\mathbf{C})\}\right) \equiv (\hat{C}, +, \cdot)\,. \tag{13}$$

Then the *canonical representation* $\rho_\mathbf{C}$ of $\mathcal{R}_\mathbf{C}$ is defined as the algebra homomorphism $\rho_\mathbf{C} : \mathcal{R}_\mathbf{C} \to End(\hat{\mathbf{C}})$, with

$$\rho_\mathbf{C}(p)\,|C\rangle := \begin{cases} \sum_{m \in \mathcal{M}_p(C)} |p_m(C)\rangle & \text{if } \mathcal{M}_p(C) \neq \emptyset \\ 0_{\hat{\mathbf{C}}} & \text{otherwise,} \end{cases} \tag{14}$$

extended to arbitrary elements of $\mathcal{R}_\mathbf{C}$ and of $\hat{\mathbf{C}}$ by linearity.

The fact that ρ_C as given in Definition 4.4 is a homomorphism is shown below.

▶ **Theorem 4.5** (Canonical Representation)**.** *For* $\mathbf{C}$ *adhesive with strict initial object,* $\rho_\mathbf{C} : \mathcal{R}_\mathbf{C} \to End(\hat{\mathbf{C}})$ *of Definition 4.4 is a homomorphism of unital associative algebras.*

Proof. See Appendix A.2. ◀

5 Recovering the blueprint: the Heisenberg-Weyl algebra

As a first consistency check and interesting special (and arguably simplest) case of rule algebras, consider the adhesive category $\mathbb{F}$ of equivalence classes of finite sets, and functions. This category might alternatively be interpreted as the category of isomorphism classes of *discrete graphs*, whose monomorphisms are precisely the injective partial morphisms of discrete graphs. Specializing to a subclass or morphisms, namely to *trivial* monomorphisms,

$$I \overset{\emptyset}{\leftharpoondown} O \equiv (I \leftarrow \emptyset \to O)\,,$$

we recover the famous Heisenberg-Weyl algebra and its canonical representation:

▶ **Definition 5.1.** Let $\mathcal{R}_0$ denote the rule algebra of DPO type rewriting for discrete graphs. Then the subalgebra $\mathcal{H}$ of $\mathcal{R}_0$ is defined as the algebra whose elementary generators are

$$x^\dagger := (\bullet \overset{\emptyset}{\Leftarrow} \emptyset)\,, \quad x := (\emptyset \overset{\emptyset}{\Leftarrow} \bullet)\,, \tag{15}$$

and whose elements are (finite) linear combinations of words in $x^\dagger$ and x (with concatenation given by the rule algebra multiplication $*_{\mathcal{R}_0}$) and of the unit element $R_\emptyset = (\emptyset \overset{\emptyset}{\Leftarrow} \emptyset)$. The canonical representation of $\mathcal{H}$ is the restriction of the canonical representation of $\mathcal{R}_0$ to $\mathcal{H}$.

The following theorem demonstrates how well-known properties of the Heisenberg-Weyl algebra (see e.g. [7, 4, 5] and references therein) follow directly from the previously introduced constructions of the rule algebra and its canonical representation. This justifies our claim that the Heisenberg-Weyl construction is a special case of our general framework.

▶ **Theorem 5.2** (Heisenberg-Weyl algebra from discrete graph rewriting rule algebra)**.**

(i) *For integers* $m, n > 0$,

$$\underbrace{x^\dagger *_{\mathcal{R}_0} \ldots *_{\mathcal{R}_0} x^\dagger}_{m\ times} = \underbrace{x^\dagger \uplus \ldots \uplus x^\dagger}_{m\ times}\,, \quad \underbrace{x *_{\mathcal{R}_0} \ldots *_{\mathcal{R}_0} x}_{n\ times} = \underbrace{x \uplus \ldots \uplus x}_{n\ times}\,, \tag{16}$$

where we define for linear rules $p_1, p_2 \in Lin(\mathbf{C})$

$$\delta(p_1) \uplus \delta(p_2) := \delta(p_1 \overset{\emptyset}{\blacktriangleleft} p_2)\,. \tag{17}$$

(ii) *The generators* $x, x^\dagger \in \mathcal{H}$ *fulfill the* canonical commutation relation

$$[x, x^\dagger] \equiv x *_{\mathcal{R}_0} x^\dagger - x^\dagger *_{\mathcal{R}_0} x = R_\emptyset\,, \quad R_\emptyset = (\emptyset \overset{\emptyset}{\leftharpoonup} \emptyset)\,. \tag{18}$$

(iii) *Every element of* $\mathcal{H}$ *may be expressed as a (finite) linear combination of so-called* normal-ordered *expressions* $x^{\dagger\,*r} * x^{*s}$ *(with* $r, s \in \mathbb{Z}_{\geq 0}$*).*

(iv) *Denoting by* $|n\rangle \equiv |\bullet^{\uplus\, n}\rangle$ *(*$n \in \mathbb{Z}_{\geq 0}$*) the basis vector associated to the discrete graph with* n *vertices in the vector space* $\hat{G}_0$ *of isomorphism classes discrete graphs, the canonical representation of* $\mathcal{H}$ *according to Definition 4.4 reads explicitly*

$$a^\dagger\,|n\rangle = |n+1\rangle\;, \quad a\,|n\rangle = \begin{cases} n \cdot |n-1\rangle & \text{if } n > 0 \\ 0_{\hat{G}_0} & \text{else} \end{cases}\;, \tag{19}$$

with $a^\dagger := \rho_{\mathcal{R}_0}(x^\dagger)$ *(the* creation operator*) and* $a := \rho_{\mathcal{R}_0}(x)$ *(the* annihilation operator*).*

Proof. See Appendix A.3. ◀

6 Applications of rule algebras to combinatorics

In this section we consider an example application, working with undirected multigraphs.

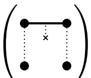
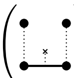
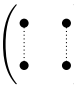
Given a set X, let $\mathcal{P}_2 X$ be the set of subsets of X of cardinality 2. Note that, unlike the ordinary powerset construction, $\mathcal{P}_2$ fails to be a covariant functor on the category of sets, since it is undefined on non-injective functions. An *undirected multigraph* is a triple $\mathcal{U} = (V, E, t : E \to \mathcal{P}_2 V)$ where V is a set of vertices, E a set of edges, and t assigns two distinct vertices to each edge. A homomorphism $f : \mathcal{U} \to \mathcal{U}'$ of undirected multigraphs consists of two functions, $f_E : E \to E'$ and $f_V : V \to V'$, such that f_V is

- *non-edge collapsing*, i.e. for all $e \in E$ with $t(e) = \{v, v'\}$, we have $f_V(v) \neq f_V(v')$, and
- *edge preserving*, i.e. for all $e \in E$ with $t(e) = \{v, v'\}$, we have $t' f_E(e) = \{f_V(v), f_V(v')\}$.

Let **uGraph** the the category of undirected multigraphs and their morphisms. It is easy to see that the empty multigraph ($V = E = \varnothing$) is a strict initial object. Moreover, it is not difficult to show that pullbacks and pushouts exist and are calculated point-wise for vertices and edges in the category of sets. It follows that **uGraph** is adhesive for similar reasons to why the usual category of directed multigraphs – which is a presheaf category – is adhesive.

For convenience, we adopt a notation in which we consider a rule algebra basis element $(O \overset{f}{\leftharpoonup} I) \in \mathcal{R}_{\mathbf{uGraph}}$ as the graph of its induced injective partial morphism $(I \overset{f}{\rightharpoonup} O) \in Inj(I, O)$ of graphs I and O, with the input graph I drawn at the bottom, O at the top, where the structure of the morphism f is indicated with dotted lines. See the example below:

▶ **Definition 6.1.** We define the algebra $\mathcal{A}$ as the one generated[2] by the rule algebra elements

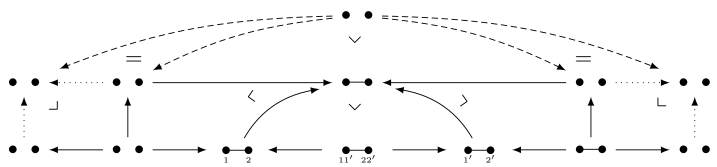
$e_+ := \frac{1}{2} \cdot \Big($  $\Big)$, $e_- := \frac{1}{2} \cdot \Big($  $\Big)$, $d := \frac{1}{2} \cdot \Big($  $\Big)$. (20)

The algebra thus defined may be characterized via its *commutation relations*, which read (with $[x, y] := x *_{\mathcal{R}} y - y *_{\mathcal{R}} x$ for $\mathcal{R} \equiv \mathcal{R}_{\mathbf{uGraph}}$)

$$[e_-, e_+] = d\,, \quad [e_+, d] = [e_-, d] = 0\,. \tag{21}$$

[2] As in the case of the Heisenberg-Weyl algebra, by "generated" we understand that a generic element of $\mathcal{A}$ is a finite linear combination of (finite) words in the generators and of the identity element $R_\emptyset$, with concatenation given by the rule algebra composition.

Here, the only nontrivial contribution (i.e. the one that renders the first commutator non-zero) may be computed from the DPO-type composition diagram[3] below (compare (5) and (6)) and its variant for the admissible match $\underset{1\ \ 2}{\bullet\!\!-\!\!\bullet} \leftarrow \underset{12'\ 21'}{\bullet\!\!-\!\!\bullet} \rightarrow \underset{1'\ 2'}{\bullet\!\!-\!\!\bullet}$:



(22)

We find an interesting structure for the representation of $\mathcal{A}$:

▶ **Lemma 6.2.** *Let $E_\pm := \rho(e_\pm)$ and $D := \rho(d)$, and for an arbitrary basis vector $|G\rangle \in \hat{\mathbb{G}}$ (with $\mathbb{G}$ denoting the set of isomorphism classes of finite undirected multigraphs), we find that the linear endomorphisms $\rho(X)$ for $X \in \{E_+, E_-, D\}$ admit a decomposition into invariant subspaces $\hat{\mathbb{G}}_n$, with $n \in \mathbb{Z}_{\geq 0}$ denoting the number of vertices of the graphs in a given subspace:*

$$\rho(X) = \bigoplus_{n \geq 0} (\rho(X))|_{\hat{\mathbb{G}}_n} \,. \tag{23}$$

Proof. The three rules that define the algebra $\mathcal{A}$ do not modify the number of vertices when applied to a given graph (via the canonical representation). ◀

One may easily verify that the operator $D = \rho(d)$ may be equivalently expressed as

$$D = \frac{1}{2} \cdot \rho\left(\begin{matrix}\bullet & & \bullet\\ \vdots & & \vdots \\ \bullet & & \bullet\end{matrix}\right) = \frac{1}{2}\left(O_\bullet O_\bullet - O_\bullet\right)\,, \quad O_\bullet := \rho\left(\begin{matrix}\bullet\\ \vdots\\ \bullet\end{matrix}\right)\,. \tag{24}$$

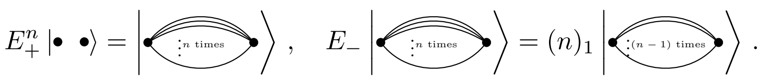
Since the diagonal operator $O_\bullet$ when applied to an arbitrary graph state $|G\rangle$ for $G \in \mathbb{G}$ effectively counts the number $n_V(G)$ of vertices of G,

$$O_\bullet\,|G\rangle = n_V(G)\,|G\rangle\,, \tag{25}$$

one finds that

$$D\,|G\rangle = \tfrac{1}{2} O_\bullet (O_\bullet - 1)\,|G\rangle = \tfrac{1}{2} n_V(G)(n_V(G) - 1)\,|G\rangle\,. \tag{26}$$

One may thus alternatively analyze the canonical representation of $\mathcal{A}$ split into invariant subspaces of D. The lowest non-trivial such subspace is the space $\hat{G}_2$ of undirected multigraphs on two vertices. It in fact furnishes a representation of the Heisenberg-Weyl algebra, with E_+ and E_- taking the roles of the creation and of the annihilation operator, respectively, and with the number vectors $|n\rangle \equiv |\bullet^{\uplus\, n}\rangle$ implemented as follows (with $(m)_n := \Theta(m-n)m!/(m-n)!$):



(27)

[3] Note that the number indices are used solely to specify the precise structure of the match, and are not to be understood as actual vertex labels or types.

But already the invariant subspace based on the initial vector $|\bullet\ \bullet\ \bullet\rangle \in \hat{\mathbb{G}}_3$ has a very interesting combinatorial structure:

$$
\begin{aligned}
E_+ |\bullet\ \bullet\ \bullet\rangle &= 3\,|\bullet\!\!-\!\!\bullet\ \ \bullet\rangle \equiv 3\,|\{1,0,0\}\rangle \\
E_+^2 |\bullet\ \bullet\ \bullet\rangle &= 3\,(|\bullet\!\!=\!\!\bullet\ \ \bullet\rangle + 2\,|\bullet\!\!-\!\!\bullet\!\!-\!\!\bullet\rangle) \equiv 3\,(|\{2,0,0\}\rangle + 2\,|\{1,1,0\}\rangle) \\
E_+^3 |\bullet\ \bullet\ \bullet\rangle &= 3\,(|\bullet\!\!\equiv\!\!\bullet\ \ \bullet\rangle + 6\,|\bullet\!\!=\!\!\bullet\!\!-\!\!\bullet\rangle + 2\,|\triangle\rangle) \\
&\equiv 3\,(|\{3,0,0\}\rangle + 6\,|\{2,1,0\}\rangle + 2\,|\{1,1,1\}\rangle) \\
&\ \vdots \\
E_+^n |\bullet\ \bullet\ \bullet\rangle &\equiv E_+^n\,|\{0,0,0\}\rangle = 3\sum_{k=0}^{n} T(n,k)\,|S(n,k)\rangle
\end{aligned}
\tag{28}
$$

Here, the state $|\{f,g,h\}\rangle$ with $f \geq g \geq h \geq 0$ and $f+g+h=n$ is the graph state on three vertices with (in one of the possible presentations of the isomorphism class) f edges between the first two, g edges between the second two and h edges between the third and the first vertex. Furthermore, $T(n,k)$ and $S(n,k)$ are given by the entry *A286030* of the OEIS database [1]. The interpretation of $S(n,k)$ and $T(n,k)$ is that each triple $S(n,k)$ encodes the outcome of a game of three players, counting (without regarding the order of players) the number of wins per player for a total of n games. Then $T(n,k)/3^{(n-1)}$ gives the probability that a particular pattern $S(n,k)$ occurs in a random sample.

It thus appears to be an interesting avenue of future research to investigate the apparently quite intricate interrelations between representation theory and combinatorics.

7 Applications of rule algebras to stochastic mechanics

One of the main motivations that underpinned the development of the rule algebra framework prior to this paper [2, 4] has been the link between associative unital algebras of transitions and continuous-time Markov chains (CTMCs). Famous examples of such particular types of CTMCs include chemical reaction systems (see e.g. [5] for a recent review) and stochastic graph rewriting systems (see [2] for a rule-algebraic implementation). With our novel formulation of unital associative rule algebras and their canonical representation for generic strict initial adhesive categories, it is possible to specify a *general stochastic mechanics framework*. While we postpone a detailed presentation of this result to future work, suffice it here to define the basic framework and to indicate the potential of the idea with a short worked example. We begin by specializing the general definition of continuous-time Markov chains (see e.g. [13]) to the setting of rewriting systems (compare [2, 5]):

▶ **Definition 7.1.** Consider an adhesive category $\mathbf{C}$ with strict initial object $o_\emptyset \in ob(\mathbf{C})$, and let $\hat{\mathbf{C}}$ denote the free $\mathbb{R}$-vector space of objects of $\mathbf{C}$ according to Definition 4.4. Then we define the space $Prob(\mathbf{C})$ as the *space of sub-probability distributions* in the following sense:

$$
Prob(\mathbf{C}) := \left\{ |\Psi\rangle = \sum_{o\in ob(\mathbf{C})} \psi_o\,|o\rangle \,\middle|\, \forall o \in ob(\mathbf{C}) : \psi_o \in \mathbb{R}_{\geq 0} \wedge \sum_{o \in ob(\mathbf{C})} \psi_o \leq 1 \right\}. \tag{29}
$$

In particular, this identifies the sequences $\{\psi_o\}_{o\in ob(\mathbf{C})} \in \ell^1_{\mathbb{R}}(ob(\mathbf{C}))$ as special types of $\ell^1_{\mathbb{R}}$-summable sequences indexed by objects of $\mathbf{C}$. Let $Stoch(\mathbf{C}) := End(Prob(\mathbf{C}))$ be the space of *sub-stochastic operators*. Then a **continuous-time Markov chain (CTMC)** is specified in terms of a tuple of data $(|\Psi(0)\rangle, H)$, where $|\Psi(0)\rangle \in Prob(\mathbf{C})$ is the *initial state*, and where $H \in End_{\mathbb{R}}(\mathcal{S}_{\mathbf{C}})$ is the *infinitesimal generator* or *Hamiltonian* of the CTMC (with $\mathcal{S}_{\mathbf{C}}$ the Fréchet space of real-valued sequences $f \equiv (f_o)_{o\in ob(\mathbf{C})}$ with semi-norms $\|f\|_o := |f_o|$). H is required to be an infinitesimal (sub-)stochastic operator, whence to fulfill the constraints

$$\begin{aligned} &H \equiv (h_{o,o'})_{o,o' \in ob(\mathbf{C})} \quad \forall o, o' \in ob(\mathbf{C}) : \\ &\quad (i)\ h_{o,o} \leq 0\,,\ (ii) \forall o \neq o' :\ h_{o,o'} \geq 0\,,\ (iii) \sum_{o'} h_{o,o'} = 0\,. \end{aligned} \tag{30}$$

Then this data encodes the *evolution semi-group* $\mathcal{E} : \mathbb{R}_{\geq 0} \to Stoch(\mathbf{C})$ as the (point-wise minimal non-negative) solution of the *Kolmogorov backwards* or *master equation*:

$$\tfrac{d}{dt}\mathcal{E}(t) = H\mathcal{E}(t)\,, \quad \mathcal{E}(0) = \mathbb{1}_{End_{\mathbb{R}}(\mathcal{S}_{\mathbf{C}})} \Rightarrow \qquad \forall t, t' \in \mathbb{R}_{\geq 0} : \mathcal{E}(t)\mathcal{E}(t') = \mathcal{E}(t + t')\,. \tag{31}$$

Consequently, the *time-dependent state* $|\Psi(t)\rangle$ of the system is given by

$$\forall t \in \mathbb{R}_{\geq 0} : \quad |\Psi(t)\rangle = \mathcal{E}(t)\,|\Psi(0)\rangle\ . \tag{32}$$

Typically, our interest in analyzing a given CTMC will consist in studying the dynamical statistical behavior of so-called observables:

▶ **Definition 7.2.** Let $\mathcal{O}_{\mathbf{C}} \subset End_{\mathbb{R}}(S_{\mathbf{C}})$ denote the space of *observables*, defined as the space of *diagonal operators*,

$$\mathcal{O}_{\mathbf{C}} := \{O \in End_{\mathbb{R}}(S_{\mathbf{C}}) \mid \forall o \in ob(\mathbf{C}) :\ O\,|o\rangle = \omega_O(o)\,|o\rangle\ ,\ \omega_O(o) \in \mathbb{R}\}\,. \tag{33}$$

We furthermore define the so-called *projection operation* $\langle| : S_{\mathbf{C}} \to \mathbb{R}$ via extending by linearity the definition of $\langle|$ acting on basis vectors of $\hat{\mathbf{C}}$,

$$\forall o \in ob(\mathbf{C}) : \quad \langle|\,o\rangle := 1_{\mathbb{R}}\,. \tag{34}$$

These definitions induce a notion of *correlators* of observables, defined for $O_1, \ldots, O_n \in \mathcal{O}_{\mathbf{C}}$ and $|\Psi\rangle \in Prob(\mathbf{C})$ as

$$\langle O_1, \ldots, O_n\rangle_{|\Psi\rangle} := \langle|\,O_1, \ldots, O_n\,|\Psi\rangle = \sum_{o \in ob(\mathbf{C})} \psi_o \cdot \omega_{O_1}(o) \cdots \omega_{O_n}(o)\,. \tag{35}$$

The precise relationship between the notions of CTMCs and DPO rewriting rules as encoded in the rule algebra formalism is established in the form of the following theorem (compare [2]):

▶ **Theorem 7.3** (Stochastic mechanics framework)**.** *Let* $\mathbf{C}$ *be an adhesive category with strict initial object, let* $\{(O_j \stackrel{r_j}{\Leftarrow} I_j) \in \mathcal{R}_{\mathbf{C}}\}_{j\in\mathcal{J}}$ *be a (finite) set of rule algebra elements and* $\{\kappa_j \in \mathbb{R}_{\geq 0}\}_{j\in\mathcal{J}}$ *a collection of non-zero parameters (called* base rates*). Then one may construct a Hamiltonian* H *from this data according to*

$$H := \hat{H} + \bar{H}\,, \quad \hat{H} := \sum_{j\in\mathcal{J}} \kappa_j \cdot \rho\left(O_j \stackrel{r_j}{\Leftarrow} I_j\right)\,, \quad \bar{H} := -\sum_{j\in\mathcal{J}} \kappa_j \cdot \rho\left(I_j \stackrel{id_{dom(r_j)}}{\Leftarrow} I_j\right)\,. \tag{36}$$

Here, for arbitrary $(I \stackrel{r}{\rightharpoonup} O) \equiv (I \stackrel{i}{\leftarrow} K \stackrel{o}{\rightarrow} O) \in Lin(\mathbf{C})$*, we define*

$$(I \xrightarrow{id_{dom(r)}} I) := (I \stackrel{i}{\leftarrow} K \stackrel{i}{\rightarrow} I)\,. \tag{37}$$

The observables *for the resulting CTMC are operators of the form*

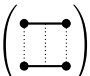
$$O_M^t = \rho\left(M \stackrel{t}{\Leftarrow} M\right)\ . \tag{38}$$

We furthermore have the jump-closure property*, whereby for all* $(O \stackrel{r}{\Leftarrow} I) \in \mathcal{R}_{\mathbf{C}}$

$$\langle|\,\rho(O \stackrel{r}{\Leftarrow} I) = \langle|\,O_I^{id_{dom(r)}}\,. \tag{39}$$

Proof. See Appendix A.4. ◀

We illustrate the framework with an example for $\mathbf{C} = \mathbf{uGraph}$ (the category of (isomorphism classes of) undirected multigraphs and morphisms thereof), where we pick the two rule algebra elements e_+ and e_- specified in (20) to define the transitions of the system. Together with two non-negative real parameters $\kappa_+, \kappa_- \in \mathbb{R}_{\geq 0}$, the resulting Hamiltonian $H = \hat{H} + \bar{H}$ reads (with $E_\pm := \rho(e_\pm)$ and $O_\bullet$ as in (24))

$\hat{H} = \kappa_+ E_+ + \kappa_- E_- \,, \quad \bar{H} = -\tfrac{1}{2}\kappa_+ O_\bullet (O_\bullet - 1) - \kappa_- O_E \,, \quad O_E := \tfrac{1}{2}\rho\Big($  $\Big) \,.$ (40)

Using the general fact that a Hamiltonian as constructed according to Theorem 7.3 verifies

$$\langle| \, H = 0 \,, \tag{41}$$

we may for example compute the time evolution of the expectation values of observables for this CTMC. Intuitively, the CTMC describes a stochastic system where edges are added and removed at random. Since these transitions do not modify the number of vertices, we immediately conclude that if the initial state $|\Psi(0)\rangle \in \mathit{Prob}(\mathbf{uGraph})$ is a *pure state*, i.e. if $|\Psi(0)\rangle = |G_0\rangle$ for some $G_0 \in \mathit{ob}(\mathbf{uGraph})$, one finds[4]

$$\forall t \geq 0 : \quad \langle| \, O_\bullet \, |\Psi(t)\rangle = \langle| \, O_\bullet \, |G_0\rangle = N_V \,, \tag{42}$$

with N_V the number of vertices of G_0. Let us analogously denote by N_E the number of edges of G_0, determined according to

$$N_E = \langle| \, O_E \, |G_0\rangle \,. \tag{43}$$

The time evolution of the moments of the edge-counting observable O_E may be computed by means of algebraic methods. Referring to [2, 5] for more extensive computations, suffice it here to demonstrate the derivation of the evolution of the average edge-count for $|\Psi(0)\rangle = |G_0\rangle$:

$$\begin{aligned}
\tfrac{d}{dt} \langle| \, O_E \, |\Psi(t)\rangle &= \langle| \, O_E H \, |\Psi(t)\rangle = \langle| \, (H O_E + [O_E, H]) \, |\Psi(t)\rangle \\
&\overset{(41)}{=} \kappa_+ \langle| \, E_+ \, |\Psi(t)\rangle - \kappa_- \langle| \, E_- \, |\Psi(t)\rangle \\
&\overset{(39)}{=} \tfrac{1}{2}\kappa_+ \langle| \, O_\bullet (O_\bullet - 1) \, |\Psi(t)\rangle - \kappa_- \langle| \, O_E \, |\Psi(t)\rangle \\
&\overset{(42)}{=} \tfrac{1}{2}\kappa_+ N_V (N_V - 1) - \kappa_- \langle| \, O_E \, |\Psi(t)\rangle \,.
\end{aligned} \tag{44}$$

Together with the initial value $\langle| \, O_E \, |\Psi(0)\rangle = N_E$, this ODE is solved (for $\kappa_M \neq 0$ and with the convention $\binom{x}{y} := 0$ for $x < y$) by

$$\langle O_E \rangle(t) \equiv \langle| \, O_E \, |\Psi(t)\rangle = e^{-t\kappa_M} \left(N_E - \tfrac{\kappa_P}{\kappa_M} \binom{N_V}{2} \right) + \tfrac{\kappa_P}{\kappa_M} \binom{N_V}{2} \xrightarrow[t \to \infty]{} \tfrac{\kappa_P}{\kappa_M} \binom{N_V}{2} \,. \tag{45}$$

Interestingly, the coefficient $\binom{N_V}{2}$ is precisely the number of edges of a complete graph on N_V vertices, Moreover, if $\kappa_P = \kappa_M$ and $N_{E*} = \binom{N_V}{2}$, $\langle O_E \rangle(t) = N_{E*} = \mathit{const}$ for all $t \geq 0$.

[4] More precisely, one may verify that $[O_\bullet, H] = 0$, whence the claim follows from $\langle| \, O_\bullet \, |\Psi(0)\rangle = N_V$ and $\tfrac{d}{dt} \langle| \, O_\bullet \, |\Psi(t)\rangle = \langle| \, O_\bullet H \, |\Psi(t)\rangle = \langle| \, (H O_\bullet + [O_\bullet, H]) \, |\Psi(t)\rangle = 0$.

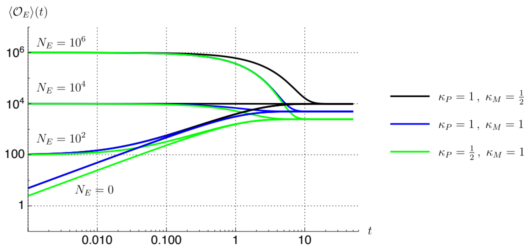


Figure 1 Time-evolution of $\langle O_E \rangle(t)$ for $|\Psi(0)\rangle = |G_0\rangle$ with $N_V = 100$.

We present in Figure 1 the time-evolution of $\langle O_E \rangle(t)$ for three different choices of parameters κ_+ and κ_-, and for four different choices each of initial number of edges N_E.

As an outlook and reference to ongoing and future work, techniques such as the ones developed in [2] and [3] in favorable cases even permit to derive the full time-dependent probability distribution of observables – in fact, in the present example, one may demonstrate that the distribution of the edge-counting observable O_E stabilizes for $t \to \infty$ onto a Poisson distribution of parameter $\frac{\kappa_P}{\kappa_M}\binom{N_V}{2}$. This result might be somewhat anticipated, in that for the special case $N_V = 2$ we found in the previous section that E_+ and E_- acting on the states with two vertices effectively yield a representation of the Heisenberg-Weyl algebra, whence in this case the process reduces to a birth-death process on edges with rates κ_+ and κ_- (see [5] for further details on chemical reaction systems).

8 Conclusion and Outlook

Based on our novel theorem on the associativity of the operation of forming DPO-type concurrent compositions of linear rewriting rules, we introduced the concept of *rule algebras*: each linear rule is mapped to an element of an abstract vector space of linear rules, on which the concurrent composition operation is implemented as a binary, bilinear multiplication operation. For every adhesive category $\mathbf{C}$, the associated rule algebra is associative, and if the category possesses a strict initial object (i.e. if $\mathbf{C}$ is an extensive category), this algebra is in addition unital. We hinted at the potential of our approach in the realm of combinatorics, and, as a first major application of our framework, we presented a *universal construction of continuous-time Markov chains* based on linear rules of extensive categories $\mathbf{C}$. It appears reasonable in light of the deep insights gained into such CTMC theories for the special cases of discrete rewriting rules [5] and multigraph rewriting rules [3, 2] to expect that our approach will lead to progress in the understanding and analysis of stochastic rewriting systems in both theory and practice.

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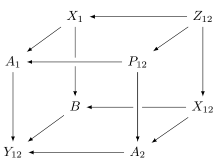
A Proofs

A.1 Proof of associativity of rule compositions

▶ **Lemma A.1.** *Let* $\mathbf{C}$ *be an adhesive category, and consider the following commutative diagram, in which all arrows are monomorphisms, and where*



- *the bottom and left faces are pushout squares, and*
- *the front and back faces are pullback squares.*

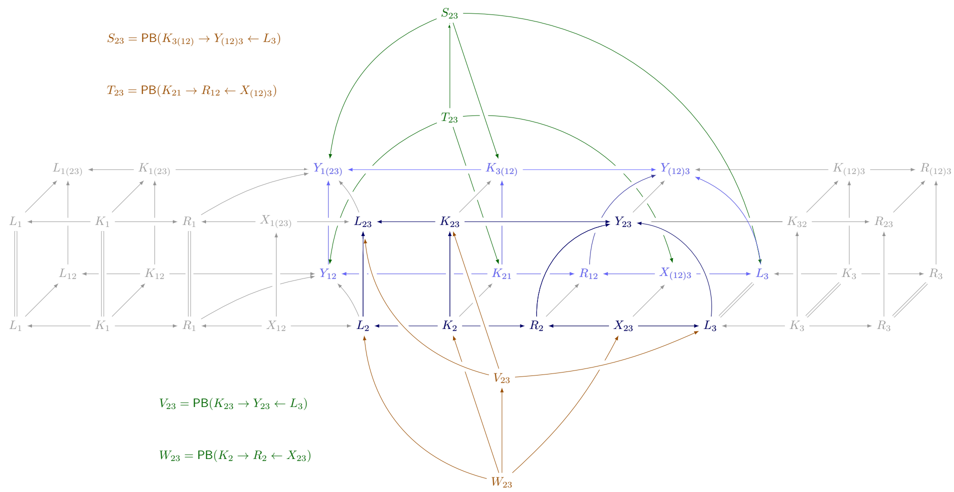
Then the right and top faces are pushout squares.

Proof. Composition of the back square and the bottom square yields a pullback square, whence according to Lemma 2.4 the top face is also a pullback square. Since thus all faces but the right one are pullbacks and the left face is a pushout square due to the VK property of $\mathbf{C}$. Analogously, since the bottom square is a pushout square and all vertical faces are pullback squares, the top face is a pushout square. ◀

▶ **Theorem 3.3** (Associativity Theorem)**.** *The composition operation* $.\overset{\cdot}{\blacktriangleleft}.$ *is* associative *in the following sense: given linear rules* $p_1, p_2, p_3 \in Lin(\mathbf{C})$*, there exists a bijective correspondence* *between pairs of admissible matches* $m_{21} \in p_2 \Vdash p_1$ *and* $m_{3(21)} \in p_3 \Vdash \left(p_2 \overset{m_{12}}{\blacktriangleleft} p_1\right)$, *and pairs of admissible matches* $m_{32} \in p_3 \Vdash p_2$ *and* $m_{(32)1} \in \left(p_3 \overset{m_{23}}{\blacktriangleleft} p_2\right) \Vdash p_1$ *such that*

$$p_3 \overset{m_{3(21)}}{\blacktriangleleft} \left(p_2 \overset{m_{21}}{\blacktriangleleft} p_1\right) = \left(p_3 \overset{m_{32}}{\blacktriangleleft} p_2\right) \overset{m_{(32)1}}{\blacktriangleleft} p_1 \,. \tag{7}$$

Proof. We refer the readers to the main text for the first part of the proof. To prove the final part, whence that the $Y_{1(23)}$ is the pushout of $R_1 \leftarrow X_{1(23)} \rightarrow L_{23}$, we construct the following extended diagram (with S_{23}, T_{23}, V_{23} and W_{23} obtained by taking the indicated pullbacks $\mathsf{PB}(\dots)$, and where the remaining new morphisms are formed as those that make the respective triangles involving the aforementioned objects commute):



Invoking Lemma A.1 twice, we may conclude that the squares $\square_{W_{23},V_{23},K_{23},K_2}$, $\square_{W_{23},V_{23},L_3,X_{23}}$, $\square_{T_{23},S_{23},K_{3(12)},K_{21}}$ and $\square_{T_{23},S_{23},L_3,X_{(12)3}}$ are pushout squares. In addition, since the squares $\square_{W_{23},V_{23},L_{23},L_2}$ and $\square_{T_{23},S_{23},Y_{1(23)},Y_{12}}$ are compositions of pushout squares, according to Lemma 2.4 they are pushout squares themselves. In order to prove the claim, we have to demonstrate that the monomorphisms of the cospan $R_1 \rightarrow Y_{1(23)} \leftarrow L_{23}$ are *jointly epimorphic*. Since Y_{12} is the pushout of $R_1 \leftarrow X_{12} \rightarrow L_2$, and since Y_{12} is included in $Y_{1(23)}$ (as encoded in the arrow $Y_{12} \rightarrow Y_{1(23)}$), the proof reduces to proving that the monomorphism $L_{23} \rightarrow Y_{1(23)}$ covers $Y_{1(23)} \setminus Y_{12}$. The proof is facilitated by taking advantage of the notion of *algebra of subobjects* available in every adhesive category (see [11] for the details). Note first that according to the structure of the auxiliary diagram constructed above, $Y_{1(23)} = Y_{12} \cup_{T_{23}} S_{23}$, while S_{23} in turn is the pushout complement of $T_{23} \rightarrow X_{(12)3} \rightarrow L_3$, whence $S_{23} = L_3 \setminus (X_{(12)3} \setminus T_{23})$. Analogously, $L_{23} = L_2 \cup_{W_{23}} V_{23}$, where V_{23} is the pushout complement of $W_{23} \rightarrow X_{23} \rightarrow L_3$, whence $V_{23} = L_3 \setminus (X_{23} \setminus W_{23})$. In addition, since $L_{23} \rightarrow Y_{1(23)}$, $L_2 \rightarrow L_{23}$ and $W_{23} \rightarrow L_2$, we conclude that $W_{23} \rightarrow T_{23}$. But since the monomorphism $X_{23} \rightarrow X_{(12)3}$ encodes that X_{23} is a subobject of $X_{(12)3}$, combining all arguments reveals that the portion of L_3 in $Y_{1(23)}$ not already covered by Y_{12} is always strictly smaller than the portion of L_3 in L_{23} not already covered by L_2, whence the claim that $R_1 \rightarrow Y_{1(23)} \leftarrow L_{23}$ is jointly epimorphic follows. In summary, we have proved that each triple of linear rules and choice of admissible overlaps $(X_{12}, X_{(12)3})$ induces an overlap pair $(X_{23}, X_{1(23)})$ as given in the construction, which concludes the proof of associativity. ◀

A.2 Proof of the homomorphism property of the canonical representations

▶ **Theorem 4.5** (Canonical Representation). *For* $\mathbf{C}$ *adhesive with strict initial object,* $\rho_{\mathbf{C}} : \mathcal{R}_{\mathbf{C}} \to End(\hat{\mathbf{C}})$ *of Definition 4.4 is a homomorphism of unital associative algebras.*

Proof. In order for $\rho_{\mathbf{C}}$ to qualify as an algebra homomorphism (of unital associative algebras $\mathcal{R}_{\mathbf{C}}$ and $End(\hat{\mathbf{C}})$), we must have (with $R_\emptyset = \delta(r_\emptyset)$, $r_\emptyset = c_\emptyset \overset{\emptyset}{\leftharpoonup} c_\emptyset$)

$$(i)\ \rho_{\mathbf{C}}(R_\emptyset) = \mathbb{1}_{End(\hat{\mathbf{C}})} \quad \text{and} \quad (ii)\ \forall R_1, R_2 \in \mathcal{R}_{\mathbf{C}} :\ \rho_{\mathbf{C}}(R_1 *_{\mathcal{R}_{\mathbf{C}}} R_2) = \rho_{\mathbf{C}}(R_1)\rho_{\mathbf{C}}(R_1)\,.$$

Due to linearity, it suffices to prove the two properties on basis elements $\delta(p), \delta(q)$ of $\mathcal{R}_{\mathbf{C}}$ and on basis elements $|C\rangle$ of $\hat{\mathbf{C}}$. Property (i) follows directly from the definition,

$$\forall C \in ob(\mathbf{C}) : \quad \rho_{\mathbf{C}}(R_\emptyset)\,|C\rangle \overset{(14)}{=} \sum_{m \in \mathcal{M}_{r_\emptyset}(C)} |(r_\emptyset)_m(C)\rangle = |C\rangle\ .$$

Property (ii) follows from Theorem 3.1 (the concurrency theorem): for all basis elements $\delta(p), \delta(q) \in \mathcal{R}_{\mathbf{C}}$ (with $p, q \in Lin(\mathbf{C})$) and for all $C \in ob(\mathbf{C})$,

$$\begin{aligned}
\rho_{\mathbf{C}}\left(\delta(q) *_{\mathbf{C}} \delta(p)\right)|C\rangle &\overset{(10)}{=} \sum_{\mathbf{d} \in q \Vdash p} \rho_{\mathbf{C}}\left(\delta\left(q \overset{\mathbf{d}}{\blacktriangleleft} p\right)\right)|C\rangle \\
&\overset{(14)}{=} \sum_{\mathbf{d} \in q \Vdash p} \sum_{e \in \mathcal{M}_{r_{\mathbf{d}}}(C)} |(r_{\mathbf{d}})_e(C)\rangle && (r_{\mathbf{d}} = q \overset{\mathbf{d}}{\blacktriangleleft} p) \\
&= \sum_{m \in \mathcal{M}_p(C)} \sum_{n \in \mathcal{M}_q(p_m(C))} |q_n(p_m(C)\rangle && (\text{via Thm. 3.1}) \\
&\overset{(14)}{=} \sum_{m \in \mathcal{M}_p(C)} \rho_{\mathbf{C}}\left(\delta(q)\right)|p_m(C)\rangle \\
&\overset{(14)}{=} \rho_{\mathbf{C}}\left(\delta(q)\right)\rho_{\mathbf{C}}\left(\delta(p)\right)|C\rangle\ .
\end{aligned}$$

◀

A.3 Proof of the relationship between discrete graph rewriting and the Heisenberg-Weyl algebra

Proof.

(i) Since there is no partial injection possible between the input of one copy and the output of another copy of $x^\dagger$ other than the trivial match, and similarly for two copies of x, the claim follows.

(ii) Computing the commutator $[x, x^\dagger] = x * x^\dagger - x^\dagger * x$ (with $* \equiv *_{\mathcal{R}_0}$) explicitly, we find that

$$x * x^\dagger = x \uplus x^\dagger + id_{\mathcal{R}_0}\,, \quad x^\dagger * x = x^\dagger \uplus x\,, \tag{46}$$

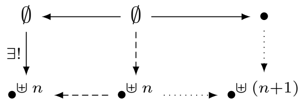
from which the claim follows due to commutativity of the operation $\uplus$ on $\mathcal{R}_0$, $x \uplus x^\dagger = x^\dagger \uplus x$.

(iii) It suffices to prove the statement for basis elements of $\mathcal{H}$. Consider thus an arbitrary composition of a finite number of copies of the generators x and $x^\dagger$. Then by repeated application of the commutation relation $[x, x^\dagger] = id_{\mathcal{R}_0}$, and since $id_{\mathcal{R}_0}$ is the unit element for $*$ on $\mathcal{R}_0$, we can convert the arbitrary basis element of $\mathcal{H}$ into a linear combination of normal-ordered elements.

(iv) Note first that by definition $|0\rangle = |\emptyset\rangle$. To prove the claim that for all $n \geq 0$

$$a^\dagger \, |n\rangle = |n+1\rangle \ ,$$

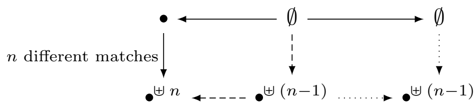
we apply Definitions 2.6 and 4.4 by computing the following diagram (compare (3)): there exists precisely one admissible match of the empty graph $\emptyset \in G_0$ into the n-vertex discrete graph $\bullet^{\uplus\, n}$, whence constructing the pushout complement marked with dashed arrows and the pushout marked with dotted arrows we verify the claim:



Proceeding analogously in order to prove the formula for the representation $a = \rho_{\mathcal{R}_0}(x)$,

$$a\,|n\rangle := \begin{cases} n \cdot |n-1\rangle & \text{if } n > 0 \\ 0_{\hat{G}_0} & \text{else,} \end{cases}$$

we find that for $n > 0$ there exist n admissible matches of the 1-vertex graph $\bullet$ into the n-vertex graph $\bullet^{\uplus\, n}$, for each of which the application of the rule $\bullet \rightharpoonup \emptyset$ along the match results in the graph $\bullet^{\uplus\,(n-1)}$:



$$\Rightarrow \ \forall n > 0 : a\,|\bullet^{\uplus\, n}\rangle = n \cdot \left|\bullet^{\uplus\,(n-1)}\right\rangle$$

Finally, for $n = 0$, since by definition there exists no admissible match from the 1-vertex graph $\bullet$ into the empty graph $\emptyset$, whence indeed

$$a\,|\emptyset\rangle = \rho_{\mathcal{R}_0}\left(\emptyset \stackrel{\emptyset}{\Leftarrow} \bullet\right) |\emptyset\rangle = 0_{\hat{G}_0} \,. \qquad ◀$$

A.4 Proof of the stochastic mechanics framework theorem

▶ **Theorem 7.3** (Stochastic mechanics framework)**.** *Let* $\mathbf{C}$ *be an adhesive category with strict initial object, let* $\{(O_j \stackrel{r_j}{\Leftarrow} I_j) \in \mathcal{R}_{\mathbf{C}}\}_{j\in\mathcal{J}}$ *be a (finite) set of rule algebra elements and* $\{\kappa_j \in \mathbb{R}_{\geq 0}\}_{j\in\mathcal{J}}$ *a collection of non-zero parameters (called* base rates*). Then one may construct a Hamiltonian* H *from this data according to*

$$H := \hat{H} + \bar{H} \,, \quad \hat{H} := \sum_{j\in\mathcal{J}} \kappa_j \cdot \rho\left(O_j \stackrel{r_j}{\Leftarrow} I_j\right) \,, \quad \bar{H} := -\sum_{j\in\mathcal{J}} \kappa_j \cdot \rho\left(I_j \stackrel{id_{dom(r_j)}}{\Leftarrow} I_j\right) \,. \tag{36}$$

Here, for arbitrary $(I \stackrel{r}{\rightharpoonup} O) \equiv (I \stackrel{i}{\leftarrow} K \stackrel{o}{\rightarrow} O) \in Lin(\mathbf{C})$*, we define*

$$(I \xrightarrow{id_{dom(r)}} I) := (I \stackrel{i}{\leftarrow} K \stackrel{i}{\rightarrow} I) \,. \tag{37}$$

The observables *for the resulting CTMC are operators of the form*

$$O_M^t = \rho\left(M \stackrel{t}{\Leftarrow} M\right) \,. \tag{38}$$

We furthermore have the jump-closure property*, whereby for all* $(O \stackrel{r}{\Leftarrow} I) \in \mathcal{R}_{\mathbf{C}}$

$$\langle | \, \rho(O \stackrel{r}{\Leftarrow} I) = \langle | \, O_I^{id_{dom(r)}} \,. \tag{39}$$

Proof. By definition, the canonical representation of a generic rule algebra element $(O \overset{r}{\leftharpoonup} I) \in \mathcal{R}_{\mathbf{C}}$ is both a row- and a column-finite object, since for every object $C \in ob(\mathbf{C})$ the set of admissible matches $\mathcal{M}_p(C)$ of the associated linear rule $p \equiv (I \overset{r}{\rightharpoonup} O)$ is finite, and since for every object $C \in ob(\mathbf{C})$ there exists only finitely many objects $C' \in ob(\mathbf{C})$ such that $C = p_m(C')$ for some match $m \in \mathcal{M}_p(C')$. Consequently, $\rho_{\mathbf{C}}(O \overset{r}{\leftharpoonup} I)$ lifts consistently from a linear operator in $End(\hat{\mathbf{C}})$ to a linear operator in $End(\mathcal{S}_{\mathbf{C}})$. Let us prove next the claim on the precise structure of observables. Recall that according to Definition 7.2, an observable $O \in \mathcal{O}_{\mathbf{C}}$ must be a linear operator in $End(\mathcal{S}_{\mathbf{C}})$ that acts diagonally on basis states $|C\rangle$ (for $C \in ob(\mathbf{C})$), whence that satisfies for all $C \in ob(\mathbf{C})$

$$O\,|C\rangle = \omega_O(C)\,|C\rangle \quad (\omega_O(C) \in \mathbb{R})\,.$$

Comparing this equation to the definition of the canonical representation (Definition 4.4) of a generic rule algebra basis element $\delta(p) \in \mathcal{R}_{\mathbf{C}}$ (for $p \equiv (I \overset{i}{\leftarrow} K \overset{o}{\rightarrow} O) \in Lin(\mathbf{C})$),

$$\rho_{\mathbf{C}}(\delta(p))\,|C\rangle := \begin{cases} \sum_{m \in \mathcal{M}_p(C)} |p_m(C)\rangle & \text{if } \mathcal{M}_p(C) \neq \emptyset \\ 0_{\hat{\mathbf{C}}} & \text{else,} \end{cases}$$

we find that in order for $\rho_{\mathbf{C}}(\delta(p))$ to be diagonal we must have

$$\forall C \in ob(\mathbf{C}) : \forall m \in \mathcal{M}_p(C) : \quad p_m(C) = C\,.$$

But by definition of derivations of objects along admissible matches (Definition 2.6), the only linear rules $p \in Lin(\mathbf{C})$ that have this special property are precisely the rules of the form

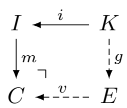
$$p^r_M = (M \overset{r}{\leftarrow} K \overset{r}{\rightarrow} M)\,.$$

In particular, defining $O^r_M := \rho_{\mathbf{C}}(\delta(p^r_M))$, we find that the eigenvalue $\omega_{O^r_M}(C)$ coincides with the cardinality of the set $\mathcal{M}_{p^r_M}(C)$ of admissible matches,

$$\forall C \in ob(\mathbf{C}) : \quad O^r_M\,|C\rangle = |\mathcal{M}_{p^r_M}(C)| \cdot |C\rangle\;.$$

This proves that the operators O^r_M form a basis of diagonal operators on $End(\mathbf{C})$ (and thus on $End(\mathcal{S}_{\mathbf{C}})$).

To prove the jump-closure property, note that it follows from Definition 2.6 that for an arbitrary *linear* rule $p \equiv (I \overset{i}{\leftarrow} K \overset{o}{\rightarrow} O) \in Lin(\mathbf{C})$, a generic object $C \in \mathbf{C}$ and a monomorphism $m : I \to C$, the admissibility of m as a match is determined by whether or not the match fulfills the gluing condition (Definition 2.3), i.e. whether or not the following pushout complement exists,



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Thus we find that with $p' = (I \overset{i}{\leftarrow} K \overset{i}{\rightarrow} I) \in Lin(\mathbf{C})$, the set $\mathcal{M}_p(C)$ of admissible matches of p in C and $\mathcal{M}_{p'}(C)$ of p' in C have the same cardinality. Combining this with the definition of the projection operator $\langle|$ (Definition 7.2),

$$\forall C \in ob(\mathbf{C}) : \quad \langle|\,C\rangle := 1_{\mathbb{R}}\,,$$

we may prove the claim of the jump-closure property via verifying it on arbitrary basis elements (with notations as above):

$$\langle|\,\rho_{\mathbf{C}}(\delta(p))\,|C\rangle = |\mathcal{M}_p(C)| = |\mathcal{M}_{p'}(C)| = \langle|\,\rho_{\mathbf{C}}(\delta(p'))\,|C\rangle\;.$$

Since $C \in ob(\mathbf{C})$ was chosen arbitrarily, we thus have indeed that

$$\langle| \, \rho_{\mathbf{C}}(\delta(p)) = \langle| \, \rho_{\mathbf{C}}(\delta(p'))\,.$$

Finally, combining all of these findings, one may verify that H as stated in the theorem fulfills all required properties in order to qualify as an infinitesimal generator of a continuous-time Markov chain. ◀