Combinatorics of Chemical Reaction Systems

Nicolas Behr (IRIF, Université Paris 7)

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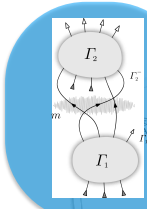
Combinatorial algebra for second-quantized Quantum Theory

Pawel Blasiak[1], Gerard H.E. Duchamp[2], Allan I. Solomon[3,4], Andrzej Horzela[1] and Karol A. Penson[3]



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Abstract

We describe an algebra $\mathcal{G}$ of diagrams that faithfully gives a diagrammatic representation of the structures of both the Heisenberg–Weyl algebra $\mathcal{H}$ – the associative algebra of the creation and annihilation operators of quantum mechanics – and $\mathcal{U}(\mathcal{L}_\mathcal{H})$, the enveloping algebra of the Heisenberg Lie algebra $\mathcal{L}_\mathcal{H}$. We show explicitly how $\mathcal{G}$ may be endowed with the structure of a Hopf algebra, which is also mirrored in the structure of $\mathcal{U}(\mathcal{L}_\mathcal{H})$. While both $\mathcal{H}$ and $\mathcal{U}(\mathcal{L}_\mathcal{H})$ are images of $\mathcal{G}$, the algebra $\mathcal{G}$ has a richer structure and therefore embodies a finer combinatorial realization of the creation–annihilation system, of which it provides a concrete model.

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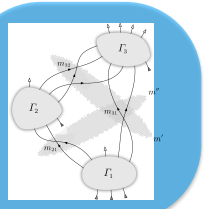

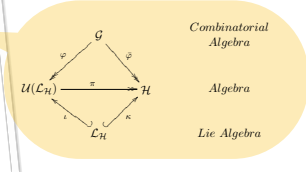

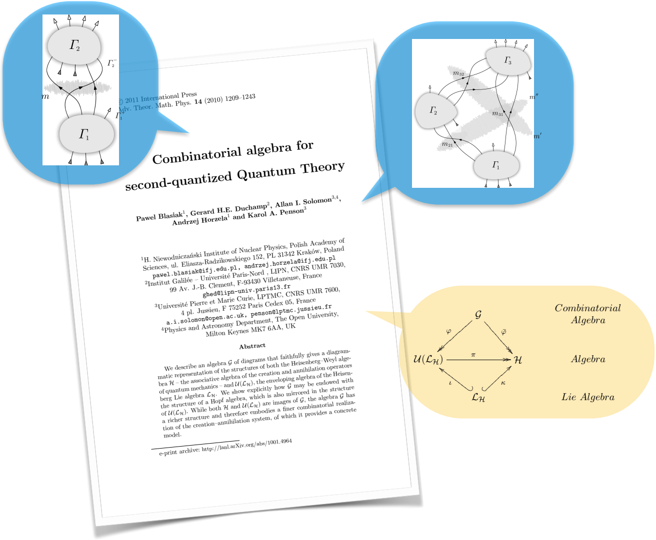

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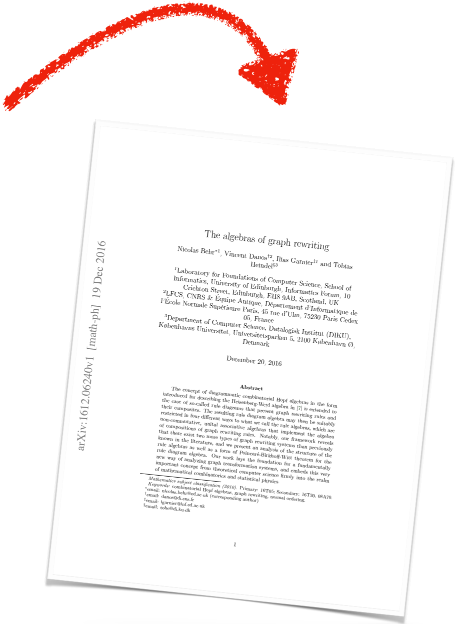
Γ_2
Γ_1
m
Γ_3
m_{32}
m_{31}
m_{21}
m''
m'
$\mathcal{G}$
φ
$\bar{\varphi}$
$\mathcal{U}(\mathcal{L}_{\mathcal{H}})$
π
$\mathcal{H}$
ι
κ
$\mathcal{L}_{\mathcal{H}}$
Combinatorial Algebra
Algebra
Lie Algebra



arXiv:1612.06240v1 [math-ph] 19 Dec 2016
The algebras of graph rewriting
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[3]Department of Computer Science, Datalogisk Institut (DIKU), Københavns Universitet, Universitetsparken 5, 2100 København Ø, Denmark
December 20, 2016
Abstract
The concept of diagrammatic combinatorial Hopf algebras in the form introduced for describing the Heisenberg-Weyl algebra in [7] is extended to the case of so-called rule diagrams that present graph rewriting rules and their composites. The resulting rule diagram algebra may then be suitably restricted in four different ways to what we call the rule algebras, which are non-commutative, unital associative algebras that implement the algebra of compositions of graph rewriting rules. Notably, our framework reveals that there exist two more types of graph rewriting systems than previously known in the literature, and we present an analysis of the structure of the rule algebras as well as a form of Poincaré-Birkhoff-Witt theorem for the rule diagram algebra. Our work lays the foundation for a fundamentally new way of analyzing graph transformation systems, and embeds this very important concept from theoretical computer science firmly into the realm of mathematical combinatorics and statistical physics.
Mathematics subject classification (2010). Primary: 16T05; Secondary: 16T30, 08A70.
Keywords: combinatorial Hopf algebras, graph rewriting, normal ordering.
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†email: danos@di.ens.fr
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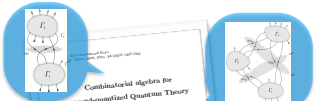
1



Combinatorial algebra for second-quantized Quantum Theory

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Combinatorics of chemical reaction systems

Nicolas Behr[a], **Gérard H. E. Duchamp**[b] **and Karol A. Penson**[a]

We propose a concise stochastic mechanics framework for chemical reaction systems that allows to formulate evolution equations for three general types of data: the probability generating functions, the exponential moment generating functions and the factorial moment generating functions. This formulation constitutes an intimate synergy between techniques of statistical physics and of combinatorics. We demonstrate how to analytically solve the evolution equations for all six elementary types of single-species chemical reactions by either combinatorial normal-ordering techniques, or, for the binary reactions, by means of Sobolev-Jacobi orthogonal polynomials. The former set of results in particular highlights the relationship between infinitesimal generators of stochastic evolution and parametric transformations fo probability distributions. Moreover, we present exact results for generic single-species non-binary reactions, hinting at a notion of compositionality of the analytic techniques.

1 Introduction

Intended as an invitation to interdisciplinary researchers and in particular to combinatorists, we present in this work an extension of the early work of Delbrück [1] on probability generating functions for chemical reaction systems to a so-called stochastic mechanics framework. While the idea to study chemical reaction systems in terms of probability generating functions is thus not new and on the contrary one of the standard techniques of this field (see e.g. [2] for a historical overview), we believe the reformulation of these techniques in terms of the stochastic mechanics formalism could lead to fruitful interaction of a broader audience of theoretical researchers. In the spirit of the ideas presented by M. Doi in his seminal paper [3], the main motivation for such a reformulation lies in a clear conceptual separation of (i) the state space of the system and (ii) the linear operators implementing the evolution of the system. Combined with insights obtained in a recent study of stochastic graph rewriting systems [4–6], one may add to this list (iii) the linear operators that implement observable quantities such as moments of number counts on states. It is only through combining this Ansatz with the standard notions of combinatorial generating functions that we find the true strengths of the stochastic mechanics approach: providing an avenue to obtain exact solutions to dynamical evolution equations. Combinatorists will recognize in our formulation of evolution equations intrinsic notions of normal-ordering problems, and indeed certain semi-linear normal-ordering techniques [7–10] will prove immensely fruitful in this direction. Chemists and other practitioners might appreciate that our solutions not only provide asymptotic information on the time-evolution of the reaction systems, but on the contrary full information on the evolution of reaction systems from any initial state at time $t = 0$ to any desired time $t = T$ (with

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Combinatorics of chemical reaction systems

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[b] *Laboratoire d'Informatique de Paris-Nord (LIPN), Institut Galilée, CNRS UMR 7030, Université Paris 13, Sorbonne Paris Cité, Villetaneuse, France; E-Mail: ghed@lipn.univ-paris13.fr*
[c] *Laboratoire de Physique Theorique de la Matière Condensée (LPTMC), CNRS UMR 7600, Sorbonne Universités, Université Pierre et Marie Curie (Paris 06), France; E-Mail: penson@lptl.jussieu.fr*

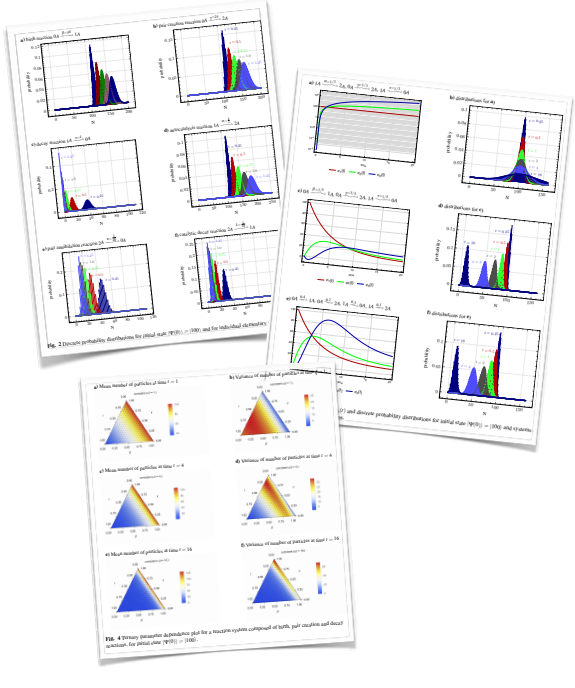


Fig. 2 Discrete probability distributions for initial state $|\Psi(0)\rangle = |100\rangle$ and for individual elementary

Fig. 4 Ternary parameter dependence plot for a reaction system composed of birth, pair creation and decay

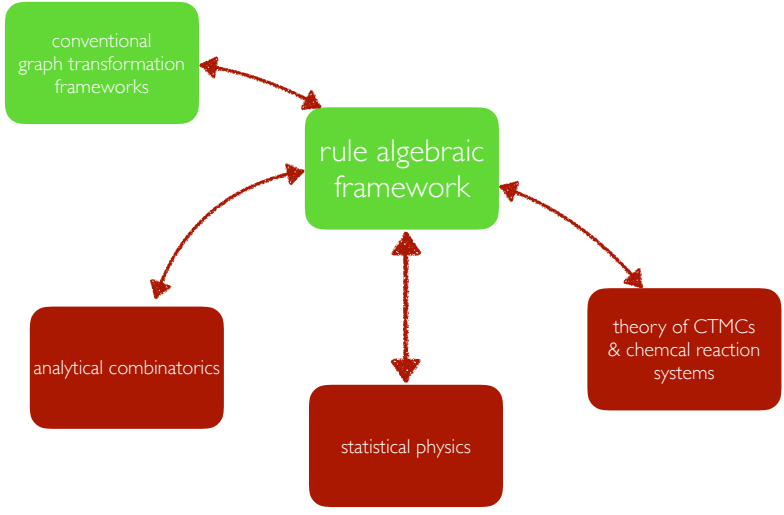
Motivation

- How do graph transformation systems (GTSs) compare to other types of stochastic systems?
- Is it possible to re-use ideas from statistical physics and combinatorics to tackle GTS computations?
- What insights may be gained by **combinatorial techniques** (normal-ordering etc.) – interesting even in the case of discrete graphs!

Idea:

Learn from the simplest case of rewriting, i.e. from the theory of **chemical reaction systems!**

Overview


conventional
graph transformation
frameworks
rule algebraic
framework
analytical combinatorics
statistical physics
theory of CTMCs
& chemcal reaction
systems

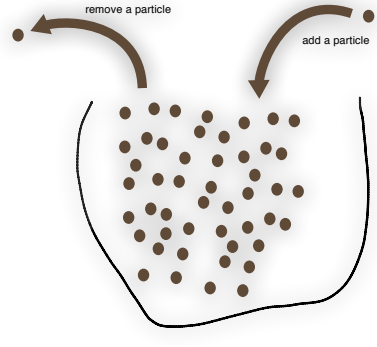
The mathematical “blueprint”: Heisenberg-Weyl algebras

The mathematical “blueprint”: the Heisenberg-Weyl algebra

- **pure state:** a **pool of** n **indistinguishable particles**

- **elementary opertions:**
  - pick a particle at random and **remove it**
  - **add a particle**

$\Rightarrow$ **basic combinatorics:**
  - **n possible ways** to **remove** a particle
  - **1 possible way** to **add** a particle



The mathematical “blueprint”: the Heisenberg-Weyl algebra

- from the theory of **bosonic Fock spaces:**

$$|n\rangle \quad \widehat{=} \quad \text{pure state of } n \text{ particles}$$

- **Ansatz:** encode the elementary operations in terms of (representations of) the **generators** of the **Heisenberg-Weyl algebra**:

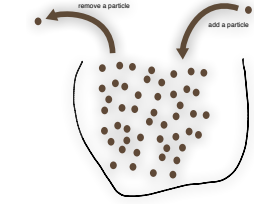
$$a\,|n\rangle := \begin{cases} n\,|n-1\rangle & \text{if } n > 0 \\ 0 & \text{else} \end{cases}$$

$$a^\dagger\,|n\rangle := |n+1\rangle \quad (n \geqslant 0)$$

- **canonical commutation relations:**

$$(aa^\dagger - a^\dagger a)\,|n\rangle = \big((n+1) - (n)\big)\,|n\rangle = |n\rangle$$

$$\Leftrightarrow \quad [a, a^\dagger] = aa^\dagger - a^\dagger a = \mathbb{1}$$

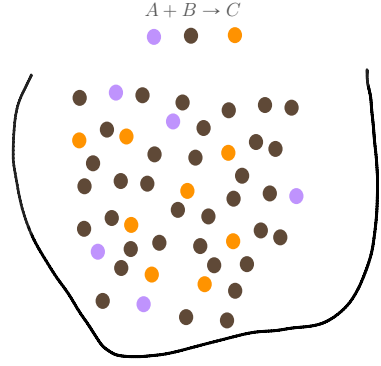


Multi-species variant

- **multi-species Heisenberg-Weyl algebra:** defined via **generators** $a_i, a_j^\dagger$ and the **canonical commutation relations**

$$[a_i, a_j] = 0 = [a_i^\dagger, a_j^\dagger], \quad [a_i, a_j^\dagger] = \delta_{i,j},$$

where $i, j \in \{1, \ldots, N\}$ (with N the **number of species**)



- **pure states:**

$$|\underline{n}\rangle \equiv |n_1, \ldots, n_N\rangle$$

- **canonical representation:**

$$a_i |\underline{n}\rangle := \begin{cases} n_i |\underline{n} - \underline{\Delta}_i\rangle & \text{if } n_i > 0 \\ 0 & \text{else} \end{cases}$$

$$a_i^\dagger |\underline{n}\rangle := |\underline{n} + \underline{\Delta}_i\rangle$$

Stochastic transition systems and continuous time Markov chain theory

The Master equation

- **Standard CTMC theory** [1]: one way to describe the CTMC's dynamics is to give a **probability distribution**

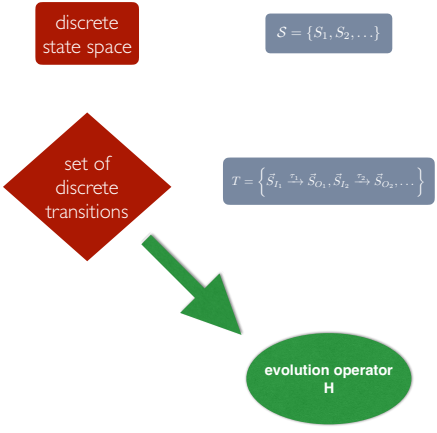
$$|\Psi(t)\rangle := \sum_{S \in \mathcal{S}} p_S(t)|S\rangle$$

of being in one of the discrete states (represented by basis vectors $|S\rangle$), and specifying the **Master equation** (aka **Schrödinger equation**)

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

where H is the **evolution operator**.

- How precisely H is determined for a given system will be intimately related to the concept of **rule algebras** in our formalism!



[1] James R. Norris. *Markov Chains*. Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge University Press, 1998

The “stochastic mechanics” viewpoint

Benefits:

$\exists$ a full-blown formalism [2][3] aka “**stochastic mechanics**” [4] for studying CTMCs:

- **Observables** O are linear operators under which each pure state is an Eigenstate,

$$O|S\rangle = \omega_O(S)|S\rangle\,.$$

- **Expectation values of observables** are computed by introducing the **dual projection vector**

$$\langle|S\rangle := 1 \quad \forall S \in \mathcal{S}\,,$$

such that for any state probability distribution $|\Psi(t)\rangle$

$$\mathbb{E}_{|\Psi(t)\rangle}(O) \equiv \langle O\rangle(t) := \langle|O|\Psi(t)\rangle\,.$$

$\Rightarrow$ **evolution of expectation values of observables** via Master equation:

$$\frac{d}{dt}\langle O\rangle(t) = \langle OH\rangle(t)\,.$$

- Additional property of the evolution operator H:

$$\langle|e^{tH}|\Psi(0)\rangle \stackrel{!}{=} 1 \quad \Rightarrow \quad \langle|H = 0\,,$$

i.e. H **preserves normalizations**.

$\Rightarrow$ analogue of the **Ehrenfest equation** of quantum mechanics:

$$\frac{d}{dt}\langle O\rangle(t) = \langle[O,H]\rangle(t)\,,$$

where $[A,B] := AB - BA$ is the **commutator**

[2] Masao Doi. “Second quantization representation for classical many-particle system”. In: *Journal of Physics A: Mathematical and General* 9.9 (1976), p. 1465

[3] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Stochastic mechanics of graph rewriting”. In: *31st Annual ACM/IEEE Symposium on Logic in Computer Science (LICS)*. 2016

[4] John C Baez and Jacob Biamonte. “A course on quantum techniques for stochastic mechanics”. In: *s arXiv:1209.3632* (2012)

A first hint at the practical advantages and potential of the framework

Proposition ([5], Prop. 3.35)

For $A, B \in End_{\mathbb{K}}(\mathcal{V})$ (with $\mathcal{V}$ a $\mathbb{K}$-vector space) and λ a formal variable,

$$e^{\lambda A} B e^{-\lambda A} = e^{ad_{\lambda A}} B\,,$$

where

$$ad_A B := [A, B] = AB - BA\,,\ ad_A^0 B := B\,.$$

[5] Brian C Hall. *Lie groups, Lie algebras, and representations: an elementary introduction.* Vol. 222. Springer, 2015

[6] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Stochastic mechanics of graph rewriting". In: *31st Annual ACM/IEEE Symposium on Logic in Computer Science (LICS).* 2016

[7] Nicolas Behr, Vincent Danos, and Ilias Garnier. *Combinatorial conversion and disassociator dynamics for stochastic rewriting systems (in preparation, ≈ Q1 2018).*

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where

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- **Application:** suppose H is an evolution operator, and let

  $$\underline{\lambda} \cdot \underline{O} \equiv \sum_i \lambda_i O_i$$

  denote a formal linear combination of observables $O_i \in \mathcal{O}$.

- Define the **moment-generating function** $\mathcal{M}(t; \underline{\lambda})$ of the CTMC as

  $$\mathcal{M}(t; \underline{\lambda}) := \left\langle e^{\underline{\lambda} \cdot \underline{O}} \right\rangle (t)\,,$$

  whence formally

  $$\left[\frac{\partial^{n_1}}{\partial \lambda_{i_1}^{n_1}} \cdots \frac{\partial^{n_k}}{\partial \lambda_{i_1}^{n_k}} \mathcal{M}(t; \underline{\lambda}) \right] \Big|_{\underline{\lambda} \to \underline{0}} = \langle O_{i_1}^{n_1} \cdots O_{i_k}^{n_k} \rangle (t)\,.$$

$\Rightarrow$ **Formal all-order moment evolution equation** [6] [7]**:**

$$\begin{aligned} \frac{d}{dt} \mathcal{M}(t; \underline{\lambda}) &= \left\langle \left| e^{\underline{\lambda} \cdot \underline{O}} H \right| \Psi(t) \right\rangle \\ &= \left\langle \left| \left(e^{\underline{\lambda} \cdot \underline{O}} H e^{-\underline{\lambda} \cdot \underline{O}} \right) e^{\underline{\lambda} \cdot \underline{O}} \right| \Psi(t) \right\rangle \\ &= \left\langle \left| \left(e^{ad_{\underline{\lambda} \cdot \underline{O}}} H \right) e^{\underline{\lambda} \cdot \underline{O}} \right| \Psi(t) \right\rangle\,. \end{aligned}$$

[5] Brian C Hall. *Lie groups, Lie algebras, and representations: an elementary introduction.* Vol. 222. Springer, 2015

[6] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Stochastic mechanics of graph rewriting". In: *31st Annual ACM/IEEE Symposium on Logic in Computer Science (LICS).* 2016

[7] Nicolas Behr, Vincent Danos, and Ilias Garnier. *Combinatorial conversion and disassociator dynamics for stochastic rewriting systems (in preparation, ≈ Q1 2018).*

Specializing to discrete graph rewriting, whence to chemical reaction systems

An interesting relation: states and observables

- **States:** so-called **number vectors**,

$$|\underline{n}\rangle \equiv |n_1, \ldots, n_N\rangle = (a_1^\dagger)^{n_1} \ldots (a_N^\dagger)^{n_N} |0, \ldots, 0\rangle$$

- **Observables** (aka **diagonal operators**): linear combinations of the opertors

$$(\underline{a}^\dagger)^{\underline{k}} \underline{a}^{\underline{k}} \equiv \prod_{i=1}^{N} (a_i^\dagger)^{k_i} a_i^{k_i}$$

(**note:** $[a_i, a_j^\dagger] = \delta_{i,j}\mathbb{1}$)

- **normal-ordering relation** (non-trivial part):

$$a_i^r (a_i^\dagger)^s = \sum_{m \geqslant 0} m! \binom{r}{m} \binom{s}{m} (a_i^\dagger)^{(r-m)} a_i^{(s-m)},$$

which has an easy interpretation in terms of rule-diagrams!

Fact (combinatorics literature!)

$$(\underline{a}^\dagger)^{\underline{s}} \underline{a}^{\underline{s}} = \sum_{\underline{k}=\underline{0}}^{\underline{s}} s_1(\underline{s}; \underline{k}) \hat{\underline{n}}^{\underline{k}}$$

$s_1(\underline{s}; \underline{k})$ – **Stirling numbers of the** 1^{st} **kind**)

$\hat{n}_i$ – **number operator** of species i,

$$\hat{n}_i := a_i^\dagger a_i\,, \quad \hat{n}_i |\underline{n}\rangle = n_i |\underline{n}\rangle$$

$\Rightarrow$ the Eigenvalues n_i of the number operators $\hat{n}_i$ of a **pure state** $|\underline{n}\rangle$ **completely characterize** the pure state!

Delbrück's insight: probability generating functions

Bargmann-Fock representation [8]

$$
\begin{array}{lcll}
|\underline{n}\rangle & \leftrightarrow & \prod_{i=1}^{N} x_i^{n_i} & \\
a_i^\dagger & \leftrightarrow & \hat{x}_i & \text{(multiplication by } x_i\text{)} \\
a_i & \leftrightarrow & \frac{\partial}{\partial x_i} & \text{(derivation by } x_i\text{)}
\end{array}
$$

- **normal-ordering relation:** for all $f \equiv f(x_1, \ldots, x_N)$,

$$\left(\hat{x}_i \frac{\partial}{\partial x_j} - \frac{\partial}{\partial x_j}\hat{x}_i\right) f = \delta_{i,j} f$$

- **probability generating function:** given a probability distribution $|\psi\rangle = \sum_{\underline{n} \geqslant 0} p_{\underline{n}} |n\rangle$,

$$|\psi\rangle \quad \leftrightarrow \quad P(x) := \sum_{\underline{n} \geqslant 0} p_{\underline{n}} \underline{x}^{\underline{n}}$$

Delbrück [9]

The **master equation** for a chemical reaction system with reactions

$$\underline{i} \cdot \underline{X} \xrightarrow{r_{\underline{i},\underline{o}}} \underline{o} \cdot \underline{X}$$

reads in the Bargmann-Fock representation

$$\frac{\partial}{\partial t} P(t; \underline{x}) = \sum_{\underline{i},\underline{o}} r_{\underline{i},\underline{o}} \left((\hat{\underline{x}})^{\underline{o}} - (\hat{\underline{x}})^{\underline{i}} \right) \left(\frac{\partial}{\partial \underline{x}} \right)^{\underline{i}} P(t; \underline{x})$$

[8] V Fock. "Verallgemeinerung und Lösung der diracschen statistischen Gleichung". In: *Zeitschrift für Physik A Hadrons and Nuclei* 49.5 (1928), pp. 339–357; Valentine Bargmann. "On a Hilbert space of analytic functions and an associated integral transform part I". In: *Communications on pure and applied mathematics* 14.3 (1961), pp. 187–214

[9] Max Delbrück. "Statistical fluctuations in autocatalytic reactions". In: *The Journal of Chemical Physics* 8.1 (1940), pp. 120–124

Aside: three types of generating functions

- **probability generating function:** given a **probability distribution** $|\psi\rangle = \sum_{\underline{n}\geqslant 0} p_{\underline{n}} |n\rangle$,

$$|\psi\rangle \quad \leftrightarrow \quad P(x) := \sum_{\underline{n}\geqslant 0} p_{\underline{n}} \underline{x}^{\underline{n}}$$

- **(exponential) moment generating function:** (with **formal parameters** $\underline{\lambda} \equiv (\lambda_1, \ldots, \lambda_N)$)

$$\mathcal{M}(t; \underline{\lambda}) := \left(e^{\underline{\lambda} \cdot \mathbb{n}} P(t; \underline{x}) \right) \Big|_{\underline{x} \to \underline{1}} \qquad (\mathbb{n}_i := \hat{x}_i \tfrac{\partial}{\partial x_i})$$

- **(exponential) factorial moment generating function:** (with **formal parameters** $\underline{\nu} \equiv (\nu_1, \ldots, \nu_N)$)

$$\mathcal{F}(t; \underline{\nu}) := \left(\sum_{\underline{k}\geqslant 0} \frac{\underline{\nu}^{\underline{k}}}{\underline{k}!} \, \underline{\hat{x}}^{\underline{k}} \left(\frac{\partial}{\partial \underline{x}} \right)^{\underline{k}} P(t; \underline{x}) \right) \Big|_{\underline{x} \to \underline{1}}$$

- **Well-known fact:** (see e.g. [10])

$$\mathcal{M}(t; \underline{\lambda}) = P(t; \underline{e^{\lambda}}), \quad \mathcal{F}(t; \underline{\nu}) = P(t; \underline{\nu} + \underline{1}) = \mathcal{M}(t; \underline{\ln(\nu + 1)})$$

[10] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of chemical reaction systems". In: *arXiv:1712.06575* (2017)

“Bonus result”: generating function evolution equations

From [11]: $\frac{\partial}{\partial t}\mathcal{M} = \mathbb{D}\mathcal{M}$, $\frac{\partial}{\partial t}\mathcal{F} = \mathbb{d}\mathcal{F}$

Table 2 Contributions $H_{(\underline{i},\underline{o})}$ to the evolution operator H, $\mathbb{D}_{(\underline{i},\underline{o})}$ to the differential operator $\mathbb{D} \equiv \mathbb{D}(\underline{\lambda}, \partial_{\underline{\lambda}})$ and $\mathbb{d}_{(\underline{i},\underline{o})}$ to $\mathbb{d} \equiv \mathbb{d}(\underline{\nu}, \partial_{\underline{\nu}})$ of individual multi-species chemical reactions $\underline{i}\cdot\underline{A} \xrightarrow{r_{\underline{i},\underline{o}}} \underline{o}\cdot\underline{A}$

Parameters	$H_{(\underline{i},\underline{o})}/r_{\underline{i},\underline{o}}$	$\mathbb{D}_{(\underline{i},\underline{o})}/r_{\underline{i},\underline{o}}$	$\mathbb{d}_{(\underline{i},\underline{o})}/r_{\underline{i},\underline{o}}$
$(\underline{o},\underline{i})$	$\left(\underline{a}^{\dagger\,\underline{o}} - \underline{a}^{\dagger\,\underline{i}}\right)\underline{a}^{\underline{i}}$	$\left(e^{\underline{\lambda}\cdot(\underline{o}-\underline{i})} - 1\right)\sum_{\underline{\ell}=\underline{0}}^{\underline{i}} \underline{S}_1(\underline{i},\underline{\ell})\left(\frac{\partial}{\partial\underline{\lambda}}\right)^{\underline{\ell}}$	$\left((\underline{\nu}+\underline{1})^{\underline{o}} - (\underline{\nu}+\underline{1})^{\underline{i}}\right)\left(\frac{\partial}{\partial\underline{\nu}}\right)^{\underline{i}}$
$(\underline{\delta}_\alpha + \underline{\delta}_\beta, \underline{0})$	$\left(a_\alpha^\dagger + a_\beta^\dagger - 1\right)$	$\left(e^{\lambda_\alpha+\lambda_\beta} - 1\right)$	$\nu_\alpha\nu_\beta + \nu_\alpha + \nu_\beta$
$(\underline{\delta}_\alpha, \underline{0})$	$a_\alpha^\dagger - 1$	$e^{\lambda_\alpha} - 1$	ν_α
$(\underline{0}, \underline{\delta}_\gamma)$	$\left(1 - a_\gamma^\dagger\right)a_\gamma$	$\left(e^{-\lambda_\gamma} - 1\right)\frac{\partial}{\partial\lambda_\gamma}$	$-\nu_\gamma\frac{\partial}{\partial\nu_\gamma}$
$(\underline{\delta}_\alpha, \underline{\delta}_\beta)$	$\left(a_\alpha^\dagger - a_\beta^\dagger\right)a_\beta$	$\left(e^{\lambda_\alpha-\lambda_\beta} - 1\right)\frac{\partial}{\partial\lambda_\beta}$	$(\nu_\alpha - \nu_\beta)\frac{\partial}{\partial\nu_\beta}$
$(\underline{\delta}_\alpha + \underline{\delta}_\beta, \underline{\delta}_\gamma)$	$\left(a_\alpha^\dagger a_\beta^\dagger - a_\gamma^\dagger\right)a_\gamma$	$\left(e^{\lambda_\alpha+\lambda_\beta-\lambda_\gamma} - 1\right)\frac{\partial}{\partial\lambda_\gamma}$	$(\nu_\alpha\nu_\beta + \nu_\alpha + \nu_\beta - \nu_\gamma)\frac{\partial}{\partial\nu_\gamma}$
$(\underline{0}, \underline{\delta}_\beta + \underline{\delta}_\gamma)$	$\left(1 - a_\beta^\dagger a_\gamma^\dagger\right)a_\beta a_\gamma$	$\left(e^{-\lambda_\beta-\lambda_\gamma} - 1\right)\left(\frac{\partial^2}{\partial\lambda_\beta\partial\lambda_\gamma} - \delta_{\beta,\gamma}\frac{\partial}{\partial\lambda_\gamma}\right)$	$-\left(\nu_\beta\nu_\gamma + \nu_\beta + \nu_\gamma\right)\frac{\partial^2}{\partial\nu_\beta\partial\nu_\gamma}$
$(\underline{\delta}_\alpha, \underline{\delta}_\beta + \underline{\delta}_\gamma)$	$\left(a_\alpha^\dagger - a_\beta^\dagger a_\gamma^\dagger\right)a_\beta a_\gamma$	$\left(e^{\lambda_\alpha-\lambda_\beta-\lambda_\gamma} - 1\right)\left(\frac{\partial^2}{\partial\lambda_\beta\partial\lambda_\gamma} - \delta_{\beta,\gamma}\frac{\partial}{\partial\lambda_\gamma}\right)$	$\left(\nu_\alpha - \nu_\beta\nu_\gamma - \nu_\beta - \nu_\gamma\right)\frac{\partial^2}{\partial\nu_\beta\partial\nu_\gamma}$

[11] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. “Combinatorics of chemical reaction systems”. In: *arXiv:1712.06575* (2017)

A seminal result on normal-ordering techniques

Theorem (Duchamp, Penson et al. [12]**)**

Let $\mathcal{H}$ be a **semi-linear operator** (in the Bargmann-Fock basis),

$$\mathcal{H} = v(\underline{\hat{x}}) + \sum_{i=0}^{N} q_i(\underline{\hat{x}})\, \partial_{x_i}\,,$$

with $q_i(\underline{\hat{x}})$ and $v(\underline{\hat{x}})$ some functions in the operators $\hat{x}_i$. Let $F(0;\underline{x})$ be an entire function in the indeterminates x_i. Define the formal power series (with formal variable λ)

$$F(\lambda;\underline{x}) := e^{\lambda\mathcal{H}}\, F(0;\underline{x})\,.$$

Then $F(\lambda;\underline{x})$ may be expressed in **closed form** as follows:

$$F(\lambda;\underline{x}) = g(\lambda;\underline{x}) F\big(0;\underline{T}(\lambda;\underline{x})\big)\,, \qquad \begin{cases} \frac{\partial}{\partial\lambda} T_i(\lambda;\underline{x}) & = q_i(\underline{T}(\lambda;\underline{x}))\,, \quad T_i(0;\underline{x}) = x_i \\ \ln g(\lambda;\underline{x}) & = \int_0^\lambda v(\underline{T}(\kappa;\underline{x}))\, d\kappa \end{cases}$$

Moreover, $e^{\lambda\mathcal{H}}$ induces a **one-parameter group** of transformations due to

$$\begin{aligned} \underline{T}(\lambda+\mu;\underline{x}) &= \underline{T}(\mu;\underline{T}(\lambda;\underline{x})) \\ g(\lambda+\mu;\underline{x}) &= g(\lambda;\underline{x}) g(\mu;\underline{T}(\lambda;\underline{x}))\,, \end{aligned}$$

[12] P Blasiak et al. "Boson normal ordering via substitutions and Sheffer-Type Polynomials". In: *Physics Letters A* 338.2 (2005), pp. 108–116

Result: exact actions of evolution semi-groups

From [13]:

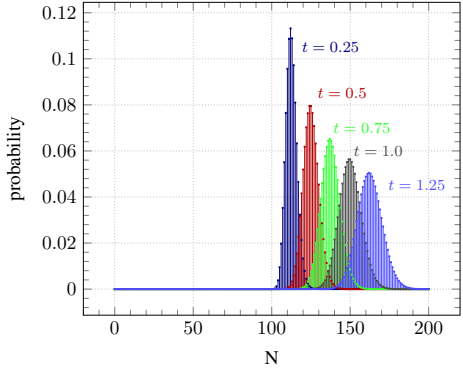
Table 3 Closed-form results for the time-dependent probability generating functions $P(t;\underline{x})$ for reaction systems of N species with a single non-binary elementary reaction; here, $S_1,\ldots,S_N$ denote the N different species, while $\underline{\Delta}_i$ ($i \in \{1,\ldots,N\}$ denotes the N-vector with coordinates $(\underline{\Delta}_i) = \delta_{i,j}$.

reaction	$\mathscr{H} = \underline{q}(\underline{x}) \cdot \partial_{\underline{x}} + v(\underline{x})$	$P(t;\underline{x}) = g(t;\underline{x})P(0;\underline{T}(t;\underline{x})$	comments
$\emptyset \xrightarrow{\alpha} S_i$	$\alpha\,(\hat{x}_i - 1)$	$Pois(\alpha t;x_i) \cdot P(0;\underline{x})$	$Pois(\mu;x) := e^{\mu(x-1)}$
$\emptyset \xrightarrow{\alpha} S_i + S_j$	$\alpha\,(\hat{x}_i\hat{x}_j - 1)$	$\left(e^{\alpha t(x_i x_j - 1)}\right) \cdot P(0;\underline{x})$	(Poisson distribution, $0 \le \mu < \infty$)
$S_i \xrightarrow{\alpha} \emptyset$	$\alpha\,(1-\hat{x}_i)\,\frac{\partial}{\partial x_i}$	$P(0;\underline{x} + (-x_i + Bern(e^{-\alpha t};x_i))\,\underline{\Delta}_i)$	$Bern(\mu;x) := (1-\mu) + x\mu$
$S_i \xrightarrow{\alpha} S_j \quad (i \neq j)$	$\alpha\,(\hat{x}_j - \hat{x}_i)\,\frac{\partial}{\partial x_i}$	$P(0;\underline{x} + (-x_i + (x_j(1-e^{-\alpha t}) + x_i e^{-\alpha t})\,\underline{\Delta}_i)$	(Bernoulli distribution, $0 \le \mu \le 1$)
$S_i \xrightarrow{\alpha} 2S_i$	$\alpha\,(\hat{x}_i^2 - \hat{x}_i)\,\frac{\partial}{\partial x_i}$	$P(0;\underline{x} + (-x_i + Geom(e^{-\alpha t};x_i))\,\underline{\Delta}_i)$	$Geom(\mu;x) := \frac{x\mu}{1-x(1-\mu)}$
$S_i \xrightarrow{\alpha} S_i + S_j \quad (i \neq j)$	$\alpha\,(\hat{x}_i\hat{x}_j - \hat{x}_i)\,\frac{\partial}{\partial x_i}$	$P(0;\underline{x} + (-x_i + x_i Pois(\alpha t;x_j)))\,\underline{\Delta}_i)$	(Geometric distribution, $0 < \mu \le 1$)
$S_i \xrightarrow{\alpha} S_j + S_k \quad (i \neq j \neq k)$	$\alpha\,(\hat{x}_j\hat{x}_k - \hat{x}_i)\,\frac{\partial}{\partial x_i}$	$P(0;\underline{x} + (-x_i + x_j x_k(1-e^{-\alpha t}) + x_i e^{-\alpha t})\,\underline{\Delta}_i)$	

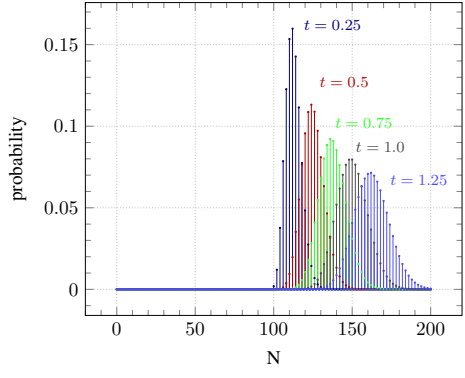
[13] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of chemical reaction systems". In: *arXiv:1712.06575* (2017)

Elementary nonary reactions – plots [13]

a) birth reaction $0A \xrightarrow{\beta=50} 1A$



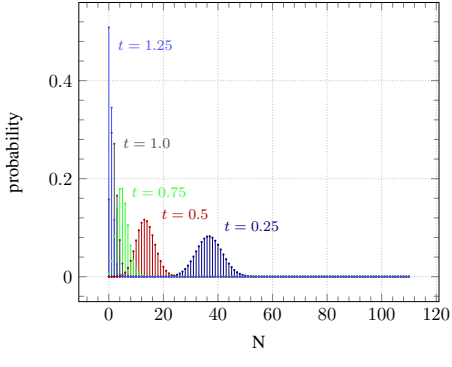
b) pair creation reaction $0A \xrightarrow{\gamma=25} 2A$



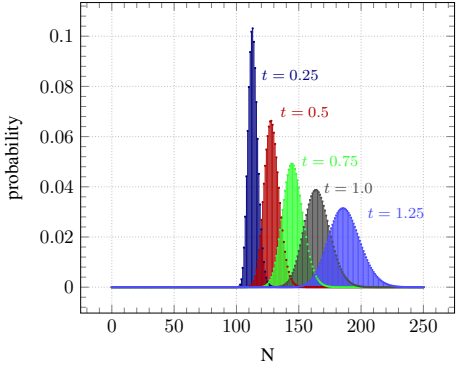
[13] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of chemical reaction systems". In: *arXiv:1712.06575* (2017)

Elementary unary reactions – plots [13]

c) decay reaction $1A \xrightarrow{\tau=4} 0A$



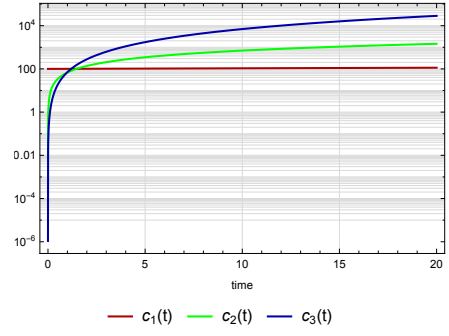
d) autocatalysis reaction $1A \xrightarrow{\alpha=\frac{1}{2}} 2A$



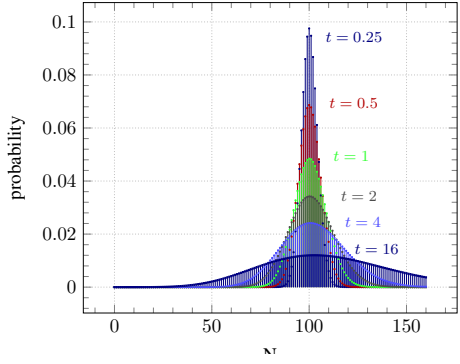
[13] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of chemical reaction systems". In: *arXiv:1712.06575* (2017)

A hint of compositionality [13]

a) $1A \xrightarrow{\alpha=1/3} 2A,\ 0A \xrightarrow{\gamma=1/3} 2A,\ 1A \xrightarrow{\tau=1/3} 0A$



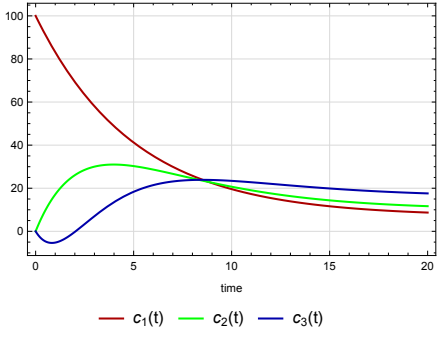
b) distributions for **a)**



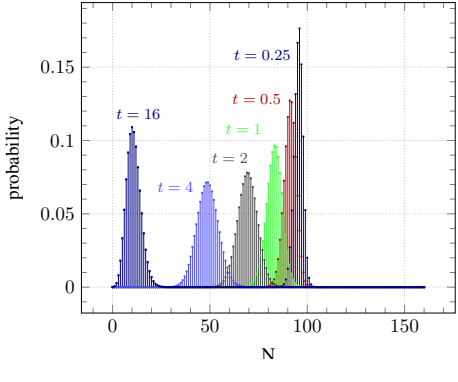
[13] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of chemical reaction systems". In: *arXiv:1712.06575* (2017)

A hint of compositionality [13]

c) $0A \xrightarrow{\beta=1/5} 1A$, $0A \xrightarrow{\gamma=3/5} 2A$, $1A \xrightarrow{\tau=1/5} 0A$



d) distributions for **c)**

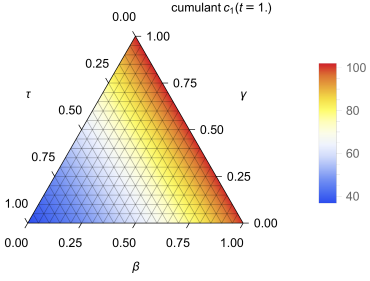


[13] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of chemical reaction systems". In: *arXiv:1712.06575* (2017)

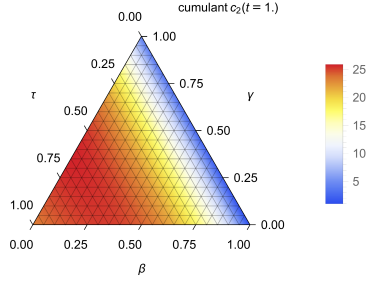
A hint of compositionality [13]

Example: ternary parameter dependence plot for a reaction system composed of **birth**, **pair creation** and **decay** reactions, for **initial state** $|\Psi(0)\rangle = |100\rangle$

a) Mean number of particles at time $t = 1$



b) Variance of number of particles at time $t = 1$

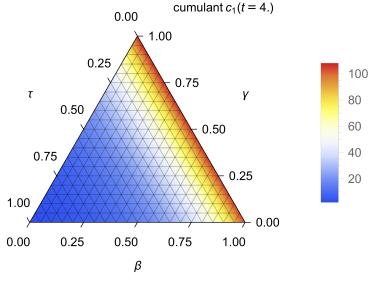


[13] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of chemical reaction systems". In: *arXiv:1712.06575* (2017)

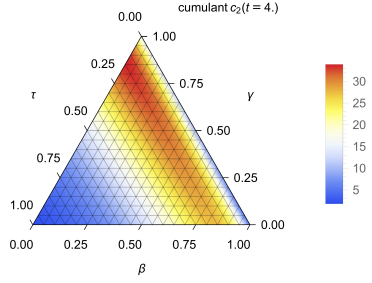
A hint of compositionality [13]

Example: ternary parameter dependence plot for a reaction system composed of **birth**, **pair creation** and **decay** reactions, for **initial state** $|\Psi(0)\rangle = |100\rangle$

c) Mean number of particles at time $t = 4$



d) Variance of number of particles at time $t = 4$

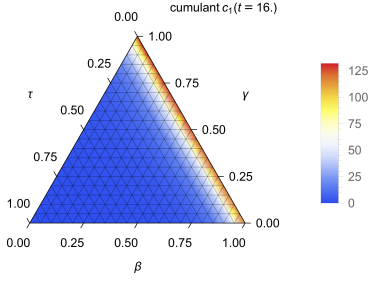


[13] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of chemical reaction systems". In: *arXiv:1712.06575* (2017)

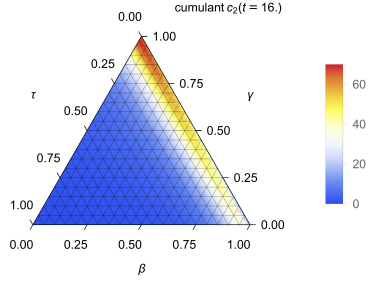
A hint of compositionality [13]

Example: ternary parameter dependence plot for a reaction system composed of **birth**, **pair creation** and **decay** reactions, for **initial state** $|\Psi(0)\rangle = |100\rangle$

e) Mean number of particles at time $t = 16$



f) Variance of number of particles at time $t = 16$



[13] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of chemical reaction systems". In: *arXiv:1712.06575* (2017)

Binary reactions and Sobolev-Jacobi orthogonal polynomials

- The precise technical details are somewhat intricate, see the our paper!
- The **basic Ansatz** is the one of McQuarrie [14], **BUT** the original Ansatz had a mathematical error...
- **Problem:** McQuarrie suggested to use the Jacobi polynomials as eigenfunction basis of the infinitesimal generator, yet for the range of parameters of interest, these are ill-posed.
- **Our solution:** the mathematical problem has been successfully treated in the 1990's by Kwon & Littlejohn [15], who introduced so-called **Sobolev-Jacobi polynomials**.
- **Aside:** This is related **normal-ordering**, too! (But one of a new kind...)

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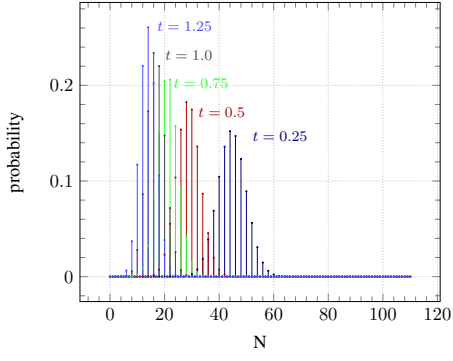
[14] Donald A McQuarrie. "Kinetics of small systems. I". In: *The journal of chemical physics* 38.2 (1963), pp. 433–436; Donald A McQuarrie, CJ Jachimowski, and ME Russell. "Kinetics of small systems. II". In: *The Journal of Chemical Physics* 40.10 (1964), pp. 2914–2921; Donald A McQuarrie. "Stochastic approach to chemical kinetics". In: *Journal of applied probability* 4.3 (1967), pp. 413–478

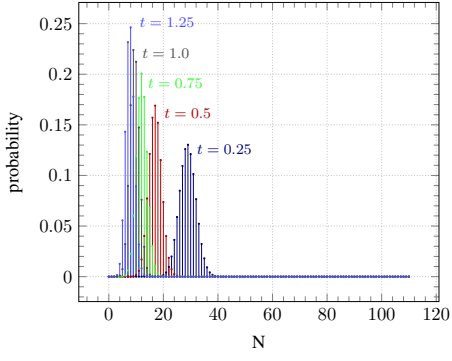
[15] KH Kwon, LL Littlejohn, and BH Yoo. "Characterizations of orthogonal polynomials satisfying differential equations". In: *SIAM Journal on Mathematical Analysis* 25.3 (1994), pp. 976–990; Kil H Kwon, LL Littlejohn, and BH Yoo. "New characterizations of classical orthogonal polynomials". In: *Indagationes Mathematicae* 7.2 (1996), pp. 199–213; Kil H Kwon and Lance L Littlejohn. "Classification of classical orthogonal polynomials". In: *J. Korean Math. Soc* 34.4 (1997), pp. 973–1008; Kil H Kwon and LL Littlejohn. "Sobolev orthogonal polynomials and second-order differential equations". In: *The Rocky Mountain journal of mathematics* (1998), pp. 547–594

Elementary binary reactions – plots [15]

e) pair annihilation reaction $2A \xrightarrow{\kappa=\frac{1}{40}} 0A$



f) catalytic decay reaction $2A \xrightarrow{\lambda=\frac{1}{10}} 1A$



[15] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of chemical reaction systems". In: *arXiv:1712.06575* (2017)

“Bonus result”: Which reactions are first-order moment-closed?

Theorem [15]

The **evolution equations for the factorial moments** $f_{\underline{n}}(t)$ read

$$\frac{d}{dt} f_{\underline{n}}(t) = \sum_{\underline{i},\underline{o}} r_{\underline{i},\underline{o}} \sum_{\underline{k}} \phi_{\underline{k}}(\underline{n};\underline{i},\underline{o}) f_{\underline{n}+\underline{i}-\underline{k}}(t)$$

$$\phi_{\underline{k}}(\underline{n};\underline{i},\underline{o}) = \left[(\underline{o})_{\underline{k}} - (\underline{i})_{\underline{k}} \right] \binom{\underline{n}}{\underline{k}} .$$

Here, we have made use of the standard conventions $\binom{x}{y} = 0$ and $(x)_y = 0$ whenever $y > x$. Specializing to $\underline{n} = \underline{\Delta}_\alpha$, i.e. to $f_{\underline{\Delta}_\alpha}$ denoting the first moment of the number vector $\hat{n}_\alpha$, one obtains the **evolution equations for the first moments** as

$$\frac{d}{dt} f_{\underline{\Delta}_\alpha}(t) = \sum_{\underline{i},\underline{o}} r_{\underline{i},\underline{o}} (o_\alpha - i_\alpha) f_{\underline{i}}(t) .$$

Therefore, the only reaction systems for which we have **first order moment closure** are **semi-linear** reaction systems, i.e. systems for which for all $(\underline{i},\underline{o})$ with rates $r_{\underline{i},\underline{o}} > 0$ we have that

$$\sum_{j \in \mathbf{S}} i_j \leqslant 1 .$$

[15] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson, “Combinatorics of chemical reaction systems”, In: *arXiv:1712.06575* (2017)

Thank you!

- John C Baez and Jacob Biamonte. “A course on quantum techniques for stochastic mechanics”. In: *s arXiv:1209.3632* (2012).
- Valentine Bargmann. “On a Hilbert space of analytic functions and an associated integral transform part I”. In: *Communications on pure and applied mathematics* 14.3 (1961), pp. 187–214.
- Nicolas Behr, Vincent Danos, and Ilias Garnier. *Combinatorial conversion and disassociator dynamics for stochastic rewriting systems (in preparation, ≈ Q1 2018)*.
- Nicolas Behr, Vincent Danos, and Ilias Garnier. *Representation theory of the rule algebras (in preparation, ≈ Q1 2018)*.

- Nicolas Behr, Vincent Danos, and Ilias Garnier. “Stochastic mechanics of graph rewriting”. In: *31st Annual ACM/IEEE Symposium on Logic in Computer Science (LICS)*. 2016.
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