



GRAPH REWRITING AND COMBINATORIAL HOPF ALGEBRA Nicolas Behr

fcsLaboratory for Foundations
of Computer Science

based on

- Nicolas Behr, Vincent Danos, and Ilias Garnier: Stochastic mechanics of graph rewriting, accepted for publication in LiCS 2016
- Nicolas Behr, Vincent Danos, Ilias Garnier, and Tobias Heindel (2016): The algebras of graph rewriting, in preparation

Categories, Logic & Physics, Scotland, University of Edinburgh, April 14th 2016

MOTIVATION

- How do graph transformation systems (GTSs) compare to other types of stochastic systems?
- Why does the conventional GTS framework seem to have so many specialized conventions?
- Is it possible to re-use ideas from statistical physics and combinatorics to tackle GTS computations?

WHY GRAPH TRANSFORMATION SYSTEMS?

- allow to encode a variety of probabilistic systems (chemical reactions, **biochemical reactions**, network dynamics, lattice models,...)
- beyond "discrete" particles!
- very flexible modelling formalism

conventional graph transformation frameworks

analytical combinatorics

statistical physics

theory of CTMCs & chemcal reaction systems



SURPRISING RESULTS

- entirely new formulation of graph rewriting syntax defined in terms of rule diagrams and their compositions rather than in terms of category theoretical concepts!
- discovery of new types of graph rewriting
- in the new framework, we can study the combinatorics of rewriting systems
- the rule algebra (of type DPO) is a generalization of and subsumes the Heisenberg-Weyl algebra

SURPRISING RESULTS

- entirely new formulation of gree's rewriting syntax defined in terms of rule diagrams ar of category theoretic
- discovery of
- in the new fraction rewriting systems

Focus of today's talk: COMBINATORICS of DISCRETE GTS's...

ncs of

the rule algebra (of type D.
 the Heisenberg-Weyl algebra

reralization of and subsumes

STOCHASTIC MECHANICS OF CHEMICAL REACTION SYSTEMS

THE HEISENBERG-WEYL

- pool of n indistinguishable particles
- basic operations:
 - pick a particle at random and **remove it**
 - add a particle
- basic combinatorics:
 - *n* **possibilities** to remove a particle
 - 1 **possibility** to add a particle



THE HEISENBERG-WEYL

- from the theory of bosonic Fock space*: introduce number vectors
 - $|n\rangle \widehat{=}$ state of exactly *n* particles
- encode the basic operations in terms of the **generators** of the **Heisenberg-Weyl algebra**:

$$\begin{split} a|n\rangle &:= \begin{cases} n|n-1\rangle & \text{if } n>0\\ 0|0\rangle & \text{else.} \end{cases}\\ a^{\dagger}|n\rangle &:= |n+1\rangle & (n\geq 0) \end{split}$$

canonical commutation relation:

$$(aa^{\dagger} - a^{\dagger}a)|n\rangle = a|n+1\rangle - na^{\dagger}|n-1\rangle$$
$$= (n+1)|n\rangle - n|n\rangle = |n\rangle$$
$$\Leftrightarrow \quad [a,a^{\dagger}] \equiv aa^{\dagger} - a^{\dagger}a = 1$$



* Pawel Blasiak et al. (2007): **Combinatorics and Boson normal ordering: A gentle introduction,** American Journal of Physics 75.7, pp. 639–646

HW part MULTI-TYPE CASE

• multi-type Heisenberg-Weyl algebra:

 $[a_i, a_j^{\dagger}] = \delta_{ij}$

• multi-type bosonic Fock space:

$$|\vec{n}\rangle \equiv |n_1, n_2, \dots\rangle \qquad (\sum_i n_i < \infty, \ n_i \in \mathbb{Z}_{\geq 0})$$

- action of the annihilators a_i and the creators a_j^{\dagger} : $a_i |\vec{n}\rangle := n_i |\vec{n} - \vec{\delta}_i\rangle, \quad a_i^{\dagger} |\vec{n}\rangle := |\vec{n} + \vec{\delta}_i\rangle$
- interpretation: the individual types (visualized as colors) are acted upon independently from one another

example for a reaction:



 $A + B \rightarrow C$

CHEMICAL REACTION SYSTEMS

$$\sum_{\tau \in T} \left(\sum_{i} s_i(\tau) X_i \xrightarrow{r_{\tau}} \sum_{j} t_j(\tau) X_j \right)$$

with: T - set of reactions; $r_{\tau} \in \mathbb{R}_{>0}$ - reaction rates; $s_i, t_j \in \mathbb{Z}_{\geq 0}$

- As presented e.g. in **Baez and Bianmonte***, there exists a precise link between multitype HW algebra and chemical reaction systems:
 - state of the system:

$$|\Psi(t)\rangle = \sum_{\vec{n}} p_{\vec{n}}(t) |\vec{n}\rangle, \quad \sum_{\vec{n}} p_{\vec{n}} = 1, \quad p_{\vec{n}}(t) \in \mathbb{R}_{\geq 0}$$

- Master equation:

$$\frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle,$$

with evolution operator

$$H := \sum_{\tau \in T} r_{\tau} \left(\vec{a}^{\dagger \, \vec{t}(\tau)} - \vec{a}^{\dagger \, \vec{s}(\tau)} \right) \vec{a}^{\vec{s}(\tau)}$$

where $\vec{a}^{\dagger t(\tau)} := \left(\prod_{i} a_{i}^{\dagger t_{i}(\tau)}\right)$ etc.

* John C Baez and Jacob Biamonte (2012): A course on quantum techniques for stochastic mechanics, arXiv preprint arXiv:1209.3632

CHEMICAL REACTION SYSTEMS

Master equation:

$$\frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle$$

formal solution:

$$|\Psi(t)\rangle = e^{tH}|\Psi(0)\rangle$$

- this is not always meaningful, but analytically solvable cases are known!
- example: birth-death reaction system

$$X \xrightarrow{1} \varnothing, \quad \varnothing \xrightarrow{\lambda} X$$

• analytic solution^{*}: for $|\Psi(0)\rangle = |N_0\rangle$, and with $\nu(t) := (1 - e^{-t})$,

$$|\Psi(t)\rangle = e^{-\nu(t)\lambda} \sum_{k=0}^{\min(N_0,n)} {\binom{N_0}{k}} e^{-kt} \nu(t)^{N_0+n-2k} \frac{\lambda^{n-k}}{(n-k)!} |n\rangle$$

* Tobias Jahnke and Wilhelm Huisinga (2007): Solving the chemical master equation for monomolecular reaction systems analytically, Journal of mathematical biology 54.1, pp. 1–26

GRAPH REWRITING

GRAPHS AND REWRITING RULES

- **graphs** = very generic graphs (multi-colored, multi edged, with self loops, directed or undirected edges?)
- **injective partial graph homomorphisms** = oneto-one mappings of vertices and edges (s.th. endpoint vertices of all edges are included)
- graph rewriting rule:

$$t: L \rightharpoonup R$$

with t – an injective partial homomorphism from finite graph L to finite graph R

• **where it begins:** a tentative depiction of graph rewriting rules...



ACTION OF REWRITING RULES ON GRAPHS



Michael Löwe (1993): **Algebraic approach to singlepushout graph transformation,** Theoretical Computer Science 109.1, pp. 181–224

- **basic idea:** to apply a rule $t : L \rightarrow R$ to a graph G,
 - I. find an occurrence of L in G (aka a **match**),
 - 2. then replace the instance of L with R as described in detail by the partial injection t
- a first hint at a notion of **representation**: in general, there are more than one possibilities to act on a given graph, so which one to choose? **answer: all of them**
- hint from HW algebra: the outcome of a rewriting operation must be some sort of linear combination of "graph states"

ACTION OF REWRITING RULES ON GRAPHS



- there exist a number of different variants of graph rewriting:
 - double pushout (DPO) rewriting (deleting/creating a vertex is only possible if no edges remain after the operation)
 - single pushout (SPO) rewriting (deleting a vertex automatically deletes all incident edges)
 - our formalism: two new variants!

Hartmut Ehrig et al. (2000): **Double-pullback graph transitions: A rule-based framework with incomplete information,** Theory and Application of Graph Transformations. Springer, pp. 85–102

Michael Löwe (1993): Algebraic approach to singlepushout graph transformation, Theoretical Computer Science 109.1, pp. 181–224

Nicolas Behr, Vincent Danos, Ilias Garnier, and Tobias Heindel (2016): **Combinatorial physics of graph rewriting,** in preparation

TOWARDS A NOTION OF ALGEBRA

• basic idea:

composition of rules via compositions of diagrams

- problem: HOW?!
- **Ansatz**: study the case of the Heisenberg-Weyl algebra in the formulation of **combinatorial Hopf algebras**

RULE DIAGRAM ALGEBRA

DIAGRAMS FOR THE HW ALGEBRA

• **Ansatz:** Let us tentatively identify the two generators of the Heisenberg-Weyl (HW) algebra with the following diagrams:

$$d_a := ullet \ , \quad d_{a^{\dagger}} := ullet \ ,$$

depicting the actions of **deleting a particle** (d_a) and **creating a particle** $(d_{a^{\dagger}})$.

Define a notion of composition along a match: let d₁, d₂ ∈ {d_a, d_{a[†]}}, and let m₁₂ denote a I:I pairing of output vertices of d₂ with input vertices of d₁, including the possibility m₁₂ = Ø. Then

$$d_1 \overset{m_{12}}{\blacktriangleleft} d_2$$

denotes the diagram resulting from drawing d_1 , d_2 and a linking arrow for each part of m_{12} .

Composition of diagrams: Let M_{d1}(d2) denote the set of matches of d2 into d1. Then the composition *p on the set of diagrams is defined as

$$d_1 *_{\mathcal{D}} d_2 := \sum_{m_{12} \in \mathcal{M}_{d_1}(d_2)} d_1 \overset{m_{12}}{\blacktriangleleft} d_2.$$

- Examples:

$$d_{a} *_{\mathcal{D}} d_{a} = \bullet \quad \bullet \equiv d_{a} \uplus d_{a}, \quad d_{a^{\dagger}} *_{\mathcal{D}} d_{a^{\dagger}} = \bullet \quad \bullet \equiv d_{a^{\dagger}} \uplus d_{a^{\dagger}}$$
$$d_{a^{\dagger}} *_{\mathcal{D}} d_{a} = \bullet \quad \bullet \equiv d_{a^{\dagger}} \uplus d_{a}, \quad d_{a} *_{\mathcal{D}} d_{a^{\dagger}} = \bullet \quad \bullet + \bullet = d_{a^{\dagger}} \uplus d_{a} + d_{e}$$

 More precisely: we define diagrams up to isomorphism, such that in particular

$$\forall d_1, d_2 \in \mathcal{D} : d_1 \uplus d_2 = d_2 \uplus d_1.$$

• For the special case of the HW-rule diagrams, it turns out that any possible rule diagram has the form

$$\forall d \in \mathcal{D}_{HW} : \exists r, s, t \in \mathbb{Z}_{\geq 0}^3 : d = d(r, s, t) = \underbrace{\mathsf{P}_{\mathsf{HW}} : \exists r, s, t \in \mathbb{Z}_{\geq 0}^3 : d = d(r, s, t) = \underbrace{\mathsf{P}_{\mathsf{HW}} : \mathsf{P}_{\mathsf{HW}} : \exists r, s, t \in \mathbb{Z}_{\geq 0}^3 : d = d(r, s, t) = \underbrace{\mathsf{P}_{\mathsf{HW}} : \mathsf{P}_{\mathsf{HW}} : \mathsf{P}_{\mathsf{HW}}$$

>purely combinatorial composition law:

$$d(r_1, s_1, t_1) *_{\mathcal{D}} d(r_2, s_2, t_2)$$

$$= \sum_{n=0}^{\min(s_1, r_2)} \frac{s_1! r_2!}{(s_1 - n)! n! (r_2 - n)!} d(r_1 + r_2 - n, s_1 + s_2 - n, t_1 + t_2 + n).$$

COMBINATORIAL HOPF ALGEBRA STRUCTURE

- **Notation:** from hereon, \mathcal{D}_{HW} is simply denoted as \mathcal{D} !
- Algebra structure: Endow the space of isomorphism classes ∂ ∈ D of rule diagrams with a vector space structure (over a field K):

$$\begin{split} \mathcal{D} &\equiv \left(\mathcal{D}, +, \cdot\right), \quad \forall d \in \mathcal{D} : d = \sum_{\mathfrak{d} \in \mathcal{D}} \kappa_{\mathfrak{d}}(d) \mathfrak{d} \\ \left(\alpha \cdot d_1 + \beta \cdot d_2\right) &:= \sum_{\mathfrak{d} \in \mathcal{D}} \left(\alpha \kappa_{\mathfrak{d}}(d_1) + \beta \kappa_{\mathfrak{d}}(d_2)\right) \mathfrak{d} \end{split}$$

i.e. we have so far that $\mathcal{D} \equiv span_{\mathbb{K}}(\{\mathfrak{d} \in \mathcal{D}).$

Binary composition law:

 $\mu: \mathcal{D} \otimes \mathcal{D} \to \mathcal{D}_{HW}: d_1 \otimes d_2 \mapsto d_1 *_{\mathcal{D}} d_2$

• Unit map:

$$\eta: \mathbb{K} \to \mathcal{D}: k \mapsto k \cdot d_{\emptyset}$$

 $\Rightarrow \mathcal{D} \equiv (\mathcal{D}, +, \cdot, \mu, \eta) \text{ is an associative, unital (noncommuta-tive) algebra.}$

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$$\begin{array}{ccc} A \otimes A \otimes A \xrightarrow{Id_A \otimes \mu} A \otimes A \\ \mu \otimes Id_A & & \downarrow^{\mu} \\ A \otimes A \xrightarrow{\mu} A \end{array} \begin{array}{c} \widehat{} \end{array} \begin{array}{c} \bigoplus \mu \\ \mu \end{array} \begin{array}{c} \widehat{} \end{array} \begin{array}{c} \bigoplus \mu \\ \widehat{} \end{array} \end{array} \begin{array}{c} \bigoplus \mu \\ \widehat{} \end{array} \begin{array}{c} \bigoplus \mu \\ \widehat{} \end{array} \end{array} \begin{array}{c} \bigoplus \mu \\ \widehat{} \end{array} \begin{array}{c} \bigoplus \mu \\ \widehat{} \end{array} \end{array} \begin{array}{c} \bigoplus \mu \\ \widehat{} \end{array} \end{array}$$







Coalgebra structure: via **decompositions** of rule diagrams!

• **Coproduct:** for a basis vector of \mathcal{D} (i.e. isomorphism class $\mathfrak{d} \in \mathcal{D}$), define

$$\Delta(\mathfrak{d}) := \sum_{\text{ways to delete superposition factors from } \mathfrak{d}_{\text{some factors deleted}} \otimes (\mathfrak{d}_{\text{deleted factors}}) ,$$

whence more concretely

 $\Delta(d(r,s,t)) = \sum_{m=0}^{r} \sum_{n=0}^{s} \sum_{\ell=0}^{t} \binom{r}{m} \binom{s}{n} \binom{t}{\ell} d(m,n,\ell) \otimes d(r-m,s-n,t-\ell).$

• counit map:

$$\varepsilon: \mathcal{D} \to \mathbb{K}: \mathfrak{d} \mapsto \begin{cases} 1_{\mathbb{K}} & \text{if } \mathfrak{d} = d_{\emptyset} \equiv d(0, 0, 0) \\ 0_{\mathbb{K}} & \text{else.} \end{cases}$$

 $\Rightarrow \mathcal{D} \equiv (\mathcal{D}, +, \cdot, \Delta, \varepsilon)$ is a coassociative, cocommutative and counital coalgebra.

Pawel Blasiak, Gerard HE Duchamp, et al. (2010): Combinatorial algebra for second-quantized Quantum Theory, Advances in Theoretical and Mathematical Physics 14.4, pp. 1209–1243

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Table 1: Bialgebra compatibility conditions, expressed in each of the three equivalent forms: via string diagrams, from the viewpoint of the algebra structure, and from the viewpoint of the coalgebra structure.



HOPF ALGEBRA STRUCTURE

Definition A.13 (Hopf algebra). A Hopf algebra $\mathcal{H} \equiv (\mathcal{H}, \mu, \eta, \Delta, \varepsilon, S)$ is a Kbialgebra \mathcal{H} equipped with a linear map $S : \mathcal{H} \to \mathcal{H}$ called the antipode such that the following diagram commutes:



In other words, S is a left and right inverse of the linear map Id under the convolution product \star :

$$S \star Id = e = Id \star S. \tag{283}$$

Corollary A.2 (Any connected filtered bialgebra is a Hopf algebra (cf. [8], Ch. 4.3, Corr. 5)). Let $\mathcal{A} \equiv (\mathcal{A}, \mu, \eta, \Delta, \varepsilon)$ be a connected filtered K-bialgebra. Then it is also a Hopf algebra, $\mathcal{A} \equiv (\mathcal{A}, \mu, \eta, \Delta, \varepsilon, S)$, with antipode S given according to (281) (via the special case $\mathcal{A} = \mathcal{H}$ and $\varphi = Id$) by

$$S(h) := Id^{\star -1}(h) = e(h) + \sum_{k=1}^{n} (e - Id)^{\star k}(h) \qquad \forall h \in \mathcal{H}^{n} \quad (n > 0).$$
(284)

Nicolas Behr, Vincent Danos, Ilias Garnier, and Tobias Heindel (2016): **The algebras of graph rewriting,** in preparation

HOPF ALGEBRA STRUCTURE

- Diagram algebra: filtration by number of connected components — for a basis diagram d(r,s,t), this would be r+s+t!
- The diagram algebra indeed fulfills all axioms of a Hopf algebra!

HOPF ALGEBRA STRUCTURE

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SUMMARY: THE FRAMEWORK SO FAR

 the rule algebra composition operations are defined via reduction of the rule diagram algebra composition operation



Combinatorial Algebra

Algebra

Lie Algebra

result: the rule algebras
 are *-algebras !!!

A HINT OF COMBINATORIAL PHYSICS

- coherent states (alternative basis for Fock space)
- formal power series
- Blasiak et al.'s results via umbral calculus and Sheffer-type sequences, leading e.g. to analytic solutions for etH for birth-death reactions
- Allan I Solomon et al. (2005): Combinatorial Physics, Normal Order and Model Feynman Graphs, Symmetries in Science XI. Springer, pp. 527–536
- Pawel Blasiak (2005): Combinatorics of boson normal ordering and some applications, arXiv preprint quant-ph/0507206
- Pawel Blasiak, Gerard HE Duchamp, et al. (2010): Combinatorial algebra for second-quantized Quantum Theory, Advances in Theoretical and Mathematical Physics 14.4, pp. 1209–1243



Nicolas Behr (2016): **Combinatorial physics of graph rewriting,** in preparation CONCLUSION

- new concise framework, first of its kind!
- subsumes HW algebras as special case in a very precise manner
- natural framework of stochastic mechanics and combinatorial physics
- **bridgehead established** between computer science, combinatorics and theoretical physics

OUTLOOK

- systematic search for analytically solvable GTSs
 - applications of sophisticated GTSs applications such as *kappa* etc
- study of the intrinsic structure of *network theory* and *game theory* expressible in terms of the rule algebra

THANKYOU!

- Nicolas Behr, Vincent Danos, and Ilias Garnier (2016): Stochastic mechanics of graph rewriting, submitted to LICS 2016
- Nicolas Behr, Vincent Danos, Ilias Garnier, and Tobias Heindel (2016): The algebras of graph rewriting, in preparation
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