COMBINATORIAL MODELS OF CREATION–ANNIHILATION

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ABSTRACT. Quantum physics has revealed many interesting formal properties associated with the algebra of two operators, A and B, satisfying the partial commutation relation $AB - BA = 1$. This study surveys the relationships between classical combinatorial structures and the reduction to normal form of operator polynomials in such an algebra. The connection is achieved through suitable graphs, or "*diagrams*", that are composed of elementary "*gates*". In this way, many normal form evaluations can be systematically obtained, thanks to models that involve set partitions, permutations, increasing trees, as well as weighted lattice paths. Extensions to q-analogues, multivariate frameworks, and urn models are also briefly discussed.

CONTENTS

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1. Introduction

The theme of our study is extremely simple. It consists in investigating some of the formal consequences of the partial commutation relation between two operators A and B (belonging to some unspecified algebra of operators):

$$[A, B] = 1. \tag{1}$$

Here $[U, V] := UV - VU$ is the Lie bracket and 1 represents the identity operator. The relation (1) will henceforth be called the *creation–annihilation axiom*. Indeed, in quantum physics[1], it is satisfied by the annihilation and creation operators, a and $a^\dagger$, which are adjoint to each other and serve to decrease or increase the number of photons by 1: in this context, one should take $A = a$ and $B = a^\dagger$.

From an algebraic standpoint, one thus considers the polynomial ring $\mathbb{C}\langle A, B\rangle$ in non-commuting indeterminates A, B, and makes systematic use of the reduction of $AB-BA-1$ to 0. (Technically, this corresponds to taking the quotient $\mathbb{C}\langle A, B\rangle/\mathcal{I}$, of the ring $C\langle A, B\rangle$ of polynomials in non-commuting indeterminates by the two-sided ideal $\mathcal{I}$ generated by $AB - BA - 1$.) It is then possible to regard (1) as a directed rewrite rule

$$AB \longrightarrow 1 + BA, \tag{2}$$

by which any non-commutative polynomial $\mathfrak{h}$ in indeterminates A, B is completely reduced to a unique *normal form*, $\mathfrak{N}(\mathfrak{h})$, where, in each monomial, all the occurrences of B precede all the occurrences of A.

For instance, the chain

$$\begin{aligned} AB\underline{AB}A &\longrightarrow AB(1+BA)A \equiv ABBAA + \underline{AB}A \\ &\longrightarrow \underline{AB}BAA + A + BAA \longrightarrow B\underline{AB}AA + A + 2BAA \\ &\longrightarrow BBAAA + 3BAA + A \end{aligned} \tag{3}$$

proves that $\mathfrak{N}(ABABA) = B^2A^3 + 3BA^2 + A$. (At each step, the pair $\underline{AB}$ involved in a reduction has been underlined.) It is precisely this non-trivial rearrangement process, known in quantum physics as *normal ordering*, which we propose to examine.

A particular realization of the commutation relation (1) is obtained by choosing some sufficiently general space $\{f(x)\}$ of smooth functions (typically, the class of $\mathcal{C}^\infty(0, 1)$ of infinitely differentiable functions over the interval $(0, 1)$, or the space

[1] The present paper deals with one or a finite number of pairs of such operators (known as "modes") , a situation that is directly relevant to the "second quantization" of quantum theory, in particular, in quantum optics; see, for instance, Louisell's book [79]. The case of a continuum of modes, which lies at the basis of quantum field theory and is associated with Feynman diagrams [39, 40, 85, 116], is not touched upon here. The developments in our study require a modicum of combinatorial theory but no *a priori* knowledge of quantum physics.

$\mathbb{C}[x]$ of polynomials in indeterminate x), on which two operators, X and D are defined:

$$(Xf)(x) = xf(x); \qquad (Df)(x) = \frac{d}{dx}f(x).$$

Then the creation–annihilation axiom is obviously satisfied by $A = D$ and $B = X$: one recovers in this way the familiar Weyl relations $[D, X] = 1$ of abstract differential algebra [101, Ch. 1]. The interest of such a differential model of creation–annihilation is that it is "*faithful*", meaning that any identity that holds in it (without *any* additional assumption regarding the space of functions) is true in all generality under (1). This differential view will prove central to our combinatorial developments.

We henceforth adopt the more suggestive differential terminology, $A \mapsto D$ and $B \mapsto X$. We shall concern ourselves here with the reduction to normal form of a variety of expressions such as

$$(XD)^n, \quad (X^2D)^n, \quad (D+X)^n, \quad (X^2D^2)^n, \quad (D^2+X^2)^n, \tag{4}$$

and many more. Observe that, by taking an *exponential generating function*, the collection of all the reductions associated with a family $(\mathfrak{H}^n)_{n\geq 0}$ is summarized by the reduction of $e^{z\mathfrak{H}}$.

Our starting point, to be developed in Section 2, is a combinatorial representation of any normal-form monomial $\mathfrak{m} = X^rD^s$ by a basic graph, called a "*gate*". The reduction of a polynomial in operators D, X (for instance, any of (4)) can then be regarded combinatorially as the process of building a whole collection of *diagrams*, which are those special *graphs* assembled from a fixed collection of elementary gates (the ones arising from the monomials in (4)). From here, as we shall see repeatedly, *obtaining the coefficients in the normal form of an operator expression is equivalent to enumerating complex graphs built from a fixed collection of gates.* In other words, we are going to explore the following *Equivalence Principle* (see Theorem 1 below for a precise formulation):

$$\boxed{\begin{array}{c}\textbf{Normal ordering}\\ \text{(operator algebra)}\end{array}} \quad \leftrightsquigarrow \quad \boxed{\begin{array}{c}\textbf{Diagram enumeration}\\ \text{(combinatorics)}\end{array}}.$$

In so doing, we build on classical works in combinatorial analysis relative to the combinatorics of differential operators; see, for instance, Joyal's theory of species [64], its exposition in the book by Bergeron, Labelle and Leroux [7], or the recent book by Flajolet and Sedgewick [47], whose notations we adopt.

The idea of using graphs to model creation–annihilation is not new. The most celebrated originator of the representation of physical processes by graphs is R.P. Feynman, who used it as a convenient book-keeping tool for perturbative expansions of quantum electrodynamics [39, 40] and the whole idea is is neatly articulated by Baez and Dolan in [3, pp. 46–49]. Seen under the interesting perspective of [3], what we propose to do is "decategorize" the abstract creation–annihilation theory by providing concrete combinatorial models of this theory. Our standpoint is however different in that we place a strong emphasis on connections with classical combinatorial structures and aim at developing exactly solvable models, hence explicit formulae. With this in mind, we tread in the steps of earlier works of Blasiak, Duchamp, Horzela, Méndez, Penson, and Solomon [10, 13, 14, 16, 18, 89] for which the present article can serve *inter alia* as a synthetic and systematic review.

$\mathfrak{H}^n$	*Structure*	*Generating function type*	
$(X+D)^n$	involutions	$e^{z^2/2}$	§3
$(XD)^n$	set partitions	e^{e^z-1}	§4
$(X^2+D^2)^n$	alternating cycles (zigzags)	$\frac{1}{\sqrt{\cos(2z)}}$	§5.1
$(X^rD)^n$	increasing trees	$\exp\left(\frac{1}{(1-(r-1)z)^{1/(r-1)}}-1\right)$	§6
$(X^2D)^n$	permutations	$\exp\left(\frac{z}{1-z}\right)$	§6.1

FIGURE 1. Some normal ordering problems relative to $\mathfrak{H}^n$, the corresponding combinatorial structures, a representative counting generating function, and the relevant section in this article.

Our purpose is to shed light on calculations developed within quantum physics and do so by means of adapted combinatorial models. For instance, set partitions (with their associated Bell and Stirling numbers) naturally arise from diagrams corresponding to powers of XD, a fact largely known in combinatorics and finite difference calculus, which is examined, under a quantum field angle, by Bender, Brody, and Meister in [5], and is further treated by Méndez, Blasiak, and Penson in [89]. Also, by providing a complete permutation model, we explain and extend calculations done by Mehta [86] that are relative to the normal ordering of

$$e^{zQ(X,D)}, \qquad \text{where} \quad Q(X,D) = \alpha D^2 + \beta X^2 + \gamma XD$$

Finally, the combinatorial approach we advocate provides, in a number of cases, a transparent alternative to the Lie algebra approach exemplifed by Wilcox [117]. Figure 1 lists a representative set of operators discussed in this paper, together with the underlying combinatorial structures and the corresponding generating function types, as summarized in each case by a prototypical instance.

Plan of the paper. Section 2 presents the basic combinatorial model of gates and diagrams, by which normal ordering is reduced to a counting problems. It also contains a brief reminder of the symbolic approach to combinatorial enumeration via generating functions (§2.4). We then consider the normal ordering problem relative to $\mathfrak{h}^n$ in increasing order of complexity of the polynomial $\mathfrak{h}$. Section 3 concerns the simplest case of linear forms in X, D, for which the natural model is seen to be that of (coloured) *involutions*. In Section 4, we proceed with the special quadratic form (XD), which is tightly coupled with *set partitions*. The general quadratic form in X, D treated in Section 5 leads to *"zigzags"*, which are structures related to *alternating permutations*, and to local order patterns in (unconstrained) permutations. Section 6 shows that semilinear operators of the form $(\phi(X)D)$ are in general modelled by simple varieties of *trees* and *forests*. Section 7 momentarily departs from our main thread and introduces *lattice path* models: it presents a direct treatment of binomial forms, including the interesting "Fermat case" $(X^r + D^r)$, which is conducive to continued fraction representations. Section 8 discusses two frameworks that are closely related to diagrams: one is the rook placement model, for which a general scanning algorithm schema provides an alternative to the methods of Section 7; the other is the planar embedding of diagrams, which leads to a systematic approach to many q–analogues of combinatorial theory. We conclude in Section 9 with a brief discussion of multivariate extensions of the gates-and-diagram model.

The present paper contains few new results. Rather, it is an attempt at a synthetic presentation of the combinatorial approach to normal ordering problems, which has been the subject of an extensive literature in recent decades. What we found striking, when preparing this paper, is the fact that *most (perhaps all?) explicitly known expansions in this orbit of questions can be put in correspondence with classical or semi-classical combinatorial models*. As we hope to demonstrate, one of the interests of the combinatorial approach in this range of problems is to bring clarity into what should be explicit and what is not likely to be.

2. **Diagrams, normal ordering, and enumeration**

In this section, we associate with each polynomial in the operators X, D a finite collection of elementary "*gates*" that are graphs with just one inner vertex, as in (5) below. We then define "*diagrams*" that are complex graphs built by assembling elementary gates according to certain rules. (Our terminology is inspired by that of digital circuits composed of elementary boolean gates.) A fundamental and easy theorem (Theorem 1) then relates the normal ordering of the powers $\mathfrak{h}^n$ of a polynomial $\mathfrak{h}$ to the enumeration of diagrams of size n that can be built out of the gates associated with $\mathfrak{h}$.

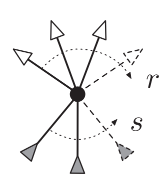
2.1. **Gates and diagrams.**

We make use of the standard definitions of graph theory, as found, for instance, in [29]. We however need to extend it somewhat. Technically, our diagrams are directed multigraphs—edges are directed, multiple edges between two vertices are allowed—that are further enriched by placing an ordering on the edges stemming from a vertex and similarly for edges leading into a vertex. (Put otherwise, we are considering graphs given together with an *embedding* into the plane.) We recall that the *indegree* and *outdegree* of a vertex are, respectively, the number of incoming and outgoing edges of that vertex. In what follows, we freely make use of graphical representations to illustrate our basic notions, while avoiding long formal developments; see Figure 2.

Definition 1. *A* gate *of type* (r, s) *consists of a vertex, called the* inner node*, to which is attached an ordered collection of* r *outgoing edges and an ordered collection of* s *ingoing edges. The vertices, not the inner node, that have indegree* 0 *are called the* inputs*; the vertices, not the inner node, that have outdegree* 0 *are called the* outputs.

A gate thus comprises $r + s + 1$ nodes in total. The input nodes are conventionally coloured in grey, the output nodes in white. For instance:

(5) gate of type (r, s) :



r outputs

s inputs.

In the graphical representation, edges are systematically (and implictly) oriented from bottom to top; they are naturally ordered among themselves, conventionally, from left to right.

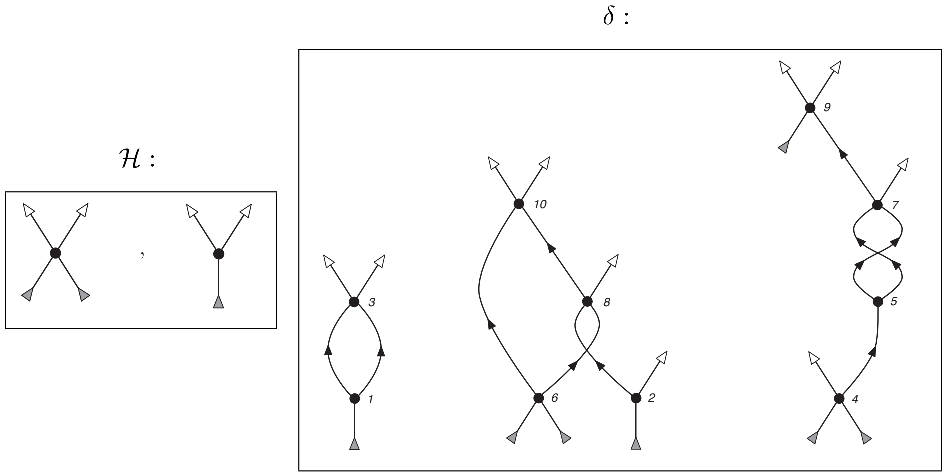


FIGURE 2. Left: a collection $\mathcal{H}$ of two gates of type $(2, 2)$ and $(2, 1)$. Right: a labelled diagram δ on the basis $\mathcal{H}$ that comprises three components.

Definition 2. *A* diagram *is a directed multigraph, which is* acyclic *(i.e., has no directed cycle) and is such that, for each vertex, an ordering has been fixed on its incoming and on its outgoing edges. In addition, there are a designated set of* inputs *(vertices with indegree* 0 *and outdegree* 1*) and a designated set of* outputs *(vertices with indegree* 1 *and outdegree* 0*). The vertices that are neither inputs nor outputs are called* inner nodes. *The* size *of a diagram is the number of inner nodes*[2] *it comprises.*

The colouring convention of gates, as in (5), is extended to the representation of diagrams; see Figure 2 for an instance. Note that a diagram is *not* necessarily connected: it may be comprised of several (weakly connected) *components*. Also, given a set $\mathcal{H}$ of gates, assimilated to a subset of $\mathbb{Z}_{\geq 0} \times \mathbb{Z}_{\geq 0}$, a diagram δ is said to have $\mathcal{H}$ as a *basis* if, for each outdegree–indegree pair (r, s) of an inner node of δ, one has $(r, s) \in \mathcal{H}$.

Finally, we need to introduce a notion of labelling, which is consistent with the standard one of combinatorial analysis [7, 47, 51, 108, 118], to which an additional *monotonicity* constraint is adjoined.

Definition 3. *A* labelled diagram *is comprised of an unlabelled diagram in the sense of Definition 2 together with an assignment of integer labels to inner nodes in such a way that:* (i) *all labels are distinct and they form an initial segment of* $\mathbb{Z}_{\geq 1}$*;* (ii) *labels* increase *along any directed path.*

Note that a labelled diagram can be interpreted as representing the complete *history* of a particular incremental construction of an unlabelled diagram by successively "grafting" gates one after the other (Figure 3), following the order given by the labels—this viewpoint will prove useful in Subsection 2.3. The enumeration

[2] In what follows, we shall discount from size outer nodes (which have size 0) and then often use the terms "vertex" and "inner node" (or simply "node") interchangeably.

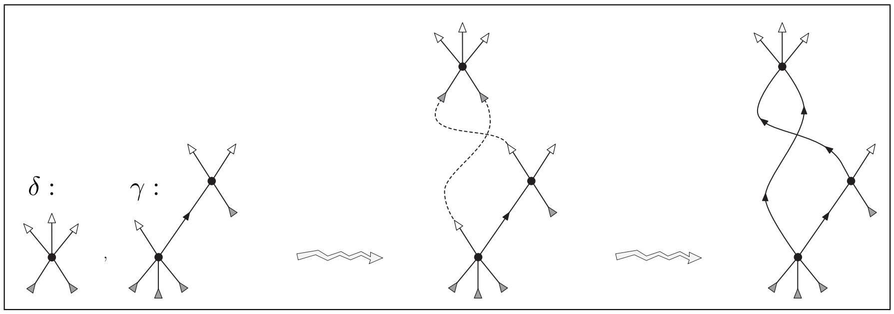


FIGURE 3. A particular grafting of a gate $\delta = X^r D^s$ (here, $r = 3, s = 2$) on a diagram γ corresponding to a term $X^a D^b$ (with $a = 3, b = 4$), in the case where two edges are matched ($t = 2$).

of labelled diagrams corresponding to a fixed basis $\mathcal{H}$ of gates is a central aspect of our approach to the creation–annihilation algebra.

2.2. **The equivalence principle.** We propose to state a general form of the *Equivalence Principle* (Theorem 1 below), in which gates and diagrams can be *weighted.* Fix a field $\mathbb{K}$, called the *domain of weigths*—it may be the field $\mathbb{C}$ of complex numbers, in the case of numeric weights, or a field $\mathbb{C}(x, y, \dots)$ of rational functions in formal variables $x, y, \dots$, in the case of symbolic weights. A *weighting* of a collection $\mathcal{H}$ of gates is an assignment of a weight $w_{r,s} \in \mathbb{K}$ to each gate of $\mathcal{H}$; equivalently, a function $w : \mathcal{H} \longrightarrow \mathbb{K}$. Such a weighting on gates induces a weighting on diagrams: *the weight $w(\delta)$ of a diagram δ is defined to be the product of the weights of the individual gates that the diagram is comprised of.* Finally, the *total weight*[3] of a class $\mathcal{D}$ of diagrams is $\sum_{\delta\in\mathcal{D}} w(\delta)$. With this convention, we state:

Theorem 1 (Equivalence Principle)**.** *Consider a polynomial $\mathfrak{h}$ with normal form*

$$\mathfrak{h} := \sum_{(r,s)\in\mathcal{H}} w_{r,s} X^r D^s. \tag{6}$$

Then the normal ordering of the power $\mathfrak{h}^n$,

$$\mathfrak{N}(\mathfrak{h}^n) = \sum_{n,a,b} c_{n,a,b} X^a D^b, \tag{7}$$

is such that the coefficient $c_{n,a,b}$ coincides with the total weight *of labelled diagrams that admit $\mathcal{H}$ as a basis weighted by w, have size n, and are comprised of $\underline{a}$ outputs and $\underline{b}$ inputs.*

The proof is deferred until the next subsection. The interest of Theorem 1 lies in the fact that it transforms an algebraic normal-ordering problem into a combinatorial enumeration problem, one that may be studied by the methods of combinatorial analysis. It is precisely our aim to explore aspects of this equivalence and the derivation of explicit normal forms, based on combinatorial theory.

We note that Theorem 1 can be rephrased in terms of generating functions. First, by (7), the quantity $\mathfrak{N}(\mathfrak{h}^n)$ is the generating polynomial of labelled diagrams

[3] Thus "total weight" extends the notion of "cardinality" or "number of elements" and determining total weights can be regarded as a (generalized) enumeration problem.

monomial $X^r D^s$	$\leftsquigarrow\rightsquigarrow$	gate of type (r,s)
polynomial $\mathfrak{h}$ in X, D	$\leftsquigarrow\rightsquigarrow$	weighted basis $\mathcal{H}$ of gates
$\mathfrak{h}^n$	$\leftsquigarrow\rightsquigarrow$	labelled diagrams of size n on $\mathcal{H}$
$e^{z\mathfrak{h}}$	$\leftsquigarrow\rightsquigarrow$	all diagrams (exp. generating function)
$(z^n X^a D^b)$	$\leftsquigarrow\rightsquigarrow$	(size $= n$, #outputs $= a$, #inputs $= b$).

FIGURE 4. The correspondences between normal forms of algebraic expressions in X, D, z (*left*) and combinatorial diagrams (*right*).

with X marking outputs, and D marking inputs: as in the case of gates, a diagram with a outputs and b inputs corresponds to a term $X^a D^b$ in the normal form. Introduce next the operator exponential

$$e^{z\mathfrak{h}} := \sum_{n\geq 0} \mathfrak{h}^n \frac{z^n}{n!},$$

which is a formal power series in z with coefficients in the polynomial ring $\mathbb{C}\langle X, D\rangle$ and the corresponding normal form

$$\mathfrak{N}(e^{z\mathfrak{h}}) = \sum_{n\geq 0} \mathfrak{N}(\mathfrak{h}^n) \frac{z^n}{n!}.$$

Then, equation (7) expresses the fundamental identity

$$\mathfrak{N}(e^{z\mathfrak{h}}) = \left(\sum_{n,a,b} c_{n,a,b} u^a v^b \frac{z^n}{n!} \right)_{\left\{ \begin{smallmatrix} u \to X \\ v \to D \end{smallmatrix} \right.} . \tag{8}$$

The sum on the right-hand side is nothing but the *exponential generating function* (EGF) of the total weight (number) of diagrams built on the weighted basis $\mathcal{H}$, where z marks size, u marks the number of outputs, and v marks the number of inputs. In writing such equalities, it is understood that all occurrences of X should be systematically written[4] to the left of all occurrences of D.

Theorem 1 thus expresses a general correspondence between the world of operators and the realm of combinatorics, which is summarized in Figure 4.

2.3. **Proof of the Equivalence Principle (Theorem 1).** For the proof of Theorem 1, a basic observation is the identity

$$(X^r D^s)(X^a D^b) = \sum_{t=0}^{s} \binom{s}{t} \binom{a}{t} t! X^{r+a-t} D^{s+b-t}. \tag{9}$$

[4] Thus, one calculates generating functions of diagrams in the usual way, then, at the end, one should group all occurrences of u before those of v, and finally perform the substitution $u \to X, v \to D$. If $G(z; u, v)$ in the generating function of diagrams, a notation often used by physicists to indicate this process is

$$: G(z; X, D) :$$

which plainly represents a commutative image, with all Xs conventionally preceding all Ds, then interpreted back as an operator in non-commuting X, D.

Without loss of generality, it suffices to consider the case $r = b = 0$. Then, with the interpretation $Df(x) = \frac{d}{dz}f(x)$ and $Xf(x) = xf(x)$, we find, by Leibniz's rule,

$$\begin{aligned}(D^sX^a)f(x) \;\equiv\; D^s(x^af(x)) &= \sum_{t=0}^{s}\binom{s}{t}(D^tx^a)(D^{s-t}f(x))\\ &= \sum_{t=0}^{s}\binom{s}{t}\binom{a}{t}t!x^{a-t}(D^{s-t}f(x)).\end{aligned}$$

The last line implies (9), upon multiplying on the left by X^r and on the right by D^b.

Let now X^aD^b be a monomial that figures explicitly in $\mathfrak{N}(\mathfrak{h}^n)$ and let X^rD^s be a monomial of $\mathfrak{h}$. The reduction to normal form of $\mathfrak{h}^{n+1}$ (viewed as $\mathfrak{h}^{n+1} = \mathfrak{h}\cdot\mathfrak{h}^n$) is obtained by applying the rule (9), then summing over all values $(r, s) \in \mathcal{H}$. Assume now, by induction that the identity (7) of Theorem 1 holds for a certain value of n, so that the coefficients of $\mathfrak{N}(\mathfrak{h}^n)$ count (with suitable weights) all diagrams of size n. The collection of legal diagrams of size $n + 1$ is obtained by grafting in all possible ways a gate of the basis $\mathcal{H}$ on a diagram of size n. If this diagram δ has a outputs and b inputs and the gate γ is of type (r, s), then the number of ways that such a grafting can be effected, when t outputs of δ are plugged into t inputs of γ is exactly

$$\binom{s}{t}\binom{a}{t}t!. \tag{10}$$

(The binomials count the choices of the t inputs of γ and the choices of the t outputs of δ that are matched; the factorial counts the possibilities of attachment.) Figure 3 displays a particular attachment of a gate of type $(3, 2)$ to a connected diagram with 3 outputs and 4 inputs.

It is then observed, from a comparison of (9) and (10) that the multiplicities induced either by a reduction of a left multiplication by X^rD^s or by adding a gate of type (r, s) are the same. Thus, the property that $\mathfrak{N}(\mathfrak{h}^{n+1})$ is the generating function of diagrams of size $n + 1$ with X marking outputs and D marking inputs is established. The property trivially holds for $\mathfrak{N}(\mathfrak{h})$, ensuring the basis of the induction. The proof of Theorem 1 is now complete.

Note 1. *The combinatorics of derivatives and Wick's Theorem.* The usual rule of calculus $Dx^n = nx^{n-1}$ has combinatorial content. For instance, $D(x^4) = 4x^3$ can be obtained as

$$D(xxxx) = \cancel{x}xxx + x\cancel{x}xx + xx\cancel{x}x + xxx\cancel{x},$$

corresponding to the formal rule: *select in all possible ways an occurrence of the variable* (x) *and replace it by a neutral element* (1). This lifts to arbitrary classes of combinatorial objects as a general "pointing–erasing" operation [47, p. 201], which applies to "atoms" (basic components of size 1, such as letters of words or vertices of graphs) that compose combinatorial structures.

Equipped with this combinatorial interpretation of D, we can proceed to revisit the normal form problem. As before X is the operator of multiplication by the variable x (i.e., $(Xf)(x) = xf(x)$, for an arbitrary function $f(x)$). Combinatorially, if f is regarded as representing an arbitrary combinatorial class whose elements are made of x-atoms, then Xf means adjoining—or "creating"— one new atom for each element of f. Consider now the normal form of an expression such as DX^2. It can be obtained by working out what DX^2f is: first X^2f adds two atoms; next, when D is applied, it must either pick up and erase one of these added X atoms or hit and destroy an atom of f. In summary, the external D either "annihilates" one occurrence of a following X or it gets directly applied to f itself. Pictorially,

$$DX^2f = \cancel{D}\cancel{X}Xf + \cancel{D}X\cancel{X}f + DXXf = 2Xf + X^2Df,$$

so that

$$\mathfrak{N}(DX^2) = 2X + X^2D.$$

Similar developments apply to arbitrary monomials in D and X, giving rise to what is known in quantum physics as *Wick's Theorem* and is usually expressed in terms of the annihilation a and creation $a^\dagger$ operators. (Here, we can interpret a as D and $a^\dagger$ as X.)

Proposition 1 (Wick's Theorem)**.** *The normal form of a monomial in X, D equals the sum of all expressions obtained by removing in all possible ways an arbitrary number of pairs $D \ldots X$ of annihilation (D) and creation (X) operators, where D precedes X, then reorganizing the resulting monomials in such a way that all Xs precede all Ds.*

Such a removal is called a *contraction*. An example of a normal form computation in this framework (with $:E:$ representing the commutative reorganization where all Xs precede all Ds, as in footnote(4)) is as follows:

$$\begin{aligned}
DXDDXD \quad = \quad & :\underbrace{DXDDXD}_{\text{no pair removed}}: \\
& + :\underbrace{\cancel{D}\cancel{X}DDXD + \cancel{D}XDD\cancel{X}D + DX\cancel{D}D\cancel{X}D + DXD\cancel{D}\cancel{X}D}_{\text{1 pair removed}}: \\
& + :\underbrace{\cancel{D}\cancel{X}\cancel{D}D\cancel{X}D + \cancel{D}\cancel{X}D\cancel{D}\cancel{X}D}_{\text{2 pairs removed}}: \\
= \quad & X^2D^4 + 4\ XD^3 + 2\ D^2.
\end{aligned}$$

(From here, the proof of Wick's Theorem is immediate: it suffices to proceed by induction on the length of the monomial to be reduced, distinguishing the two cases $\mathfrak{N}(Xw)$ and $\mathfrak{N}(Dw)$, where w in an arbitrary monomial in X, D.)

The procedure that underlies Wick's Theorem may involve a large number of steps, as it amounts to enumerating all possible *sets* of contractions. The computational complexity is thus exponential in the worst case. By contrast, the combinatorial approach based on diagrams provides a graphical means to track down patterns in the diversity of Wick's contractions, which can then be effectively used to achieve a reduction in computational complexity and, in several cases, lead to closed-form solutions.

Next, we can interpret gates in the same vein: D^s corresponds to selecting a sequence of s distinct atoms and replacing each of them by the neutral element, whereas X^r means adding r new atoms. A derivative (D) then "hooks" on atoms (X) or it "jumps" to the right. A particular labelled diagram composed of gates $(\gamma_1, \ldots, \gamma_n)$, with γ_j associated with $X^{r_j}D^{s_j}$, then corresponds to a particular expansion of

$$(X^{r_n}D^{s_n}) \cdots (X^{r_2}D^{s_2})(X^{r_1}D^{s_1}).$$

Identities such as (9) then receive a natural interpretation and the construction of diagrams can be entirely developed in this way from first principles—this approach will be revisted in Section 8, when we discuss the q-difference operator Δ. .... ■

Note 2. *Duality.* There is an easy but important duality in reductions to normal forms. For noncommutative expressions in the two variables X, D, define an *antimorphism* φ by the rules

$$\varphi(X) = D, \quad \varphi(D) = X, \quad \varphi(U \cdot V) = \varphi(V) \cdot \varphi(U), \tag{11}$$

together with an extension to polynomials by linearity. Thus, for a monomial $\mathfrak{m}$, its image $\varphi(\mathfrak{m})$ is obtained by exchanging the rôles of X and D as well as reading letters backwards. It is then observed that the basic quantity $DX - XD - 1$ is invariant under φ. As a

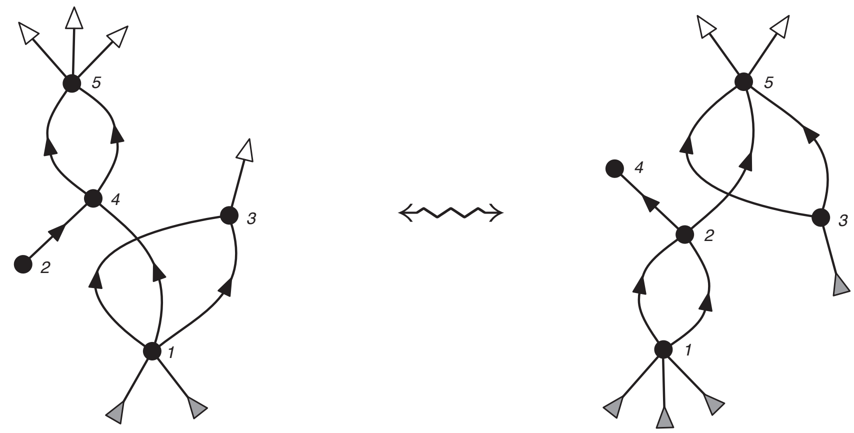


FIGURE 5. A diagram (left) and its dual (right).

consequence, any identity $\mathfrak{U} = \mathfrak{V}$ (modulo $DX - XD = 1$) over terms $\mathfrak{U}, \mathfrak{V}$ in X, D immediately implies a *dual identity* $\varphi(\mathfrak{U}) = \varphi(\mathfrak{V})$.

This duality has a natural graph interpretation. Define the *dual graph* $\widetilde{\Gamma}$ by reverting the arrows in Γ, relabeling the vertices $\bullet$ in reverse order (*i.e.*, $1, 2, ..., n-1, n$ are changed into $n, n-1, ..., 2, 1$ respectively). The result is again a legitimate graph. See Figure 5 for illustration. Clearly, the dual graph is made of a basis of gates that is dual to the one of the original graph.

A consequence of the foregoing considerations is that the normal forms of $\mathfrak{h}^n$ and of $\varphi(\mathfrak{h})^n$ involve the same coefficients, with the coefficient of X^aD^b in $\mathfrak{N}(\mathfrak{h}^n)$ being identical to that of X^bD^a in $\mathfrak{N}(\varphi(\mathfrak{h})^n)$. In this way, for instance, the normal forms we develop below for $(X^2D)^n$ immediately translate to the case of $(XD^2)^n$. (In physical contexts, duality is often associated with hermitian conjugacy; see Mikhailov's article [91, §3] for several examples). .... ■

Note 3. *The combinatorics of Taylor's formula.* Here is a basic illustration of the combinatorics of derivatives. It is well known, from several areas of analysis and the calculus of finite differences[5], that the exponential of a derivative plays the rôle of a translation operator—also known as "shift". Specifically, with the notations of Note 1, we consider the operator

$$T_y := e^{yD}. \tag{12}$$

Symbolically, we have, corresponding to Taylor's formula:

$$T_y \cdot f(x) = \sum_{n\geq 0} \frac{y^n}{n!} D^n f(x) = \sum_{n\geq 0} \frac{y^n}{n!} f^{(n)}(x) = f(x+y). \tag{13}$$

It is piquant to note that the formula admits a transparent combinatorial interpretation, in view of Note 1. Think of $f(x)$ as being the generating function of a class $\mathcal{F}$ of combinatorial objects, themselves composed of atoms represented by x:

$$f(x) = \sum_{\phi\in\mathcal{F}} x^{|\phi|}.$$

---

[5] See, e.g., the treatises of Jordan [60, pp. 13–14] and Milne-Thomson [92, p. 33]. The interest of this symbolic view is *inter alia* to lead to an immediate proof of (a form of) the Euler–Maclaurin summation formula by a computation of $(e^{yD} - 1)^{-1}$; cf [92, p. 260].

The application of the operator $\frac{1}{n!}D^n$ means: "select in all possible ways an unordered collection of n atoms in each elements of $\mathcal{F}$ and replace these by neutral elements". The application of $\frac{1}{n!}y^nD^n$ then translates as follows: "select in all possible ways a collection of n atoms of type x in each elements of $\mathcal{F}$ and replace these by y-atoms". The exponential e^{yD} then corresponds to choosing an *arbitrary* number of x and replacing them by y, the outcome being exactly the bivariate generating function $f(x+y)$. Thus, seen from combinatorics, Taylor's formula

$$f(x+y) = \sum_{n\geq 0} \frac{y^n}{n!} f^{(n)}(x)$$

simply expresses *the decomposition of a bicolouring process according to the number of atoms whose colour is changed.* Figuratively:

$$\text{Bicolour}_{x,y}[\mathcal{F}] \quad \equiv \quad \bigcup_{n=0}^{\infty} \text{"change } n \text{ occurrences of } x \text{ into } y \text{ in elements of } \mathcal{F}(x)\text{"}.$$

(This exercise appears, for instance, explicitly as Note III.31 in [47, p. 201].) .... ■

Note 4. *Normal forms and PDEs.* The reduction of powers of differential operators to normal form is of interest in the analysis of certain types of *partial differential equations* (PDEs). Consider the *initial value problem*, also known as *"Cauchy problem"*,

$$(14) \qquad \begin{cases} \dfrac{\partial}{\partial t}F(x,t) = \Gamma\, F(x,t), & \text{with} \quad \Gamma \in \mathbb{C}[x,\partial], \quad \partial \equiv \partial_x = \frac{\partial}{\partial x} \\ F(x,0) = f(x), \end{cases}$$

where Γ is a differential operator, which is a polynomial in x and ∂_x. The solution is determined by the initial data $f(x)$ at time $t=0$. An equation of this sort is sometimes referred to as an *evolution equation*, with the specific choice of the linear differential operator Γ serving to model various physical contexts. Classical examples, in the one-dimensional case, are the heat equation,

$$(15) \qquad \frac{\partial F}{\partial t} = \frac{\partial^2 F}{\partial x^2},$$

and the Schrödinger equation with time-independent potential $V \equiv V(x)$:

$$(16) \qquad i\hbar\frac{\partial F}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 F}{\partial x^2} + V(x)F.$$

With the notations of (14), introduce the *Ansatz*

$$(17) \qquad F = e^{t\Gamma}\, f,$$

where the operator exponential is classically defined as

$$(18) \qquad e^{t\Gamma} := \sum_{n=0}^{\infty} \frac{t^n}{n!}\Gamma^n.$$

Proceeding formally, we verify that

$$(19) \qquad \frac{\partial F}{\partial t} = \left(\frac{\partial}{\partial t}e^{t\Gamma}\right) f = \Gamma e^{t\Gamma} f = \Gamma\, F,$$

while, by construction, F reduces to f at $t=0$. (Analytically, sound uses of such operator exponentials can be based on the theory of operator semigroups; see, for instance, the book by Engel and Nagel [37], and especially its Chapter 6, for an accessible discussion.)

If now the normal form of the powers Γ^n can somehow be regarded as known,

$$e^{t\Gamma} = \sum_{n=0}^{\infty} \frac{t_n}{n!} A_n, \quad \text{with} \quad A_n = \sum_{\alpha,\beta} a^{(n)}_{\alpha,\beta} x^\alpha \partial^\beta,$$

then, a formal solution of the evolution equation (14) is

$$F(x,t)=\sum_{n=0}^{\infty}\frac{t^n}{n!}\sum_{\alpha,\beta}a^{(n)}_{\alpha,\beta}x^\alpha\partial^\beta f. \tag{20}$$

It is naturally a nontrivial matter to make analytic sense of (20), which often proves to be a *divergent* expansion, but the formal solution (20) should at least provide valuable clues as to the kind of special function involved in the *analytic* solution of the evolution equation (14). . . . . ■

Note 5. *The heat equation.* To illustrate the usefulness of operator calculus, we briefly show how to rederive[6] formally the solution of the heat equation (15) in the present perspective. In accordance with the Ansatz (17), one should consider the operator exponential $e^{t\partial^2}$.

We choose[7] to examine the effect of the exponential-of-the-Laplacian $e^{t\partial^2}$ on the collection of base functions $\{e^{i\omega x}\}$, so that

$$e^{t\partial^2}\cdot e^{i\omega x}=\sum_{n\geq 0}\frac{t^n}{n!}\left((i\omega)^{2n}e^{i\omega x}\right)=e^{-t\omega^2}e^{i\omega x}.$$

Then, if $f(x)$ is a Fourier integral,

$$f(x)=\int_{-\infty}^{+\infty}e^{-i\omega x}\phi(x)\,d\omega,$$

Equation (20) yields by linearity the *formal* solution

$$F(x,t)=\int_{-\infty}^{+\infty}e^{-i\omega x}\left(e^{-t\omega^2}\phi(\omega)\right)\,d\omega.$$

The function $F(\,\cdot\,,t)$ thus appears as the Fourier transform of the product of the two functions $e^{-t\omega^2}$ and $\phi(\omega)$. This, by well known properties of the Fourier transform, which exchanges convolutions and ordinary product, leads (formally still) to the celebrated "heat kernel" solution

$$F(x,t)=\frac{1}{\sqrt{4\pi t}}\int_{-\infty}^{+\infty}\exp\left(-\frac{(x-y)^2}{4t}\right)f(y)\,dy. \tag{21}$$

In this particular case of the heat equation, the normal form problem relative to $(\partial^2)^n$ is trivial. Nonetheless, the derivation above demonstrates the type of usage of operator exponentials, once these can be made sufficiently "explicit". It is one of our goals to develop a combinatorial toolbox for the simplification of such exponentials, which could then serve as a preamble to the analysis of more complicated types of PDEs. . . . . ■

2.4. **Combinatorial enumeration.** Throughout this paper, we appeal to general methods of combinatorial analysis relative to the enumeration of labelled objects and extensively base our discussion on the standard conventions of the book *Analytic Combinatorics* [47, Ch. 2]. If $\mathcal{C}$ is a combinatorial class formed of labelled objects (typically, diagrams), we systematically let $\mathcal{C}_n$ be the subclass of objects of

---

[6] What follows is extremely classical material (see, e.g., [34, pp. 107–109]), only slightly rearranged to suit our needs.

[7] This choice actually corresponds to an eigenfunction expansion in disguise. For instance, if Γ has known eigenvalues $\{\lambda\}$ with eigenfunctions $\{v(x)\}$, then $e^{t\Gamma}\,v(x)=e^{t\lambda}v(x)$, from which solutions can be composed by linearity.

size n, with C_n the corresponding cardinality. The *exponential generating function* (EGF) of the class is

$$C(z) := \sum_{n\geq 0} C_n \frac{z^n}{n!} = \sum_{c\in\mathcal{C}} \frac{z^{|c|}}{|c|!}.$$

What we want to do is construct complex combinatorial classes from simpler ones. The initial classses include the *atomic class* $\mathcal{Z}$, which comprises a single element of size 1 and has EGF z, as well as the neutral class $\mathcal{E}$, which consists of a single element of size 0 and has EGF 1

Disjoint unions, henceforth written plainly as '+', clearly correspond to sums of EGFs:

$$\mathcal{C} = \mathcal{A} + \mathcal{B} \qquad \Longrightarrow \qquad C(z) = A(z) + B(z). \tag{22}$$

The *labelled product* $\mathcal{C} = \mathcal{A} \star \mathcal{B}$ of two labelled classes is obtained by taking all the ordered pairs (α, β), with $\alpha \in \mathcal{A}$ and $\beta \in \mathcal{B}$, then relabelling them in all order-consistent ways so as to obtain a well-labelled pair (α', β'). We then have the correspondence

$$\mathcal{C} = \mathcal{A} \star \mathcal{B} \qquad \Longrightarrow \qquad C(z) = A(z) \cdot B(z). \tag{23}$$

It is then possible to form the class of all (labelled) *sequences* ('SEQ'), *sets* ('SET'), and *cycles* ('CYC') with components in $\mathcal{A}$, the corresponding EGFs being given by the following dictionary:

$$\left\{\begin{array}{lll} \mathcal{C} = \textsc{Seq}(\mathcal{A}) & \Longrightarrow & C(z) = \dfrac{1}{1 - C(z)} \\ \mathcal{C} = \textsc{Set}(\mathcal{A}) & \Longrightarrow & C(z) = \exp(C(z)) \\ \mathcal{C} = \textsc{Cyc}(\mathcal{A}) & \Longrightarrow & C(z) = \log \dfrac{1}{1 - C(z)}\,. \end{array}\right. \tag{24}$$

These basic constructions suffice to transcribe the normal form problem in simpler cases such as $(X + D)$ in Section 3 and (XD) in Section 4.

Finally, we shall need the modified *"boxed product"* construction, $\mathcal{C} = (\mathcal{A}^\square \star \mathcal{B})$, which corresponds to the subset of ordered pairs $(\alpha, \beta) \in (\mathcal{A} \star \mathcal{B})$, such that the *smallest* label is constrained to belong to the α component; see Greene's thesis [54], as well as the accounts in [7, Ch. 7] and [47, §II.6.3]. The translation rule from constructions to EGFs is

$$\mathcal{C} = (\mathcal{A}^\square \star \mathcal{B})\,, \quad \Longrightarrow \quad C(z) = \int_0^z \left(\frac{d}{dt} A(t)\right) \cdot B(t)\, dt. \tag{25}$$

This covers in particular the *min-rooting* operation, which attaches an external atom to a $\mathcal{B}$–structure and assigns to it the smallest label: the construction is simply $(Z^\square \star \mathcal{B})$ and it corresponds to an integration operator $\int_0^z B(t)\, dt$. The same translation applies to the dual boxed product $\mathcal{C} = (\mathcal{A}^{\blacksquare} \star \mathcal{B})$, where it is now the *largest* label that is constrained to belong to the $\mathcal{A}$-component. We shall make much use of these constructions, which correspond to a decomposition according to the first or last gate of a diagram: they are used typically in Section 5, relative to $(X^2 + D^2)$, and Section 6, relative to $(X^2 D)$.

All the rules above extend to *multivariate* generating functions: these contain extra parameters, which can keep track of various additive characteristics of structures [47, Ch. III].

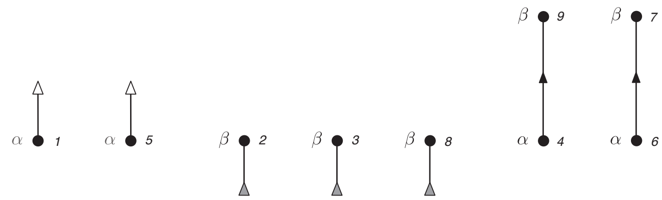


FIGURE 6. A particular $(X+D)$–diagram.

In the next sections, we are precisely going to make use of the dictionary formed by (22), (23), (24), and (25) in order to enumerate various classes of diagrams associated (via Theorem 1) with the normal ordering of terms in the operators X, D.

3. **Linear forms $(X + D)$, involutions, and generalizations**

This section is dedicated to the normal ordering of expressions of the form $(a(X) + D)^n$ and $(a(D) + X)^n$, with $a(\,\cdot\,)$ a polynomial, starting with the easier case $(X + D)^n$. Thus, the schema is that of a base form in X and D, which is linear in at least one of the operators X, D. The combinatorial models turn out to be *special coloured permutations* (involutions and generalizations), for which the introduction of diagrams easily leads to fully explicit forms.

3.1. **The basic linear case** $(X + D)$**.** Linear forms in the operators X and D, namely, operators of the form

$$\Gamma = \alpha X + \beta D,$$

can serve to illustrate the usefulness of diagrams with minimal apparatus. In accordance with the developpements of Section 2, we are talking here of diagrams based on two types of gates: a gate X has no input and one output; a gate D has one input and no output:

By inspection of all the possible ways of assembling gates, it is immediately seen that a diagram must be comprised of three types of components: isolated X–gates, isolated D–gates, and pairs DX, where a D is hooked to an earlier arrived X. In the labelled case, the isolated X and D may receive arbitrary labels, while the "saturated" DX pairs are only constrained by the fact that the label of the X is smaller than the label of the D; see Figure 6.

Combinatorially, the class of all diagrams is thus specified by

$$\mathcal{G} = \mathrm{SET}(\alpha\mathcal{Z} + \beta\mathcal{Z} + \alpha\beta\,\mathrm{SET}_2(\mathcal{Z})),$$

when the multiplicative weights α, β are taken into account. Here, the $\textsc{Set}_2$ construction[8] describes an unordered pair of two labels whose arrangement is immaterial: the smaller label is necessarily attached to an X-gate, the larger one to a D-gate; see Figure 6. The generating function of all weighted diagrams is accordingly

$$G(z) = e^{(\alpha+\beta)z+\alpha\beta z^2/2}. \tag{26}$$

An equivalent way of phrasing this result is as an equality,

$$\mathfrak{N}\left(e^{z(\alpha X+\beta D)}\right) = e^{\alpha\beta z^2/2} \cdot e^{\alpha z X} \cdot e^{\beta z D}, \tag{27}$$

where the right-hand side is to be interpreted as a standard expansion in the commuting indeterminates X, D. A straight expansion then yields an explicit form of (27),

$$\sum_{k,\ell,m\geq 0} \frac{z^{2k}}{2^k\, k!}(\alpha\beta)^k \frac{z^\ell}{\ell!}\alpha^\ell X^\ell \frac{z^m}{m!}\beta^m D^m,$$

which, after collection of the coefficient of z^n, can be summarized as follows[9].

Proposition 2. *The normal form of $(\alpha X+\beta D)^n$ satisfies*

$$\mathfrak{N}\left((\alpha X+\beta D)^n\right) = \sum_{\ell,m} I_{\ell,m}^{(n)} X^\ell D^m,$$

where, for $n-\ell-m$ odd, the coefficients $I_{\ell,m}^{(n)}$ are 0, while, for $n-\ell-m$ even, they satisfy

$$I_{\ell,m}^{(n)} = \frac{n!}{2^{(n-\ell-m)/2}((n-\ell-m)/2)!\,\ell!\,m!}\alpha^{(n+\ell-m)/2}\beta^{(n+\ell+m)/2}.$$

In combinatorics, a permutation σ containing only cycles of sizes 1 and 2 is known as an *involution* (it satisfies $\sigma^2 = \mathbf{1}$). The specification and exponential generating functions are accordingly

$$\mathcal{I} = \textsc{Set}(\mathcal{Z} + \textsc{Cyc}_2(\mathcal{Z})), \qquad I(z) = e^{z+z^2/2};$$

see, e.g., [47, p. 122]. The numbers $I_{\ell,m}^{(n)}$ therefore enumerate coloured involutions, where singleton cycles can receive any one of two colours (corresponding either to an X or a D). In other words: *the natural combinatorial model for the normal ordering of $(X+D)^n$ is that of (bicoloured) involutions.*

The classical result expressed by Proposition 2 is usually derived in the context of Lie groups by means of the Baker–Campbell–Hausdorff formula [50, 55], since, in this case, nested Lie brackets of higher order vanish. Indeed, it is known in this theory that, if the commutator $C = [A, B]$ commutes with both A and B, one has the general identity[10] (see [50, p. 463] and [55, p. 64]):

$$e^{z(A+B)} = e^{zA} \cdot e^{z^2/2[B,A]} \cdot e^{zB}.$$

[8] In this particular case, a $\textsc{Cyc}_2$ construction can equivalently be used, given the obvious combinatorial isomorphism $\textsc{Set}_2(\mathcal{Z}) \cong \textsc{Cyc}_2(\mathcal{Z})$.

[9] Proposition 2 is a classical result: it is for instance derived by means of operator calculus methods in Wilcox's paper [117, Eq. (10.43)], published in 1967.

[10] Formulae of this sort are sometimes known as "disentanglement formulae" [26].

Note 6. *Solution of a special PDE by normal ordering of* $(X+D)^n$. The partial differential equation of interest is

$$\frac{\partial F}{\partial t} = \frac{\partial F}{\partial x} + xF, \tag{28}$$

with initial value condition $F(x,0) = f(x)$. This is of the form considered when discussing operator exponentials in Note 4, p. 12, here with $\Gamma = (X+D)$. The operator solution $e^{t\Gamma} f$, under the normal ordering provided by Equation (27) above, becomes

$$e^{t\Gamma} f = e^{t^2/2} \cdot e^{tx} \cdot e^{tD} f.$$

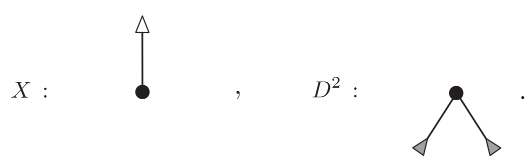
We know (from the earlier Note 3, p. 11) that the exponential of a derivative is a shift, $e^{tD} f(x) = f(x+t)$, so that the solution to (28) is the fully explicit

$$F(x,t) = e^{t^2/2+xt} f(x+t), \tag{29}$$

whose validity is easily checked directly.

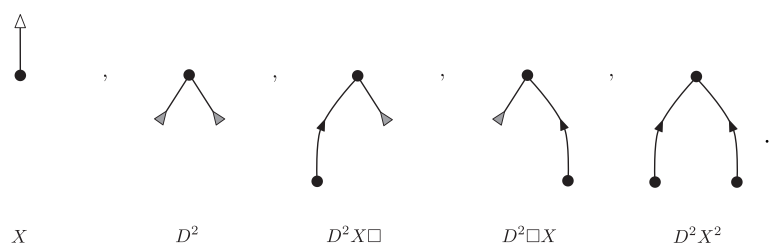
No claim is made that the PDE (28) is hard to solve, and, indeed, it succumbs easily to the method of characteristics, which is generally applicable to linear and quasilinear PDEs [109, §1.15]. It is nonetheless instructive to observe the way the reduction to normal ordering (with the right factor e^{tD}) could automatically put us on the tracks of a general solution. . . . . ■

3.2. **Generalizations to** $(X + D^r)$ **and** $(X^r + D)$**.** We next examine the case of the operator $(X + D^2)$. According to the main theorem, one should consider diagrams built out of two types of gates: D^2–gates have two inputs and no output; X–gates have, as usual, one output and no input:



It is then easily realized that the only possibilities for connected diagrams are given by the following list:

(30)



For instance, D^2X^2 represents a connected component that is "saturated", in the sense that the two inputs of a D^2–gate are connected to the (earlier arrived) outputs of two X–gates; similarly, $D^2X\Box$ depicts a component, for which the output of an X–gate is plugged into the first input of a D^2–gate, while the second input remains free; and so on.

We can then look at the balance of inputs and outputs corresponding to each of the gates of the list (30). For instance, a $D^2X\Box$ component has one input gate (a dangling D) and no output, so that it is equivalent to a D, in terms of the balance between number of inputs and number of outputs. Proceeding systematically, we determine the following table for all the possible types of connected components:

(31)

type :	D^2	X	$D^2\square X$	$D^2X\square$	D^2X^2
size :	1	1	2	2	3
balance :	D^2	X	D	D	1.

Next, we should examine the number of ways of placing labels on connected components. In the case of a $D^2\square X$ or $D^2X\square$, the size equals 2, but the D^2–gate is necessarily associated with the largest label; thus, any such component is a $\text{SET}_2(\mathcal{Z})$, itself combinatorially equivalent to a $\text{CYC}_2(\mathcal{Z})$. In the case of a saturated component D^2X^2, two possible orderings are to be considered, since the first input of D^2 is associated with either the earlier arrived X or with the later X; in this case, the component turns out to be equivalent to a $\text{CYC}_3(\mathcal{Z})$. Thus, using now, as standard *commuting* formal variables, u to mark components with a dangling output (X) and v to mark components with a dangling input (D), we have, for the various components, the specifications:

(32)

type :	D^2	X	$D^2\square X$	$D^2X\square$	D^2X^2
specification :	$v^2\mathcal{Z}$	$u\mathcal{Z}$	$v\,\text{CYC}_2(\mathcal{Z})$	$v\,\text{CYC}_2(\mathcal{Z})$	$\text{CYC}_3(\mathcal{Z})$.

There results that the class of all diagrams is described by

$$\mathcal{G} = \text{SET}\left(v^2\mathcal{Z} + u\mathcal{Z} + v\,\text{CYC}_2(\mathcal{Z}) + v\,\text{CYC}_2(\mathcal{Z}) + \text{CYC}_3(\mathcal{Z})\right),$$

with corresponding EGF

$$G(z;u,v) = \exp(v^2z + uz + vz^2/2 + vz^2/2 + z^3/3). \tag{33}$$

In other words, the model is now that of *(multicoloured) permutations, all of whose cycles are of length at most three, where, in addition, singletons and doubletons can be of any of two colours.*

The very same reasoning applies to the normal ordering of $(X^2+D)^n$. The diagrams are isomorphic to the earlier ones, with inputs and outputs being exchanged and time being reversed. That is, the rôles of X and D in (33) are simply to be exchanged—this is a special case of the general *duality* discussed in Note 2, p. 10. In summary:

Proposition 3. *The normal orderings corresponding to the base operators (D^2+X) and (X^2+D) satisfy*

$$\begin{cases} \mathfrak{N}\left(e^{z(D^2+X)}\right) & = & e^{z^3/3+zX}\cdot e^{z^2D+zD^2} \\ \mathfrak{N}\left(e^{z(X^2+D)}\right) & = & e^{z^3/3+z^2X+zX^2}\cdot e^{zD}. \end{cases} \tag{34}$$

Finally, the explicit normal forms associated with $(D+a(X))$ and $(X+a(D))$, for $a(\,\cdot\,)$ a polynomial, are accessible via a combinatorial calculus that suitably extends (31) and (32): the combinatorial model now involves permutations with cycles of length at most r. We leave it as an exercise to the reader to work out details and state[11]:

[11] Mikhailov [90] has a simple proof based on operator algebra in [90], and he refers to earlier works of Witschel (1975) and Yamazaki (1952).

Proposition 4. *The normal ordering corresponding to the base operators $(a(D)+X)$ and $(a(X)+D)$ are given by*

$$\left\{\begin{array}{lcl} \mathfrak{N}\left(e^{z(a(D)+X)}\right) & = & e^{zX}\cdot\exp\left(\int_0^z a(v+w)\,dw\right)\Big|_{v\mapsto D} \\ \mathfrak{N}\left(e^{z(a(X)+D)}\right) & = & \exp\left(\int_0^z a(X+w)\,dw\right)\cdot e^{zD}. \end{array}\right. \tag{35}$$

In the pure binomial case of (D^r+X) and (X^r+D), the normal forms further simplify[12] as

$$\left\{\begin{array}{lcl} \mathfrak{N}\left(e^{z(D^r+X)}\right) & = & e^{zX}\cdot\exp\left(\frac{1}{r+1}\left[(D+z)^{r+1}-D^{r+1}\right]\right) \\ \mathfrak{N}\left(e^{z(X^r+D)}\right) & = & \exp\left(\frac{1}{r+1}\left[(X+z)^{r+1}-X^{r+1}\right]\right)\cdot e^{zD}, \end{array}\right.$$

which gives back (27) and (34), when $m=1,2$.

Note 7. *Another PDE.* The usual consequences for PDEs also hold, with the further simplification that e^{tD} is a shift and that, for the quadratic case at least, the exponential of the Laplacian can be made explicit in the Fourier basis of complex exponentials. For instance, the general PDE schema

$$\frac{\partial F}{\partial t}=\frac{\partial F}{\partial x}+a(x)F,$$

admits the solution

$$F(x,t)=e^{Q(x,t)}f(x+t),\qquad Q(x,t):=\int_0^t a(x+w)\,dw.$$

In particular, $a(x)=x^2$ corresponds to $Q(x,t)=t^3/3+tx^2+t^2x$. .... ■

4. The special quadratic form (XD), set partitions, and derivative products

This section is dedicated to the normal ordering of the powers $(XD)^n$, a problem which has been recognized for a long time to be tightly coupled to set partitions and Stirling numbers of the second kind. In Appendix A, we summarize the main results contained in the rather remarkable thesis memoir of Heinrich Scherk, defended in 1823: the reduction of $(XD)^n$ figures there explicitly! We also consider, in this section, the related quadratic form $XD+g(X+D)$. Finally, we show that the combinatorial approach advocated here extends rather easily to powers of operators such as X^2D^2, X^3D^3, and so on, which relates to several combinatorial enumeration problems of independent interest.

4.1. **The form (XD) and set partitions.**

By the general isomorphism theorem, the operator (XD) corresponds to a gate with one input and one output:

XD :

With these, we can form chains where the input of an XD–gate is connected to the output of a previously arrived XD–gate. When time stamps are put on the

[12] These formulae have also been found independently by Karol Penson (unublished, 2004).

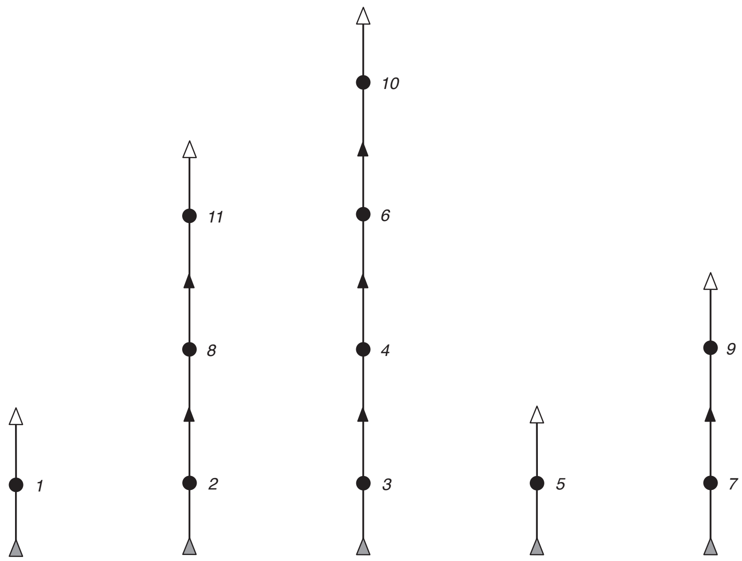


FIGURE 7. A particular diagram associated with (XD).

vertices of the gates, a connected component becomes an increasing linear graph (see, e.g., [47, p. 99]), in the sense that vertices are linearly arranged and labelled in increasing order, with the additional condition that size needs to be at least one: see Figure 7. Representing chains (connected components) from bottom to top, here is a particular representation—edges between adjacent elements, which are redundant, are omitted:

$$\begin{array}{ccccc} & & 10 & & \\ & 11 & 6 & & \\ & 8 & 4 & & 9 \\ 1 & 2 & 3 & 5 & 7. \end{array}$$

Under this form one recognizes the classical structure of set partitions, where a partition of a set is a subdivision of the elements of the set into indistinguishable non-empty *classes*, also known as "blocks" [23, 47, 53]. (Here the components have been presented in increasing order of their leading elements.)

Components can be equivalently regarded as non-empty unordered collections of labels (non-empty "urns" in the terminology of [47, p. 99]); that is, they are specified by $\mathcal{K} = \textsc{Set}_{\geq 1}(\mathcal{Z})$. An arbitrary graph built out of XD–gates is then an unordered collection of such components, so that the corresponding class is $\textsc{Set}(\mathcal{K})$. With z marking the size of a graph (its number of gates, equivalently, vertices) and u marking the number of connected components (here equal to the number of inputs *and* to the the number of outputs), we thus have for diagrams the specification

$$\mathcal{G} = \textsc{Set}\left(u\,\textsc{Set}_{\geq 1}(\mathcal{Z})\right),$$

hence the corresponding generating function

$$G(z,u) = e^{u(e^z-1)}. \tag{36}$$

The generating functions solve the corresponding enumeration problems. By an expansion of (36) taken at $u = 1$, the total number ϖ_n of partitions of a set of cardinality n satisfies the "Dobiński relation"

$$\varpi_n = n![z^n]e^{e^z-1} = e^{-1}\sum_{\ell\geq 0}\frac{\ell^n}{\ell!}, \tag{37}$$

a quantity known in combinatorics as a *Bell number* [23]. The number of partitions of n elements into k classes is the *Stirling number of the second kind*, nowadays usually denoted by $\left\{{n \atop k}\right\}$, whose value is [23, 47, 53]

$$\left\{{n \atop k}\right\} = n![z^n u^k]e^{u(e^z-1)} = \frac{n!}{k!}[z^n](e^z-1)^k = \frac{1}{k!}\sum_{j=0}^{n}\binom{k}{j}(-1)^{k-j}j^n, \tag{38}$$

as can be immediately verified from a series expansion of (37).

Back to the normal ordering problem, each connected component of a diagram, i.e., each chain of XD–gates, has one input and one output, so that the balance of a single component is of the form XD, the balance of k components being accordingly X^kD^k. We then have:

Proposition 5. *The normal ordering associated with $e^{z(XD)}$ involves the Stirling partition numbers:*

$$\begin{aligned}\mathfrak{N}\left(e^{z(XD)}\right) &= e^{u(e^z-1)}\Big|_{\langle u^k\mapsto X^kD^k\rangle} \\ &= \sum_{n\geq 0}\frac{z^n}{n!}\left[\sum_k\left\{{n \atop k}\right\}X^kD^k\right] \quad = \quad \sum_{k\geq 0}\frac{1}{k!}\left(e^z-1\right)^k X^kD^k.\end{aligned} \tag{39}$$

Note 8. *Yet another PDE.* Proceeding as before, we obtain from (39), that the PDE

$$\frac{\partial F}{\partial t} = x\frac{\partial F}{\partial x}$$

with initial condition $F(x,0) = f(x)$ possesses the solution

$$F(t,x) = \sum_{k\geq 0}(e^t-1)^kX^k\frac{D^k}{k!}f(x) = f(x(e^t-1)+x) = f(xe^t),$$

whose *a posteriori* verification is immediate. .... ■

Note 9. *History.* The origin of the Stirlng partition numbers $\left\{{n \atop k}\right\}$ and their cognates, the Sirling cycle numbers $\left[{n \atop p}\right]$, lies in eighteenth century calculus. The classical way of defining them is as the coefficients expressing, in the polynomial algebra $\mathbb{C}[x]$, the change of basis between the canonical basis x^n and the factorial basis $x^{\underline{n}} \equiv x(x-1)\cdots(x-n+1)$ or its trivial variant $x^{\overline{n}} = x(x+1)\cdots(x+n-1)$. Indeed, one has [53, pp. 248–249]:

$$x^n = \sum_k\left\{{n \atop k}\right\}x^{\underline{k}}, \qquad x^{\overline{n}} = \sum_k\left[{n \atop k}\right]x^k\,. \tag{40}$$

(In a different circle of ideas, Stirling numbers are known to probabilists as a way of relating factorial moments and standard power moments [28, p. 47].) Upon examining the effect on coefficients of power series, it is then seen that Stirling coefficients serve to express the connection between powers $(x\partial_x)^n$ and standard derivatives, via $x^k\partial_x^k$, which is exactly what we derived by elementary combinatorics in (39). An equivalent operator

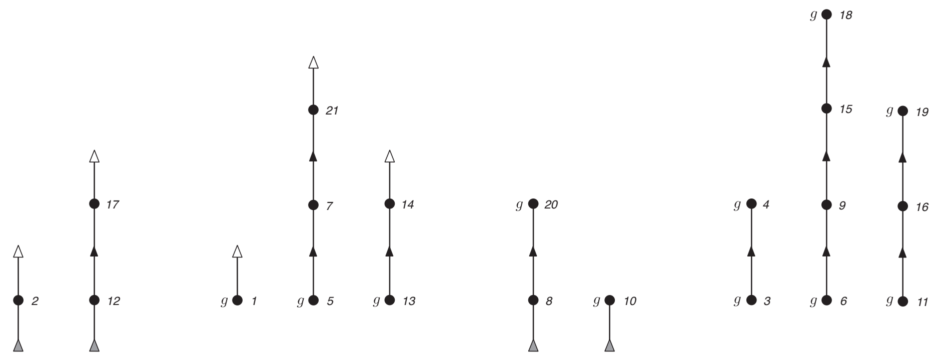
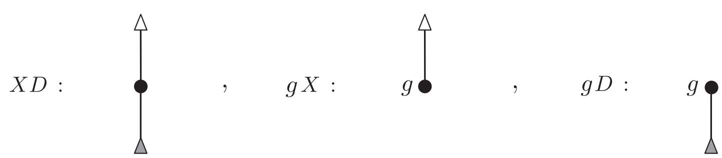


FIGURE 8. A sample diagram associated with $(XD+g(X+D))$.

formulation appears as an exercise[13] in Comtet's book [23, Ex. 2, p. 220]. (Some of these properties were already familiar to Scherk in 1823; cf Appendix A, p. 64.)

In the context of quantum physics, the combinatorial connections between the normal ordering of $(a^\dagger a)^n$ and Stirling numbers have been recognized early: see, for instance, the papers of Wilcox [117, p. 978], for an algebraic perspective, and especially Katriel [67], for the combinatorial connection. (See also references therein to earlier works by Schwinger and others.) This thread has given rise to a large body of subsequent literature. In particular, Bender, Brody, and Meister explicitly discuss Bell numbers in the context of diagrams in [5], although their approach differs substantially from ours, as they focus on interpretations of the schema $e^{\phi(D)}e^{\xi(X)}$. The relations between set partitions, diagrams and Stirling numbers are used as a lead example by Baez and Dolan [3] to illustrate the process of "decategorifying" (!) the creation–annihilation theory. We examine below, in Subsection 4.2, further interesting extensions of the combinatorial approach that are due to Blasiak *et al.* . . . . ■

Note 10. *Normal forms relative to* $(XD+g(X+D))$. We briefly discuss this case, which is treated by Wilcox [117] and Louisell [79] by means of operator calculus, as it illustrates the versatility of the combinatorial method. The gates are now of the three types X, D and XD:



The connected components are similar to those relative to (XD), with, in addition, the possibility that a line graph can be "capped" with a D, or "cupped" with an X, or both capped and cupped; they are consequently of *four* possible types, see Figure 8. Hence, one can write directly the specification of graphs as

$$\mathcal{G} = \text{SET}\left((uv+ug+vg)\,\text{SET}_{\geq 1}(\mathcal{Z}) + g^2\,\text{SET}_{\geq 2}(\mathcal{Z})\right),$$

where u and v mark inputs and outputs, respectively. The corresponding multivariate EGF is then

$$G(z;u,v) = e^{(x+g)(y+g)(e^z-1)}e^{-g^2 z}.$$

[13] This interesting exercise also contains the reduction of $(X^{a+1}D)^n$ and its connection with $\{(1-at)^{1/a}-1\}$ [with the minor typo of a missing exponent of n], which we shall encounter later in Section 6; see also Riordan [98, §6.6] for related operational calculus derivations.

(This case prefigures the planted-tree construction of Subsection 6.3, p. 39.) .... ■

4.2. **The product form** (X^2D^2)**.** This subsection and the next one serve to revisit the combinatorial works of Blasiak, Horzela, Penson, Solomon, and coauthors [10, 14, 17, 18, 89]. See also Schork's synthetic study [103], which furthermore includes some q-analogues. To avoid cumbersome notations, we start with a discussion of the operator X^2D^2. What is at stake is understanding the structure of reductions such as

$$\left\{\begin{array}{lcl} (X^2D^2) & = & X^2D^2 \\ (X^2D^2)^2 & = & 2X^2D^2 + 4X^3D^3 + X^4D^2 \\ (X^2D^2)^3 & = & 4X^2D^2 + 32X^3D^3 + 38X^4D^4 + 12X^5D^5 + X^6D^6, \end{array}\right. \tag{41}$$

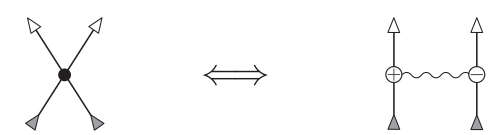
where the sums of the coefficients form a sequence $\varpi_n^{2,2}$, which starts as

$$(\varpi_n^{2,2}) = 1, 7, 87, 1657, 43833, 1515903, 65766991, 3473600465, \dots . \tag{42}$$

These numbers appear as Sequence *OEIS* **A020556** in Sloane's *Online Encyclopedia of Integer Sequences* [104], henceforth abbreviated as "*OEIS*". The triangle of coefficients in the expansion of powers of (X^2D^2) as in (41) is Sequence *OEIS* **A078739**.

By the combinatorial isomorphism, we now have one kind of gate, namely, X^2D^2; that is, a gate has two input edges and two output edges. Such a gate thus picks up two previously existing outgoing edges and generates two new outgoing edges, the local balance of the number of links (edges) being clearly null; in other words, we can view a gate as simply "propagating" two existing links. It is then of advantage to align edges vertically and represent an X^2D^2–gate by a horizontal vector: the orientation conventionally serves to distinguish the first input from the second input; these inputs can be conveniently tagged by a $\oplus$ and a $\ominus$ sign, respectively, as in the following diagram:

(43) X^2D^2 :



When such gates are stacked on top of one another, they then give rise to piles of vectors that can be viewed as (weird!) "scaffoldings"; see Figure 9. (This structure is loosely evocative of Viennot's theory of "heaps of pieces" [114].)

Bilabelled structures. Let $\mathcal{S}_{n,k}$ be the collection of all diagrams comprised of n gates of type X^2D^2 that have k inputs and let $\left\{ {n \atop k} \right\}_{2,2} \equiv S_{n,k}$ be the corresponding cardinality. We consider the class $\mathcal{S}_k = \bigcup_n \mathcal{S}_{n,k}$, which it is now our goal to enumerate. This can be achieved by considering *bilabelled* objects, that is, objects carrying two kinds of labels. In the case at hand, we consider the extended class $\widehat{S}_k$, where *inputs* bear independent labels, $1', \dots, k'$, which are indicated by a prime ("primed"), in order to distinguish them from the usual gate/vertex labels. The labelled product extends trivially—distribute independently both types of labels. It translates straightforwardly as a product of *biexponential generating functions*, of the form

$$f(z, \zeta) = \sum_{n,\nu} f_{n,\nu} \frac{z^n}{n!} \frac{\zeta^\nu}{\nu!}, \tag{44}$$

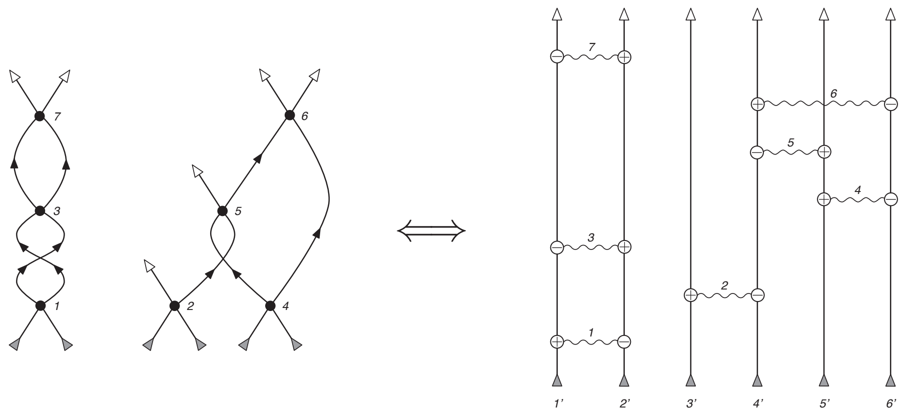


FIGURE 9. The scaffolding representation of an X^2D^2 graph.

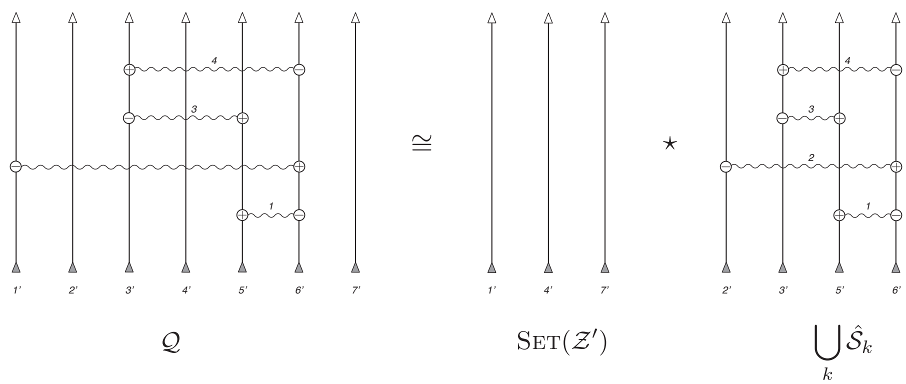


FIGURE 10. A graphical rendering of the isomorphism expressed by (45): on the left appear "relaxed" scaffoldings; on the right the product form that isolates unused inputs and a proper scaffolding.

where the powers of z and ζ record, respectively, the number of standard and primed labels.

Let $\widehat{\mathcal{S}}_{n,k}$ be the class of diagrams of size n with k labelled inputs. In terms of cardinalities, we have $\widehat{S}_{n,k} = k! S_{n,k}$. (Indeed, in a standard, singly labelled diagram of $\mathcal{S}_{n,k}$, all inputs are *distinguishable*, say, according to the time they are first used, and by considering the first input, tagged "$\oplus$", before the second one, tagged "$\ominus$"; there are thus exactly $k!$ ways to superimpose an input labelling on a diagram.) We then claim the identity

$$\mathcal{Q} = \textsc{Set}(\mathcal{Z}') \star \left(\bigcup_k \widehat{\mathcal{S}}_k \right) \tag{45}$$

Here, $\mathcal{Z}'$ represents an atom that carries a primed label, but no standard ("unprimed") label; the class $\mathcal{Q}$ is a relaxed version of $\bigcup_k \widehat{\mathcal{S}}_k$ in which extra (primed–labelled) inputs are allowed; the labelled product '$\star$' is, in accordance with our previous discussion, taken to distribute both kinds of labels.

In order to justify (45), observe that the left hand side describes all possible sequences of choices of pairs of distinct prime-tagged elements amongst a set of cardinality k, with the possibility of some of the elements to be unused; the factor $\mathrm{SET}(\mathcal{Z}')$ in the right hand side simply gathers all these unused inputs, with the sum there corresponding to legal (bilabelled) diagrams; see Figure 10.

We next effect the translation into bivariate generating functions, here taken to be of the form (44). Thus, z records gates and ζ records inputs. (Note the subtle difference between ζ, as a carrier of primed labels, and u, as a plain unlabelled marker in earlier developments relative to (XD).) By the definition of $\mathcal{Q}$, we have

$$Q(z,\zeta) = \sum_{n,k=0}^{\infty} [k\cdot(k-1)]^n \frac{\zeta^k}{k!}\frac{z^n}{n!}.$$

Equation (45) then translates as the biexponential generating function identity

$$e^{\zeta} \sum_{n,k=0}^{\infty} k! S_{n,k} \frac{\zeta^k}{k!}\frac{z^n}{n!} = \sum_{n,k=0}^{\infty} [k\cdot(k-1)]^n \frac{\zeta^k}{k!}\frac{z^n}{n!},$$

which solves to give explicitly (with $\left\{ {n \atop k} \right\}_{2,2} \equiv S_{n,k}$)

$$\sum_{n,k=0}^{\infty} \left\{ {n \atop k} \right\}_{2,2} \zeta^k \frac{z^n}{n!} = e^{-\zeta} \sum_{n,k=0}^{\infty} [k\cdot(k-1)]^n \frac{\zeta^k}{k!}\frac{z^n}{n!}. \tag{46}$$

Collecting the coefficient of z^n and expanding the result as a binomial convolution leads to the following statement [18].

Proposition 6. *The normal ordering associated to $e^{z(X^2D^2)}$ satisfies*

$$\mathfrak{N}\left(e^{z(X^2D^2)}\right) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \sum_k \left\{ {n \atop k} \right\}_{2,2} X^k D^k, \tag{47}$$

where the generalized Stirling numbers $\left\{ {n \atop k} \right\}_{2,2}$ are

$$\left\{ {n \atop k} \right\}_{2,2} = \frac{1}{k!} \sum_{j=2}^{k} (-1)^{k-j} \binom{k}{j} [j\cdot(j-1)]^n. \tag{48}$$

This calculation also implies a Dobiński-type formula for the generalized Bell numbers of (42),

$$\varpi_n^{2,2} = e^{-1} \sum_{\ell\geq 2} \frac{[\ell(\ell-1)]^n}{\ell!}, \tag{49}$$

an identity given in [18] which is further generalized in Proposition 7 below. The formulae (48) and (49) are seen neatly to extend their standard counterparts[14]

[14] A similar, simplified, treatment can also be inflicted to the usual Stirling numbers. Let $\mathcal{W}$ be the bilabelled class of all finite words over the labelled alphabet $\{1', 2', \dots\}$. The biexponential generating function is $W(z,\zeta) = \sum_{n,k} k^n (\zeta^k/k!)(z^n/n!) = \exp(\zeta\cdot e^z)$. With $\mathcal{Q}$, as defined above, representing a stock of "unused" letters, we have the identity $\mathcal{W} = \mathcal{Q} \star \mathcal{R}$, where $\mathcal{R}$ is the class of "gapless" words, in the sense that their letters form an initial segment of $\{1', 2', \dots\}$. (The class $\mathcal{R}$ is isomorphic to the class of "surjections" [47, §II.3], also known as ordered set partitions or preferential arrangements.) We then have $W(z,\zeta) = e^{\zeta} R(z,\zeta)$, which implies $R = e^{-\zeta} W$ giving back $R(z,\zeta) = \exp(\zeta(e^z - 1))$, which is both a biexponential generating function of surjections and the usual bivariate exponential generating function of set partitions; cf Equation (36), with the substitution $\zeta \mapsto u$.

in (38) and (37). Finally, expanding by the binomial theorem the quantities $[j(j-1)]^n$ in (48) or $[\ell(\ell-1)]^n$ in (49) serves to relate the generalized and basic families of numbers:

$$\left\{ {n \atop k} \right\}_{2,2} = \sum_{r=0}^{n} (-1)^{n-r} \binom{n}{r} \left\{ {n+r \atop k} \right\}, \qquad \varpi_n^{2,2} = \sum_{r=0}^{n} (-1)^{n-r} \binom{n}{r} \varpi_{n+r}.$$

Note 11. *Matrix enumeration and diagrams.* Let $\mathcal{M}^{\pm}_{n,k}$ be the collection of matrices with n rows and k columns, having all their entries in $\{0, \pm 1\}$, such that the following conditions are met: (i) there is exactly one $+1$–entry and one -1–entry in each row; (ii) no column consists solely of 0s. The corresponding cardinality satisfies

$$M^{\pm}_{n,k} = k! \left\{ {n \atop k} \right\}_{2,2},$$

as the set of matrices is clearly isomorphic to diagrams relative to X^2D^2 with *labelled* inputs (the column numbers)—these constitute the class $\widehat{S}_k$ above.

Similarly, let $\mathcal{M}^{+}_{n,k}$ be the collection of matrices with n rows and k columns, having all their entries in $\{0, 1\}$, such that the following conditions are met: (i) there are exactly two 1–entries in each row; (ii) no column consists solely of 0s. The corresponding cardinality satisfies

$$M^{+}_{n,k} = 2^{-n} k! \left\{ {n \atop k} \right\}_{2,2},$$

since this is equivalent to killing the orientation of gates.

The counts of matrices without restrictions on the number of rows are then, respectively,

$$M^{\pm}_{n} = \sum_{k=2}^{2n} k! \left\{ {n \atop k} \right\}_{2,2}, \qquad M^{+}_{n,k} = \frac{1}{2^n} \sum_{k=2}^{2n} k! \left\{ {n \atop k} \right\}_{2,2}.$$

The sequence of values $(M^{+}_{n})_{n\geq 1}$ starts as

$$1, 13, 409, 23917, 2244361, 308682013, 58514835289.$$

It has number *OEIS* **A055203**, with a description, "The number of different relations between n intervals on a line", which is easily related to our previous discussion. Also, perhaps more picturesquely: "Imagine you have n events of non-zero duration, in how many different ways could those events overlap in time?". (The *OEIS* refers to some unpublished work of S. Schwer relative to temporal logics and formal linguistics.) .... ■

Note 12. *Coupon collection with group drawings.* In probability theory, the coupon collector problem asks for the distribution of the number of samplings with replacement from a finite set $\mathcal{E}$, which are needed till a complete collection of the elements of $\mathcal{E}$ is obtained. If T is this random time and m is the cardinality of $\mathcal{E}$, one has

$$\mathbb{P}_m[T \leq n] = \frac{m!}{m^n} \left\{ {n \atop m} \right\} = \sum_{k=0}^{m} \binom{m}{k} (-1)^k \left(\frac{k}{m} \right)^n, \tag{50}$$

since the event $\{T \leq n\}$ corresponds to a sequence of n choices (each with m possibilities), such that each of the m possibilities is chosen at least once. (The $m!$ factor corresponds to the fact that *ordered* set partitions are to be considered, since the m elements of $\mathcal{E}$ are distinguishable.) See Feller's book [38] for a classical probabilistic derivation and [47, pp. 116–117] for a treatment cast within the framework of analytic combinatorics. It is also well known that the expected time for a complete collection satisfies

$$\mathbb{E}_m[T] = 1 + \frac{1}{2} + \cdots + \frac{1}{m} = \mathrm{H}_m = \log m + \gamma + o(1).$$

The coupon collector problem *with group drawings* is the variant problem, where one now draws from $\mathcal{E}$ in *groups* of r *distinct* elements. Here $r = 2$. This problem is, once more, a variant of those previously considered, and one finds

$$\mathbb{P}_m[T \le n] = \frac{m!}{(m(m-1))^n} \left\{ {n \atop m} \right\}_{2,2} = \sum_k \binom{m}{k} (-1)^k \left(\frac{k(k-1)}{m(m-1)} \right)^n,$$

which exhibits a pleasant similarity to the basic case (50). This formula was obtained by Stadje [106] by means of a subtle use of the inclusion–exclusion principle combined with suitable combinatorial identities—the derivation above seems to us much more transparent. Analytic methods then make it possible to derive the expected value [31]

$$\mathbb{E}_m[T] = \frac{m(m-1)}{2m-1} \left(H_m + \frac{1}{2m-1} - \frac{(-1)^m}{(m+1)\binom{2m-1}{m+1}} \right) = \frac{1}{2}\log m + \frac{\gamma}{2} + o(1).$$

This analysis is itself intimately related to that of the number of isolated vertices under the Erdős–Rényi random graph model [19, §7.1]. . . . . ■

Note 13. *Set partitions and contiguites.* Here is yet another interpretation of generalized Stirling numbers. Given a partition π of $\{1, \dots, n\}$, a pair $(j, j+1)$ is called a *contiguity* of π if j and $j+1$ belong to the same block. By extension, we also say that the number j is a contiguity.

In a diagram, we can view the gate bearing label j as being associated to two inputs labelled $2j-1$ and $2j$. In this way, the set of labels becomes $\{1, \dots, 2n\}$. We now consider partitions of $\{1, \dots, 2n\}$ and, given a gate, group in a single block all inputs that correspond to the same thread (i.e., are "vertically aligned"). The rules corresponding to the formation of diagrams then imply the following: *diagrams formed from X^2D^2 gates that are of size n are in bijective correspondence with set partitions of size $2n$, where continguities of odd values 1,3,5,. . . , are forbidden.* Thus the total number of such set partitions is the generalized Bell number $\varpi_n^{2,2}$ of (49).

This raises the question of enumerating set partitions according to the number of contiguities. The number $\widetilde{B}_n$ of those *without* any contiguity turns out to be the shifted (standard) Bell number ϖ_{n-1}, where ϖ_n is defined in (37). This can be shown from the relation

$$\widetilde{\mathcal{B}}^{\square} \star \mathcal{U} = \mathcal{B}, \qquad \mathcal{U} = \textsc{Set}(\mathcal{Z}),$$

which expresses the fact that an arbitrary partition (the class $\mathcal{B}$ of *all* set partitions) can be obtained from a contiguity-free partition (the class $\widetilde{\mathcal{B}}$) by gluing extra atoms (from $\mathcal{U}$) *after* their immediate predecessors (hence the appearance of the box operator in $\widetilde{\mathcal{B}}^{\square}$). From this specification and the general translation rules seen earlier, a simple computation provides the EGF: by (25), we have (with here $B_n \equiv \varpi_n$, so that $B(z) = e^{e^z-1}$)

$$\int \widetilde{B}'(z)e^z = B(z), \qquad \text{implying} \quad \widetilde{B}(z) = \int B(z) = \sum_{n\ge1} B_{n-1}\frac{z^n}{n!}.$$

This solves the enumeration problem, as $\widetilde{B}_n = B_{n-1}$. It is seen from here that

$$\int e^{uz}\widetilde{B}'(z) = e^{e^z+(u-1)z-1}$$

enumerates set partitions according the number of contiguities, marked by u. Consequently, *in the class of all set partitions, the statistics of contiguities and of singleton blocks are identical.* (An analogous process serves to relate derangements to the class of all permutations.) . . . . ■

In summary, the orbit of equivalences mentioned above (matrices, coupon collector, set partitions) justifies considering the generalized Stirling numbers $\left\{ {n \atop k} \right\}_{2,2}$ as basic quantities of combinatorial analysis.

4.3. **Higher order forms** (X^rD^r)**.** The discussion relative to X^2D^2 extends to X^rD^r and more generally to *balanced polynomials*, which are of the form

$$\mathfrak{h} = \sum_{\ell=1}^{r} \eta_\ell X^\ell D^\ell, \tag{51}$$

where $\eta = (\eta_j)$ is a sequence of arbitrary coefficients. We state:

Proposition 7 ([10, 17, 18])**.** *Let* $\mathfrak{h}$ *be a balanced polynomial in the sense of* (51)*. The* $\mathfrak{h}$*-Stirling numbers defined as the coefficients in the expansion*

$$\mathfrak{h}^n = \sum_k \left\{ {n \atop k} \right\}_{\mathfrak{h}} X^k D^k$$

admit the explicit form

$$\left\{ {n \atop k} \right\}_{\mathfrak{h}} = \frac{1}{k!} \sum_{j=1}^{k} (-1)^{k-j} \binom{k}{j} h(j)^n, \qquad h(x) := \sum_{\ell \geq 1} \eta_\ell \cdot x(x-1)\cdots(x-\ell+1). \tag{52}$$

Proof. A combinatorial proof based on gates and graphs proceeds along the same line as what has been done for X^2D^2. See the diagram of (43) and Figure 10. What happens is that each rung of a scaffolding is now comprised of an ℓ-arrangement (for some ℓ satisfying $1 \leq \ell \leq r$) of labelled inputs: the number of possibilities for each rung to be connected to j inputs is then exactly $h(j)$. Then, with $\widehat{\mathcal{S}}_k$ the collection of scaffoldings with k labelled inputs and $\mathcal{Q}$ the relaxed scaffoldings that may have unused labelled inputs, the relation (45) still holds (see also Figure 10). We then have the equality of double exponential generating functions

$$e^x \cdot \sum_{n,k} k! \left\{ {n \atop k} \right\}_{\mathfrak{h}} \frac{x^k}{k!} \frac{z^n}{n!} = \sum_{n,k} h(j)^n \frac{x^j}{j!} \frac{z^n}{n!}. \tag{53}$$

This last relation is equivalent to the statement upon extracting the coefficient of x^kz^n. □

The note below provides a typical alternative derivation taken from [10, 17, 18] and based on simple algebra; see also [103, §3].

Note 14. *Algebraic reduction of* $(X^rD^r)^n$. The idea is to apply $(X^rD^r)^n$ to the exponential function e^x. We write $\left\{ {n \atop k} \right\}_{r,r} := \left\{ {n \atop k} \right\}_{\mathfrak{h}}$, for $\mathfrak{h} = X^rD^r$. On the one hand, we have

$$(X^rD^r)^n\, e^x = \sum_k \left\{ {n \atop k} \right\}_{r,r} X^kD^ke^x = \sum_k \left\{ {n \atop k} \right\}_{r,r} x^ke^x, \tag{54}$$

by the definition of the $\left\{ {n \atop k} \right\}_{r,r}$ numbers and the fact that $D^ke^x = e^x$. On the other hand,

$$(X^rD^r)^n\, e^x = \sum_j \left[j(j-1)\cdots(j-r+1)\right]^n \frac{x^j}{j!}, \tag{55}$$

by the Taylor expansion of e^x. The comparison of (54) and (55) yields

$$\sum_k \left\{ {n \atop k} \right\}_{r,r} x^k = e^{-x} \sum_j \left[j(j-1)\cdots(j-r+1)\right]^n \frac{x^j}{j!},$$

which is equivalent to the statement of Proposition 7 in the case $\mathfrak{h} = X^rD^r$. .... ■

Schork reviews the numbers of Note 14 in [103] and discusses as well some q-analogues (see also the early work of Katriel and Kibler [72], the papers by Méndez and Rodriguez [87, 88], and Section 8.2 below). The normal form problem for $(X^rD^s)^n$ unites the case of $(X^rD^r)^n$ discussed above and the case of $(X^rD)^n$, which is closely related to trees: we shall accordingly discuss it later, in Note 18 of Subsection 6.2, p. 38. Relative to these and other cases, we note that Mikhailov [90] obtained the normal orderings of

$$(X+D)^n,\ (D^r+X)^n,\ (D+N)^n,\ (D^2+N)^n,$$

where $N = XD$; his end-formulae are "combinatorial", but his derivations are essentially algebraic. See also Katriel [68] for related material.

5. Quadratic forms $(X^2 + XD + D^2)$, zigzags, and permutations

The normal forms associated with $(X^2 + D^2)$ are related to evolution equations of the form

$$\frac{\partial}{\partial t}\psi(x,t) = \frac{\partial^2}{\partial x^2}\psi(x,t) + x^2\psi(x,t)$$

(in the case of the Schrödinger equation, this corresponds to a quantum harmonic oscillator, i.e., a quadratic potential) and are of great importance in quantum optics, where "squeezing" is introduced by means of quadratic forms in annihilation and creation operators. It is then not a surprise that the normal form problem for (powers of) quadratic forms should have been studied early, and, for instance, a paper by Mehta [86] published in 1977 contains results equivalent to our Propositions 8 and 9 below; see also Wilcox [117, §10] (published in 1967). The derivations in the cited paper are entirely operator-algebraic. As we show here, such normal forms follow routinely from the representation by diagrams in conjunction with standard methods of combinatorial analysis. This approach, which, to the best of our knowledge is new, furthermore reveals connections with alternating permutations (Subsection 5.1) as well as with general permutations classified according to local order patterns (Subsection 5.2).

5.1. The circle form $(X^2 + D^2)$ and zigzags. For the operator $(X^2 + D^2)$, the associated gates have either two outgoing (X^2) or two ingoing lines (D^2); these are then shaped like a "cup" or a "cap":

A general graph relative to $(X^2 + D^2)$ consists of (weakly) connected components, and each connected component involves caps and cups in alternation: we shall refer to them as "zigzags"; see Figure 11. Note that since the inputs and outputs of gates are distinguishable, edges may cross. It is then easily realized that zigzags can be of one of four types, depending on the excess of the number of free outputs over the number of free inputs—values for this excess can be $-2, 0, +2$— with, in addition, for excess 0, the fact that diagrams may be either "closed" or "open". This gives rise to four different types of connected components, which we denote by $\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}$. In summary, with $\mathcal{G}$ be the class of all graphs relative to $(X^2 + D^2)$, u marking the

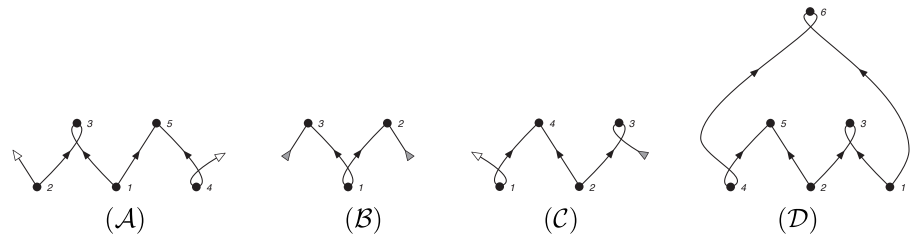


FIGURE 11. The four classes of connected components (zigzag's) $\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}$ relative to $(X^2 + D^2)$.

number of outputs, and v marking the number of inputs, the decomposition into connected components is expressed by

$$\mathcal{G} = \text{SET}\left(u^2\mathcal{A} + v^2\mathcal{B} + uv\mathcal{C} + \mathcal{D}\right), \tag{56}$$

Removal of the vertex with the largest label (in the case of $\mathcal{A}, \mathcal{C}, \mathcal{D}$) or with the smallest one (in the case of $\mathcal{B}$) shows that a zigzag can be decomposed into one or two smaller zigzags. This is expressed by the formal specification

$$\left\{\begin{array}{lcl} \mathcal{A} & = & \mathcal{Z} + 4\,(\mathcal{A} \star \mathcal{Z}^{\blacksquare} \star \mathcal{A}) \\ \mathcal{B} & = & \mathcal{Z} + 4\,(\mathcal{B} \star \mathcal{Z}^{\square} \star \mathcal{B}) \\ \mathcal{C} & = & 4\,(\mathcal{A} \star \mathcal{Z}^{\blacksquare} \star (\mathcal{C} + \mathcal{E})) \\ \mathcal{D} & = & 2\,(\mathcal{Z}^{\blacksquare} \star \mathcal{A})\,. \end{array}\right. \tag{57}$$

The multiplicities (2 and 4, as the case may be) reflect the various possibilities of attachments: for instance, in the case of type $\mathcal{D}$, there are clearly two ways of attaching the largest label to a previously existing zigzag of type $\mathcal{A}$. (The class $\mathcal{E}$ is comprised of a unique "neutral" element of size 0; the class $\mathcal{Z}$ consists of a single atom of size 1.)

The decomposition into connected components (56) gives

$$G(z; u, v) = \exp\left(u^2 A(z) + v^2 B(z) + uv\, C(z) + D(z)\right), \tag{58}$$

while the combinatorial specification (57) give rise to integral equations:

$$\left\{\begin{array}{ll} A(z) = z + 4\displaystyle\int_0^z A(t)^2\,dt, & B(z) = z + 4\displaystyle\int_0^z B(t)^2\,dt, \\ C(z) = 4\displaystyle\int_0^z A(t)\cdot(C(t)+1)\,dt, & D(z) = 2\displaystyle\int_0^z A(t)\,dt\,. \end{array}\right. \tag{59}$$

The equivalent differential equations,

$$\left\{\begin{array}{ll} \partial_z\, A(z) = 1 + 4\,A(z)^2\ , & \partial_z\, B(z) = 1 + 4\,B(z)^2\ , \\ \partial_z\, C(z) = 4\,A(z)\cdot(C(z)+1)\ , & \partial_z\, D(z) = 2\,A(z)\ , \end{array}\right.$$

(with the initial conditions $A(0) = B(0) = C(0) = D(0) = 0$) admit separation of variables, hence they have closed-form solutions:

$$\left\{\begin{array}{ll} A(z) = \frac{1}{2}\,\tan(2z), & B(z) = \frac{1}{2}\,\tan(2z), \\ C(z) = \cos(2z)^{-1} - 1, & D(z) = -\frac{1}{2}\,\ln(\cos(2z))\,. \end{array}\right. \tag{60}$$

(Note that equality of generating functions $A(z) = B(z)$ mirrors the isomorphism between classes $\mathcal{A}$ and $\mathcal{B}$, which can be seen explicitly by a horizontal reflection of zigzags and a relabelling of the vertices according to $1, \ldots, m \mapsto m, \ldots, 1$.)

Collecting the results of (58) and (60), we obtain:

Proposition 8. *The generating function of all graphs associated with* $(X^2 + D^2)$ *admits the explicit form*

$$G(z; u, v) = \frac{1}{\sqrt{\cos(2z)}} \cdot \exp\left(\tfrac{1}{2}(u^2 + v^2)\tan(2z) + uv(\sec(2z) - 1)\right). \tag{61}$$

Note 15. *Zigzags and alternating permutations.* The enumeration of zigzags is closely related to one of the most classical problems of combinatorial analysis; namely, the enumeration of alternating permutations; see [23, pp. 258–259] and [108, pp. 73–75]. (We follow the presentation in [47, §II.6.3].) Let a permutation $\sigma = \sigma_1 \cdots \sigma_n$ be written as a word (so that σ_i represents $\sigma(i)$). The permutation σ is said to be *alternating* if $\sigma_1 < \sigma_2$, $\sigma_2 > \sigma_3$, and so on, with an alternating pattern of rises ($\sigma_{2j-1} < \sigma_{2j}$) and falls ($\sigma_{2j} < \sigma_{2j+1}$). Let $\mathcal{S}$ and $\mathcal{T}$ be, respectively, the EGF of even-sized and odd-sized permutations. By a maximum based decomposition analogous to what we have seen before, the specifications are

$$\mathcal{T} = (\mathcal{T} \star \mathcal{Z}^{\blacksquare} \star \mathcal{T}); \qquad \mathcal{S} = \{\epsilon\} + (\mathcal{T} \star \mathcal{Z}^{\blacksquare} \star \mathcal{S}).$$

Hence, via integral and differential relations, the well-known solutions:

$$\begin{array}{lclcll} S(z) & = & \sec(z) & = & 1 + 1\,\dfrac{z^2}{2!} + 5\,\dfrac{z^4}{4!} + 61\,\dfrac{z^6}{6!} + \cdots & (\textit{OEIS}\ \mathbf{A000364}) \\ T(z) & = & \tan(z) & = & z + 2\,\dfrac{z^3}{3!} + 16\,\dfrac{z^5}{5!} + 272\,\dfrac{z^7}{7!} + \cdots & (\textit{OEIS}\ \mathbf{A000182}). \end{array}$$

Also of interest are *alternating cycles* defined to be directed cycles whose edges have alternatively increasing and decreasing end points. These are necessarily of even size with specification $\mathcal{U} = (\mathcal{Z}^{\blacksquare} \star \mathcal{T})$, so that $U(z) = \int T(z)$ and $U(z) = \log\sec(z)$ whose coefficients are a shifted version of the tangent numbers $n!\,[z^n]\tan(z)$. The undirected cycle version has EGF $V(z) = \frac{1}{2}\log\sec(z) + \frac{1}{4}z^2$, so that (undirected) graphs whose components are (undirected) alternating cycles have EGF

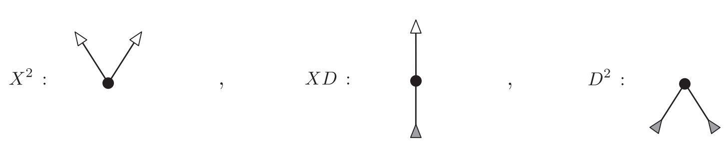
$$W(z) = \frac{e^{z^2/4}}{\sqrt{\cos(z)}} = 1 + 1\,\frac{x^2}{2!} + 4\,\frac{x^4}{4!} + 38\,\frac{x^6}{6!} + 710\,\frac{x^8}{8!} + \cdots,$$

which is not found in the *OEIS*. For reasons discussed below, in Section 7, several of these numbers have OGFs that admit explicit *continued fraction* representations. .... ■

5.2. **The general quadratic form** $(\alpha\, D^2 + \beta\, X^2 + \gamma\, XD)$**.** We treat here diagrams corresponding to the general quadratic form

$$\alpha\, D^2 + \beta\, X^2 + \gamma\, XD,$$

which introduce extra gates having one ingoing and one outgoing line (compare with Subsection 5.1):



Hence, the graphs again have the structure of open and closed zig-zags, but now with ascents and descents of arbitrary length, see Fig. 12. Additionally, parameters α, β and γ keep track, respectively, of the statistics of valleys, peaks and rises/falls in the construction. The analysis of this case closely follows the scheme given in Subsection 5.1. We state:

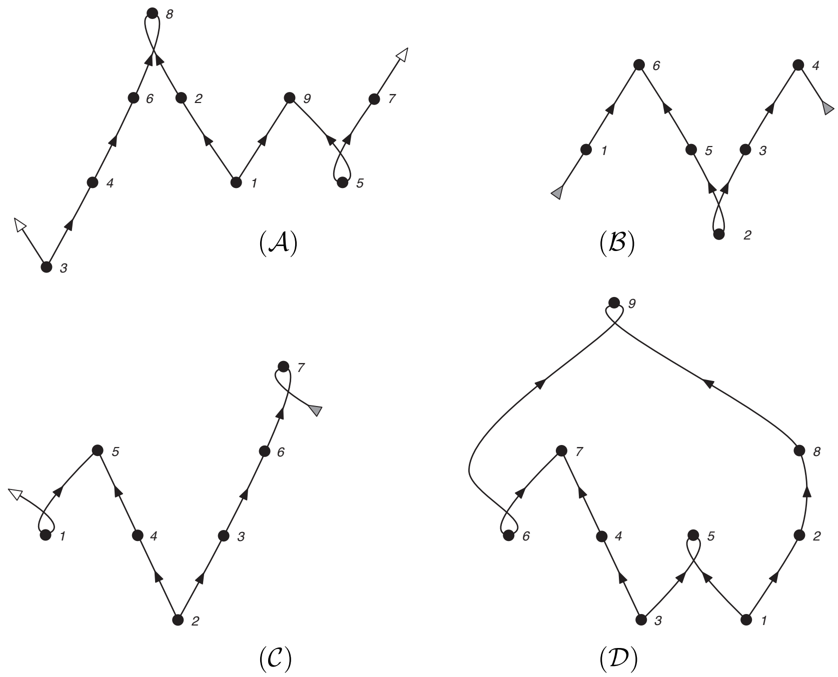


FIGURE 12. The four classes of connected components $\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}$ associated with $(\alpha\, D^2 + \beta\, X^2 + \gamma\, XD)$.

Proposition 9. *The generating function of all graphs associated with* $(\alpha D^2 + \beta X^2 + \gamma XD)$ *admits the explicit form*

$$
\begin{aligned}
G(z; u, v) \quad &= \quad \exp\left(\left(\frac{u^2}{4\alpha} + \frac{v^2}{4\beta}\right)(\delta\, \tan(\delta\, z + \theta) - \gamma)\right) \\
&\qquad \cdot \exp\left(uv\left(\frac{\cos(\theta)}{\cos(\delta\, z + \theta)} - 1\right)\right) \cdot e^{\frac{\gamma}{2} z} \sqrt{\frac{\cos(\theta)}{\cos(\delta\, z + \theta)}},
\end{aligned} \tag{62}
$$

where

$$\delta = \sqrt{4\alpha\beta - \gamma^2}, \qquad \theta = \arctan(\gamma/\delta). \tag{63}$$

Proof. The decomposition into connected components gives, for the class of all diagrams:

$$\mathcal{G} = \textsc{Set}\left(u^2\, \mathcal{A} + v^2\, \mathcal{B} + uv\; \mathcal{C} + \mathcal{D}\right). \tag{64}$$

The specification of the four types of components paralells that of (57):

$$
\left\{
\begin{array}{lcl}
\mathcal{A} & = & \beta\; \mathcal{Z} + 2\gamma\; \mathcal{Z}^{\blacksquare} \star \mathcal{A} + 4\alpha\; \mathcal{A} \star \mathcal{Z}^{\blacksquare} \star \mathcal{A}\,, \\
\mathcal{B} & = & \alpha\; \mathcal{Z} + 2\gamma\; \mathcal{Z}^{\square} \star \mathcal{B} + 4\beta\; \mathcal{B} \star \mathcal{Z}^{\square} \star \mathcal{B}\,, \\
\mathcal{C} & = & \gamma\; \mathcal{Z} + \gamma\; \mathcal{Z}^{\blacksquare} \star \mathcal{C} + 4\alpha\; \mathcal{A} \star \mathcal{Z}^{\blacksquare} \star (\mathcal{C} + \mathcal{E})\,, \\
\mathcal{D} & = & 2\alpha\; \mathcal{Z}^{\blacksquare} \star \mathcal{A}\,.
\end{array}
\right.
$$

The translation into equations binding EGFs is now automatic. First, we have

$$G(z; u, v) = \exp\left(u^2\, A(z) + v^2\, B(z) + uv\; C(z) + D(z)\right).$$

Next,

$$\begin{cases} A(z) &=& \beta\, z + 2\,\gamma \displaystyle\int_0^z A(t)\,dt + 4\,\alpha \int_0^z A(t)^2\,dt, \\ B(z) &=& \alpha\, z + 2\,\gamma \displaystyle\int_0^z A(t)\,dt + 4\,\beta \int_0^z B(t)^2\,dt, \\ C(z) &=& \gamma\, z + \gamma \displaystyle\int_0^z C(t)\,dt + 4\,\alpha \int_0^z A(t)\cdot(C(t)+1)\,dt, \\ D(z) &=& 2\,\alpha \displaystyle\int_0^z A(t)\,dt\,. \end{cases}$$

The corresponding differential equations are

$$\begin{cases} \partial_z\, A(z) &=& \beta + 2\gamma\, A(z) + 4\alpha\, A(z)^2\ , \\ \partial_z\, B(z) &=& \alpha + 2\gamma\, B(z) + 4\beta\, B(z)^2\ , \\ \partial_z\, C(z) &=& (\gamma + 4\alpha\, A(z))\cdot(C(z)+1)\ , \\ \partial_z\, D(z) &=& 2\alpha\, A(z)\,, \end{cases}$$

with initial conditions $A(0) = B(0) = C(0) = D(0) = 0$. There is again separation of variables. However, as examplified by the case of $\mathcal{A}$, one now needs to solve (with $y = A(z)$)

$$\frac{dy}{\beta + 2\gamma y + 4\alpha y^2} = dz,$$

which neccessitates factoring the quadratic form in the denominator, hence solving a quadratic equation: this introduces the auxiliary quantities (63). The solutions found are

$$\begin{cases} A(z) &=& \dfrac{\delta}{4\alpha}\,\dfrac{\gamma + \delta\,\tan(\delta\, z)}{\delta - \gamma\,\tan(\delta\, z)} - \dfrac{\gamma}{4\alpha} &=& \dfrac{\delta}{4\alpha}\,\tan(\delta\, z + \theta) - \dfrac{\gamma}{4\alpha}\ , \\ B(z) &=& A(z)\big|_{\alpha\leftrightarrow\beta}\ , \\ C(z) &=& \cos(\delta\, z) - \frac{\gamma}{\delta}\sin(\delta\, z) - 1 &=& \dfrac{\cos(\theta)}{\cos(\delta\, z + \theta)} - 1\ , \\ D(z) &=& -\frac{1}{2}\ln\big(\cos(\delta\, z) - \frac{\gamma}{\delta}\sin(\delta\, z)\big) - \frac{\gamma}{2}\, z &=& \frac{1}{2}\ln\left(\dfrac{\cos(\theta)}{\cos(\delta\, z+\theta)}\right) - \frac{\gamma}{2}\, z\ . \end{cases}$$

from which the statement results. □

Note 16. *Generalized Eulerian numbers.* In the same way that zigzags are closely reated to alternating permutations, the diagrams considered here are closely related to a quadrivariate statistics on permutations; namely that of the number of peaks, valleys, double rises, and double falls [51, Ex. 3.3.46, p. 195]. For instance, Carlitz and Scoville [21] found the corresponding multivariate EGF,

$$\frac{e^{\alpha_2 z} - e^{\alpha_1 z}}{\alpha_2 e^{\alpha_1 z} - \alpha_1 e^{\alpha_2 z}}, \qquad \alpha_1\alpha_2 = u_1 u_2, \quad \alpha_1 + \alpha_2 = u_3 + u_4$$

(u_1, u_2, u_3, u_4 mark, respectively, the four types of elements listed above), which suitably generalizes the bivariate EGF of Eulerian numbers (*OEIS* **A008292** and [23, p. 244]),

$$A(z,u) = \frac{1-u}{1 - u e^{z(1-u)}}. \tag{65}$$

which enumerates permutations according to the number of rises (do $u_1 = u_3 u$, $u_2 = u_4 = 1$). See [47, p. 202] for a derivation along the lines above. The corresponding OGFs also have explicit continued fraction expansions [41], which are closely related to the combinatorial aproach of the present study—see Subsection 7.1. .... ■

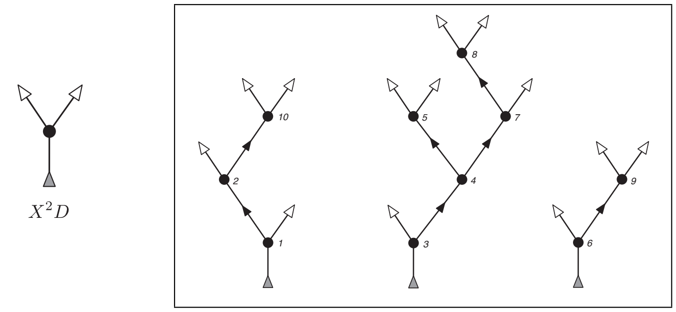


FIGURE 13. The basic gate $\mathbb{Y}$ associated with X^2D (left) and a corresponding diagram (right box).

6. The semilinear forms $(\phi(X)D)$ and increasing trees

We consider here first-order differential operators of the general form $\phi(X)D + \rho(X)$, where ϕ is a nonlinear polynomial of arbitrary degree. The general combinatorial model is that of increasing trees, which were discussed early by Leroux and Viennot [76, 77] and further developed by Bergeron, Labelle, and Leroux in their reference text [7, Ch. 5]. (The subject is treated under the combinatorial–analytic angle by Bergeron *et al.* [6].) In the physics literature, Lang [74] seems to have been among the first to discuss the normal ordering associated with X^rD; see also his later paper [75]. Then Blasiak *et al.* [11, 15] discovered the relationship between general abstract varieties of increasing trees, as in [6], and the forms $(\phi(X)D)$, which we propose to examine now. It is pleasant to note that the developments of this section also serve to answer several algebraic–combinatorial questions first raised by Scherk in 1823; see the discussion relative to Figure 26, p. 69, of the Appendix.

6.1. The form (X^2D) and increasing trees. In the case of the operator XD^2, the gates have one input and two outputs. They are thus shaped as a letter "$\mathbb{Y}$"; see Figure 13. By successively grafting outputs of such $\mathbb{Y}$'s to inputs of other $\mathbb{Y}$'s, we obtain graphs that are necessarily acyclic, so that each connected component is a *tree*. These trees are *plane trees* (there is a distiction between left and right outgoing edges); they are *binary*, by design; and, finally, they are increasing in the sense that labels increase along any branch stemming from the root. Such trees are quite well known in combinatorial theory under the name of *binary increasing trees*, their importance being due to the fact that they are in bijective correspondance with permutations. See for instance [47, §II.6.3] or [107].

We commence with the class $\mathcal{T}$ of binary increasing trees. A tree in $\mathcal{T}$ is obtained by starting with a root that bears the smallest label; then, each of the two output edges is either left untouched or it is attached recursively to a similar tree. Within the language of specifications summarized in Section 2, this is expressed as follows ("ϵ" represents a neutral structure of size 0):

$$\mathcal{T} = (\mathcal{Z}^{\square} \star (\{\epsilon\} + \mathcal{T}) \star (\{\epsilon\} + \mathcal{T}))\,.$$

The translation to EGFs is then

$$T(z) = \int_0^z (1 + T(w))^2\, dw,$$

which, by differentiation, leads to the equation

$$T'(z) = (1 + T(z))^2, \qquad T(0) = 0.$$

Since this last differential equation admits separation of variables, we find $T'/(1 + T)^2 = 1$, hence $-1/(1 + T) = z - 1$; that is,

$$T(z) = \frac{z}{1-z} \equiv \sum_{n=1}^{\infty} n! \frac{z^n}{n!}.$$

This verifies that $T_n = n!$: binary increasing trees are equinumerous with permutations. (Combinatorially, here are two easy combinatorial arguments: (i) the number of choices for successively adding a new gate is $1, 2, 3, 4, 5, \ldots$; (ii) a permutation is obtained when node labels are read in infix, i.e., left-to-right, order. The formal relation with *binary* trees, is well explained combinatorially by Leroux–Viennot [76, 77]: see also [7, Ex. 12, p. 383].)

Now, a connected diagram has one input (the link into the root) and $(n+1)$ free outputs, if n is the number of nodes ($\mathbb{Y}$–gates associated with (X^2D)) of the tree. Thus, the trivariate EGF, where u marks outputs and v marks inputs is

$$vuT(uz) = \frac{vu^2z}{1 - uz}.$$

The EGF of all diagrams is accordingly

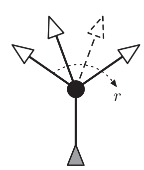
$$G(z; u, v) = \exp\left(\frac{vu^2z}{1 - uz}\right).$$

In particular, the total number of diagrams of size $n \geq 1$ is

$$n![z^n]G(z; 1, 1) = n![z^n]e^{z/(1-z)} = \sum_{k=1}^{n-1} \binom{n-1}{k-1} \frac{n!}{k!}.$$

The sequence starts as $1, 1, 3, 13, 73, 501, 4051, 37633$, and is *OEIS* **A000262** ("sets of lists"); see also [47, p. 125] ("fragmented permutations"). We are indeed enumerating unordered forests of increasing binary trees, equivalently, sets of nonempty permutations, i.e., structures of type $\textsc{Set}(\textsc{Seq}_{\geq 1}(\mathcal{Z}))$.

This approach applies almost verbatim to the operator X^rD, with $r \geq 2$. In this case, we are dealing with r–ary trees, where each node has r outgoing edges:



X^rD

The differential equation becomes $T' = (1 + T)^r$, with solution

$$T = [1 - (r-1)z]^{-1/(r-1)} - 1, \quad \text{and} \quad n![z^n]T(z) = n!\binom{n + 1/(r-1) - 1}{n}. \tag{66}$$

The balance betwen the number of outputs and size is dealt with as before (with an r-ary tree of n internal nodes having $n(r-1) + 1$ ougoing edges). So:[15]

[15] Interestingly enough, Comtet has a form equivalent to the one we give, as an exercise in his book [23, Ex. 2, p. 220] relative to "Lie derivatives and operational calculus".

Proposition 10. *The EGF of diagrams associated with* (X^rD) *is*

$$G(z;u,v) = \exp\left(\frac{uv}{[1-(r-1)u^{r-1}z]^{1/(r-1)}} - uv\right).$$

For $r=2$*, the normal forms associated with* $\mathfrak{h} = (X^2D)$ *simplify to*[16]

$$\mathfrak{N}(\mathfrak{h}^n) = \sum_{\ell=1}^{n-1} \binom{n-1}{k-1}\frac{n!}{k!} X^{n+k}D^k.$$

For $r \geq 3$*, one has* $\mathfrak{N}(\mathfrak{h}^n) = \sum_k \gamma_{n,k} X^{k+(r-1)n}D^k$*, with*

$$\gamma_{n,k} = \frac{n!}{k!}\sum_{\ell=0}^{k}(-1)^{k-\ell}\binom{k}{\ell}\binom{n+\ell/(r-1)-1}{k}(r-1)^n.$$

Combinatorially, the number of possibilities for successively adding a new gate is now $1, r, (2r-1), \ldots$, which is consistent with (66). The derivation given above, via EGFs, has however been adopted since it is the only one applicable to the general case $(\phi(X)D)$, as we see next. The total number of graphs for $r=3,4$ starts as

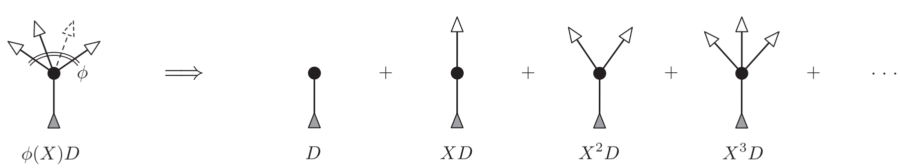
$r=3:\quad 1, 4, 25, 211, 2236, 28471, 422899, 7173580, \ldots$ *OEIS* **A049118**
$r=4:\quad 1, 5, 41, 465, 6721, 117941, 2433145, 57673281, \ldots$ *OEIS* **A049119**,

and these coefficients are expressible as binomial sums; see Lang's study [74] for an early discussion of these numbers revisited in [75] and the papers [11, 15] by Blasiak *et al.* for relations with the normal ordering problem.

6.2. **The general case** $(\phi(X)D)$**.** In this case, we must consider a polynomial

$$\phi(y) = \sum_{j=0}^{R} \phi_j y^r,$$

with gates of the form X^jD, any such gate being assigned weight ϕ_r. The corresponding increasing trees can thus have various types of internal nodes, as dictated by $\phi(y)$. Graphically:



In combinatorial terms, this defines a *variety of increasing trees*: the basic and asymptotic theory of these being the subject of the paper [6].

The graphs associated with $\phi(X)D$ are still (unordered) forests of increasing trees, themselves denoted by $\mathcal{T}$, or $\mathcal{T}^\phi$, whenever the dependency on ϕ needs to be

[16] The coefficients, up to sign, are sometimes known as "Lah numbers" (*OEIS* **A008297** and [100, p. 44]), the Lah polynomials being essentially Laguere polynomials.

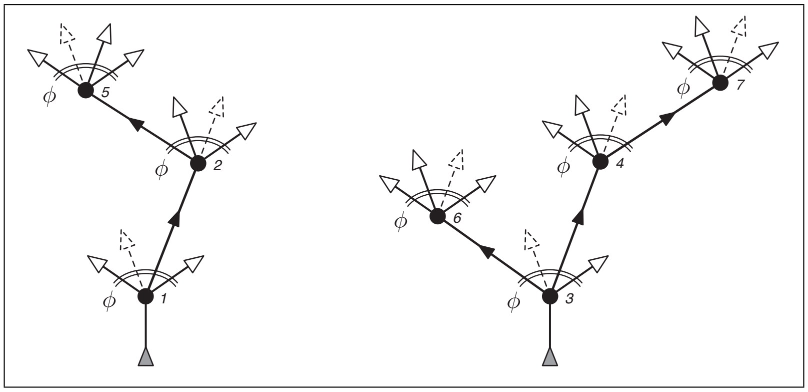


FIGURE 14. A diagram with some $\phi(X)D$ that is comprised of two rooted trees.

made explicit. The basic equation for the EGF $T = T(z,u)$, with u a marker for "unsaturated" outgoing edges is then (Figure 14)

$$\mathcal{T} = \sum_{j=0}^{R} \phi_r \left(\mathcal{Z}^{\square} \star \overbrace{(u+\mathcal{T}) \star \cdots \star (u+\mathcal{T})}^{r \text{ times}} \right) \tag{67}$$

Thus, we have

$$T(z,u) = \int_0^z \phi(u + T(w,u))\, dw, \qquad \text{implying} \quad \frac{\partial}{\partial z} T(z,u) = \phi(u + T(z,u)),$$

and separation of variables yields, with u a parameter:

$$\int_0^{T(z,u)} \frac{d\tau}{\phi(u+\tau)} = z.$$

We can now conclude as follows.

Proposition 11. *Define*

$$\Phi(y) := \int_{y_0}^{y} \frac{d\tau}{\phi(\tau)}, \tag{68}$$

where y_0 is an arbitrary nonnegative constant chosen so that $\phi(y_0) \neq 0$. Let $T \equiv T^{\phi}(z,u)$ be defined as the solution of

$$T \ : \qquad \Phi(T+u) - \Phi(u) = z, \quad \textit{with } T(0,u) = 0. \tag{69}$$

Then the multivariate EGF of all diagrams relative to $(\phi(X)D)$ is

$$G(z;u,v) = \exp\left(vT^{\phi}(z,u)\right).$$

Proposition 11 provides a solution to the general problem posed by Scherk in his doctoral dissertation [102, §8] of 1823: see our Appendix A, p. 69. The remarks relative to Scherk's thesis, p. 68 below, provide a concrete illustration of the combinatorics of increasing trees in relation to the normal form of $(\phi(X)D)^n$.

On another register, it is shown in [6] that the singular structure of $T(z,1)$ can be systematically determined, from which there follow many *asymptotic* distributional analyses of parameters, including path length, node-degre profile, root degree, and so on. However, as regards explicit forms that are of concern for us here, only a few functions $\phi(y)$ are susceptible to exact expressions; for instance,

$$y^r, \quad (1+y)^r, \qquad (ay^2+by+c), \quad y(y+1)\cdots(y+r-1). \tag{70}$$

Note 17. *Some solvable varieties* [6, §2]. First, (X^2D+D), corresponding to $\phi(y)=y^2+1$, leads to a solvable case:

$$G(z;u,v)=\exp\left(\frac{v(1+u^2)\tan z}{1-u\tan z}\right), \qquad G(z;1,1)=\exp\left(\frac{2\tan(z)}{1-\tan z}\right).$$

The coefficients $n![z^n]G(z;1,1)$ are of the form $2^n a_n$, where

$$(a_n)=1,1,2,6,23,107,583,3633,25444,197620,\ldots$$

is *OEIS* **A000772** ["the number of elevated(!) increasing binary trees"]. More generally, any quadratic polynomial leads to a solvable model.

On another register, if $\phi(y)$ has only *rational roots*, then its partial fraction expansion only involves rational coefficients. The inversion problem is then of the type

$$\sum_j r_j \log(1-\alpha_j T^j)=z, \qquad r_j,\alpha_j\in\mathbb{Q}.$$

Thus, by inversion, T *is an algebraic function of* e^z. This is in particular the case for Stirling polynomials, such as $\phi(y)=(y+1)(y+2)(y+3)$, for which

$$T(z,1)=-2+\frac{2}{\sqrt{4-3e^{2z}}}=6z+66\frac{z^2}{2!}+1158\frac{z^3}{3!}+28290\frac{z^4}{4!}+\cdots.$$

(This last example is from [6, p. 30].)

Other interesting cases for combinatorics are $\phi(y)=e^y$ and $\phi(y)=(1-y)^{-1}$, leading, respectively, to increasing Cayley trees (so-called "recursive" trees) and increasing Catalan trees ("plane ordered recursive trees", also known as "PORTs"); see [6, §1]. The corresponding EGFs, $T(z)=T(z,1)$ are

$$\begin{cases} T(z) &= \log\dfrac{1}{1-z} &= \displaystyle\sum_{n\ge1}(n-1)!\frac{z^n}{n!} & \big(\phi(y)=e^y\big) \\ T(z) &= 1-\sqrt{1-2z} &= \displaystyle\sum_{n\ge1}\big(1\cdot3\cdots(2n-3)\big)\frac{z^n}{n!} & \big(\phi(y)=(1-y)^{-1}\big). \end{cases}$$

We will not discuss them further as they are out of our scope, since they concern non-polynomial forms (see however Scherk's result relative to the normal ordering of (e^XD), Proposition A.2, in the Appendix).. .... ■

Note 18. *Algebraic reduction of* X^rD^s *after* [10, 18]. One may apply the same procedure as in Note 14, p. 28, to obtain coefficients of the normal form of $(X^rD^s)^n$ written as

$$(X^rD^s)^n=X^{n(r-s)}\sum_k \left\{ {n \atop k} \right\}_{r,s} X^rD^s$$

We first assume that $r\ge s$. The action of X^rD^s on the exponential e^x is

$$(X^rD^s)^n\,e^x=X^{n(r-s)}\sum_k \left\{ {n \atop k} \right\}_{r,s} X^kD^ke^x=\sum_k \left\{ {n \atop k} \right\}_{r,s} x^ke^x, \tag{71}$$

equivalently,

$$(X^rD^s)^n\,e^x=\sum_j\prod_{p=1}^n (j+(p-1)(r-s))^{\underline{s}}\;\frac{x^{j+n(r-s)}}{j!}. \tag{72}$$

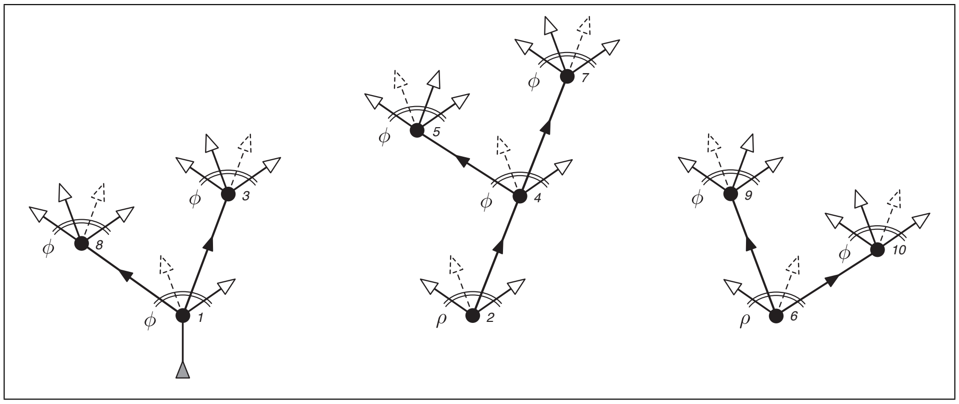


FIGURE 15. A particular diagram (forest) associated to a form $(\phi(X)D + \rho(X))$, comprised of one rooted tree and two planted trees.

Then the comparison of (71) and (72) produces

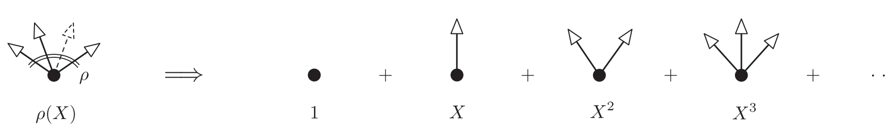
$$\sum_k \left\{ n \atop k \right\}_{r,s} x^k = e^{-x} \sum_j \prod_{p=1}^{n} (j + (p-1)(r-s))^{\underline{s}} \; \frac{x^j}{j!},$$

and extraction of coefficients yields

$$\left\{ n \atop k \right\}_{r,s} = \frac{1}{k!} \sum_{j=s}^{k} (-1)^{k-j} \binom{k}{j} \prod_{p=1}^{n} (j + (p-1)(r-s))^{\underline{s}}, \tag{73}$$

a formula, of which, remarkably enough, Scherk had non-trivial cases (see Proposition A.3, p. 70). The case $r < s$ gives rise to similar coefficients, as results from the duality argument of Note 2, p. 10. .... ■

6.3. **The form $(\phi(X)D + \rho(X))$ and planted trees.** We now have gates of the form X^s (arising from the monomials contained in $\rho(X)$) in addition to the earlier ones, of form $X^r D$ that originate with $\phi(X)D$. In combinatorial terms, there is thus the additional possibility of "planting" any combination of members of the family of increasing trees $\mathcal{T}^\phi$ on a root, whose outdegree has possibilities dictated by the monomials of $\rho(X)$. Graphically:



A connected component is then either a planted tree $\mathcal{R}^\phi$, or a rooted tree of $\mathcal{T}^\phi$.

The corresponding specification is (with $\mathcal{T}^\phi$ as before):

$$\left\{ \begin{array}{lcll} \mathcal{R}^\phi & = & \displaystyle\sum_{s \geq 0} \rho_s \left(\mathcal{Z}^\square \star \left(u + \mathcal{T}^\phi\right)^s \right) & \text{(planted trees)} \\ \mathcal{G} & = & \textsc{Set}\left(\mathcal{R}^\phi + v\mathcal{T}^\phi\right) & \text{(all graphs).} \end{array} \right.$$

We then have:

Proposition 12. *The graphs associated with the normal ordering of* $(\phi(X)D + \rho(X))$ *have the trivariate generating function*

$$G(z;u,v) = e^{R^\phi(u,z)} \cdot e^{vT^\phi(u,z)}, \qquad \textit{where} \quad R^\phi(u,z) := \int_0^z \rho\left(u + T^\phi(u,t)\right) dt,$$

and T^ϕ *is specified by* (68) *and* (69)*.*

Note 19. *Yet another PDE.* In the case of the PDE

$$\frac{\partial}{\partial z} F(x,z) = \phi(x) \frac{\partial}{\partial x} F(x,z), \tag{74}$$

with initial value condition $f(x,0) = f(x)$, the solution (cf Proposition 11) can be described in the following suggestive way.

> *Let* $Q(y)$ *be the primitive function of* $1/\phi(y)$ *and* $Q^{(-1)}(x)$ *denote its inverse; the solution of* (74) *is*
>
> $$F(x,z) = f(Q^{(-1)}(z + Q(x))).$$

This is, for instance, the form given by Dattoli *et al.* in [27], Equation (I.2.18), p. 6; Equation (I.2.25) of that paper treats the general case of Proposition 12 above. See also the discussion in [15], especially the formula (1) there. We shall briefly return to the combinatorics of increasing trees, when we discuss multivariate extensions of these results in Section 9, Note 25, p. 62 below. . . . . ■

7. Binomial forms $(X^a + D^b)$, lattice path models, and continued fractions

The purpose of this section is to develop *from first principles* combinatorial models that are now expressible as *lattice paths.* The approach is an alternative to the gates-and-diagrams model of previous sections, though it is strongly related—we shall indeed present a correspondence in Subsection 8.1. The main focus here is on the reduction of powers of the "*binomial forms*" $(X^a + D^b)$. Contrary to what has been the case until now, the reductions are often far from being explicit, in terms of either coefficients or generating functions. Nonetheless, this section reveals interesting connections with other areas of combinatorics. In this context, the "*Fermat forms*" $(X^r + D^r)$ stand out, due to a simple relation with a yet mysterious class of *continued fractions.*

7.1. **Normal ordering and lattice paths.** We first revisit briefly the normal ordering problem. Given the (not necessarily normal) representation H of an operator, which may be a power $\mathfrak{h}^n$ or a generating function $e^{z\mathfrak{h}}$, its normal ordering is, by definition, of the form

$$\mathfrak{N}(H) = \sum_{\alpha,\beta \in \mathbb{Z}_{\geq 0}} c_{\alpha,\beta} X^\alpha D^\beta,$$

for a family of constants $c_{\alpha,\beta} \equiv c_{\alpha,\beta}(H)$ that depends on H. Of special interest for our subsequent discussion is the *constant term* $c_{0,0}$, which we shall rewrite as

$$\mathbf{C.T.}(H) \equiv c_{0,0}(H).$$

Note that, since D^β, for $\beta \geq 1$ is cancelled by a constant, we have

$$\mathfrak{N}(H\,\mathbb{1}) = \sum_\alpha c_{\alpha,0} X^\alpha,$$

where '$H\,f$' represents the application of the operator H to the function $f \equiv f(x)$ and $\mathbb{1}$ denotes the constant function equal to unity. We then have the obvious constant-term identity

$$\textbf{C.T.}(H) = H \circ \mathbb{1}\big|_{X=0}\,. \tag{75}$$

In this section, we shall mostly be concerned with *constant term identities.*

There is a known way to represent the normal ordering process as a *transformation* of *lattice paths* in the cartesian plane $\mathbb{Z}_{\geq 0} \times \mathbb{Z}_{\geq 0}$. This is for instance reviewed in the elegant discussion of Varvak [112]; see also Subsection 8.1 below for a quick review. Our approach has some analogy, but it also differs in essential aspects.

First, we note that the linear differential operator D is characterized by the way it acts on the canonical basis $\{x^k\}_{k=0}^{\infty}$ of monomials, in which it is represented[17] by the infinite matrix

$$\mathbf{D} = \begin{bmatrix} 0 & 1 & \cdot & \cdot & \cdot & \cdots \\ \cdot & 0 & 2 & \cdot & \cdot & \cdots \\ \cdot & \cdot & 0 & 3 & \cdot & \cdots \\ \cdot & \cdot & \cdot & 0 & 4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \qquad \mathbf{D}_{i,j} = j \cdot [\![\, i = j-1 \,]\!], \quad i,j \geq 0.$$

Similarly, the linear multiplication operator is represented by the matrix

$$\mathbf{X} = \begin{bmatrix} 0 & \cdot & \cdot & \cdot & \cdot & \cdots \\ 1 & 0 & \cdot & \cdot & \cdot & \cdots \\ \cdot & 1 & 0 & \cdot & \cdot & \cdots \\ \cdot & \cdot & 1 & 0 & \cdot & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \qquad \mathbf{X}_{i,j} = [\![\, i = j+1 \,]\!], \quad i,j \geq 0.$$

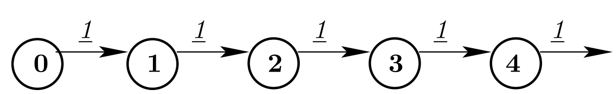
If $\mathbf{H}$ is the matrix obtained from an $\{X,D\}$–operator H by the substitutions $X \mapsto \mathbf{X}$ and $D \mapsto \mathbf{D}$, then, the constant term of H is obtained as

$$\textbf{C.T.}(H) = (1,0,0,\ldots)\,\mathbf{H}\,(1,0,0,\cdots)^{\mathbf{t}}; \tag{76}$$

that is, the constant term of H equals the upper left corner element of $\mathbf{H}$.

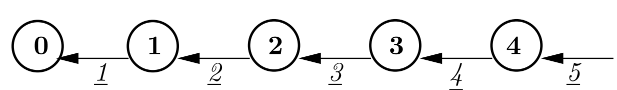
We can now avail ourselves of the basic isomorphism between matrix products and paths in graphs (see, e.g., [9, p. 9] or [47, §V.5.1]). We consider here *digraphs* (directed graphs), whose vertices are the integers $\mathbb{Z}_{\geq 0}$. The graphs also have edges that are allowed to bear *multiplicities*, with the multiplicity of a path being the product of the multiplicities of the edges that it comprises. Then, the *transposed* matrix $\widetilde{\mathbf{X}}$ is the incidence matrix of the following graph (with edge-weights underlined)

$\widetilde{\mathbf{X}}$:



while the transposed $\widetilde{\mathbf{D}}$ corresponds to

$\widetilde{\mathbf{D}}$:



[17] Given a predicate P, we denote by $[\![\, P \,]\!]$ its *indicator*, whose value is 1 if P is true and 0 otherwise (Iverson's notation).

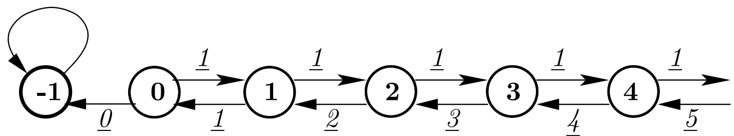


FIGURE 16. The Weyl graph corresponding to $(X+D)$.

The analogy with the way X and D operate is striking—just *interpret state* $\mathbf{k}$ *as representing the quantity* x^k.

Of special interest is the graph similarly constructed from the matrix $(\widetilde{\mathbf{X}}+\widetilde{\mathbf{D}})$ associated to the operator $(X+D)$; it is displayed in Figure 16 and we propose to call it the *Weyl graph.* To each monomial $\mathfrak{f}=\mathfrak{f}_1\cdots\mathfrak{f}_n$ in X,D, we associate a path $\pi(\mathfrak{f})$ obtained by scanning $\mathfrak{f}$ *backwards* and transcribing each letter as either a leftward move (for a D) or a rightward move (for an X):

$$\pi(\mathfrak{f})=\pi_1\cdots\pi_n, \qquad \text{where} \quad \pi_j=\begin{cases}\text{a leftward move } (\widetilde{\mathbf{D}}) \text{ if } \mathfrak{f}_{n-j}=D\\ \text{a rightward move } (\widetilde{\mathbf{X}}) \text{ if } \mathfrak{f}_{n-j}=X.\end{cases} \tag{77}$$

Multiplicities along a path are to be cumulated multiplicatively, as said. In addition, a D-move from vertex 0 is simply to be interpreted as carrying a weight 0 (since $D\cdot\mathbb{1}=0$), which must then make the weight of the whole path to vanish—to take care of this case, its is convenient to add a *"sink node"* (tagged by $-\mathbf{1}$ in Figure 16) to our graph. With these conventions, we can state:

Proposition 13. *Consider a non-commutative monomial* $\mathfrak{f}$ *in* X,D*. The constant term of its normal form is nonzero if and only if the associated path* $\pi(\mathfrak{f})$ *in the Weyl graph of Figure 16, starting from vertex* 0*, returns to vertex* 0*. In that case, this constant term is equal to the multiplicative weight of the path* $\pi(\mathfrak{f})$ *as described in* (77)*.*

Proof. The constant term is given by the matrix form of (76). Here the matrix $\mathbf{H}$ is the one corresponding to the product $\mathfrak{f}_1\cdots\mathfrak{f}_n$ of the Xs and Ds that $\mathfrak{f}$ is composed of. This constant term also equals the upper left corner of the transposed matrix $\widetilde{\mathbf{H}}=\pi_1\cdots\pi_n$ (see Equation (77)). Then, the classical isomorphism between matrix products and graphs yields the statement. $\square$

For instance, $\mathfrak{f}=XXDD$ has $\mathbf{C.T.}(\mathfrak{f})=0$, which corresponds to the fact that, in the reversed form $DDXX$, the first D takes us to the sink state. For $\mathfrak{g}=DDXX$, we have $\mathbf{C.T.}(\mathfrak{g})=2$, since, to the reverse form $XXDD$, there corresponds a path

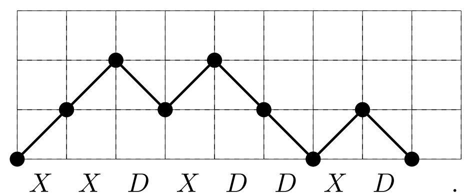
$$0 \xrightarrow{X} 1 \xrightarrow{X} 2 \xrightarrow{D} 1 \xrightarrow{D} 0,$$

with multiplicity $1\times1\times2\times1=2$. By design, this agrees with the interpretation of state k as a token for the monomial x^k:

$$\mathbf{C.T.}(DDXX)=(DDXX)\circ\mathbb{1}=2, \qquad \text{since} \quad 1 \xrightarrow{X} x \xrightarrow{X} x^2 \xrightarrow{D} 2x \xrightarrow{D} 2.$$

This interpretation also gives back the basic property that the constant term of a monomial $\mathfrak{f}=\mathfrak{f}_1\cdots\mathfrak{f}_n$ is nonzero iff each suffix $\mathfrak{f}_j\cdots\mathfrak{f}_n$ has at least as many Xs as Ds *and* the number of Xs in $\mathfrak{f}$ equals the number of Ds.

Finally, a path in the graph $\mathbb{Z}_{\geq 0}$, with edges of the form $(j,j+1)$ and $(j,j-1)$ is classically interpreted as a *lattice path of Dyck type* [108, p. 221], that is, a polygonal line in the cartesian plane $\mathbb{Z} \times \mathbb{Z}$: start from the origin and simply associate a North-East move ("ascent") $\binom{+1}{+1}$ to a rightward step and a South-East move ("descent") $\binom{+1}{-1}$ to a leftward step. *The multiplicity of such a path is the product of the (starting) altitudes of descents.* For instance to $\mathfrak{h} = DXDDXDXX$, there corresponds, by reversion, the path $\pi = XXDXDDXD$ in the Weyl graph, which gives rise to the Dyck representation



.

The multiplicity in this case is $\mathbf{C.T.}(\mathfrak{h}) = 1 \times 1 \times 2 \times 1 \times 2 \times 1 \times 1 \times 1 = 4$.

7.2. **Fermat forms $(X^r + D^r)$ and continued fractions.** Motzkin paths[18] are lattice paths that, in addition to ascents $\binom{+1}{+1}$ and descents $\binom{+1}{-1}$, are also allowed to contain level steps $\binom{+1}{0}$. Flajolet [41] has built elements of a combinatorial theory of continued fractions, which can be viewed as based on the following generating function of Motzkin paths:

$$F(\mathbf{a}, \mathbf{d}, \boldsymbol{\ell}) = \cfrac{1}{1 - \ell_0 - \cfrac{a_0 d_1}{1 - \ell_1 - \cfrac{a_1 d_2}{1 - \ell_2 - \cfrac{a_2 d_3}{\ddots}}}}. \tag{78}$$

(See also [47, §V.4] for a concise exposition.) Here the variables a_j, d_j, and ℓ_j mark, respectively, the ascents, descents, and level steps, with (starting) altitude equal to j. A substitution

$$a_j \mapsto \alpha_j z, \quad d_j \mapsto \delta_j z, \quad \ell_j \mapsto \lambda_j z, \tag{79}$$

then yields the ordinary generating function of Motzkin paths when multiplicities $(\alpha_j, \delta_j, \lambda_j)$ are present, with z marking length. In this case, the continued fraction of (78) becomes

$$F(z) = \cfrac{1}{1 - \lambda_0 z - \cfrac{\alpha_0 \delta_1 z^2}{1 - \lambda_1 z - \cfrac{\alpha_1 \delta_2 z^2}{1 - \lambda_2 z - \cfrac{\alpha_2 \delta_3 z^2}{\ddots}}}}, \tag{80}$$

which is known as a *Jacobi fraction* or *J–fraction* [94, 115]

We note that the continued fractions in (78) and (80) are *ordinary generating functions*, whereas we have been considering so far *exponential* generating functions

[18] Such paths are associated to an enriched Weyl graph in which self loops of the form (j, j) are permitted.

in association with $e^{z\mathfrak{h}}$. The connection is via the formal *Laplace transform* $\mathcal{L}$ defined as

$$\mathcal{L}\left[\sum_{n=0}^{\infty} f_n \frac{z^n}{n!}\right] = \sum_{n=0}^{\infty} f_n z^n,$$

which is (formally; sometimes asymptotically, or even analytically) representable by

$$\mathcal{L}[\varphi(z)] = \int_0^{\infty} e^{-t}\varphi(tz)\, dt.$$

Thus, we shall obtain here constant term identities for the OGF

$$\mathcal{L}\left[e^{z\mathfrak{h}}\right] \equiv \frac{1}{1 - z\mathfrak{h}},$$

instead of the more customary $e^{z\mathfrak{h}}$.

As a first illustration, we revisit the normal ordering problem relative to $\mathfrak{h} = (X + D)$. The constant term of $e^{z\mathfrak{h}}$ is in this case the EGF of "closed" diagrams; i.e., diagrams with no free input or output that are relativ to X–gates and D–gates. For size $2n$, these are enumerated by the odd factorials, $1 \cdot 3 \cdots (2n-1)$, with EGF equal to $e^{z^2/2}$, as we saw already. On the other hand, the interpretation as lattice paths, with weights (79) of the form

$$\alpha_j = 1, \quad \delta_j = j, \quad \ell_j = 0, \tag{81}$$

leads to a continued fraction (80) that must correspond to the OGF of odd factorials. We thus obtain:

Proposition 14. *The normal ordering of* $(X + D)$ *corresponds to the continued fraction expansion*

$$\begin{array}{lcl} \mathbf{C.T.}\left(\dfrac{1}{1 - z(X+D)}\right) & \equiv & \mathbf{C.T.}\left(\mathcal{L}\left[e^{z(X+D)}\right]\right) \\ = \displaystyle\sum_{n\geq 0} \left[1 \cdot 3 \cdots (2n-1)\right] z^{2n} & = & \cfrac{1}{1 - \cfrac{1\cdot z^2}{1 - \cfrac{2 \cdot z^2}{1 - \cfrac{3 \cdot z^2}{\ddots}}}}. \end{array}$$

Analytically, this formal continued fraction is easily derived as a special case of Gauß's expansion of the quotient of contigous ${}_2F_1$ hypergeometric functions [94, 115]. Asymptotically, it is associated with the expansion at infinity of the Gaussian error function. Combinatorially, its proof [41] reduces to a bijection originally due to Françon and Viennot [48], itself based on a linear scan of the arch diagram representation of involutions (see, e.g., [47, Ex. 5.10, p. 333]). The expansion of Proposition 14 is finally tightly coupled with Hermite polynomials, hence the name "Hermite histories" chosen by Viennot for Motzkin–Dyck paths weighted according to (81).

We next turn to the general normal ordering problem of the *Fermat form* $(X^r + D^r)$, with r a natural integer.

Proposition 15. *The normal ordering of* $(X^r + D^r)$ *corresponds to the continued fraction expansion (with* $x^{\overline{r}} = x(x+1)\cdots(x+r-1)$*)*

$$\begin{aligned}
\mathbf{C.T.}\left(\frac{1}{1-z(X^r+D^r)}\right) &\equiv \mathbf{C.T.}\left(\mathcal{L}\left[e^{z(X^r+D^r)}\right]\right) \\
&= \cfrac{1}{1-\cfrac{1^{\overline{r}}\cdot z^2}{1-\cfrac{(r+1)^{\overline{r}}\cdot z^2}{1-\cfrac{(2r+1)^{\overline{r}}\cdot z^2}{\ddots}}}}.
\end{aligned}$$

Proof. What is involved is the collection of all Dyck paths in the Weyl graph, such that Xs and Ds go by groups of r identical letters; for instance $X^3X^3D^3X^3D^3D^3$, for $r=3$. Then, only vertices whose values are multiples of r are reachable. By grouping steps r by r, these paths are seen to be equivalent to paths in the nearest-neighbour graph with vertex set $\mathbb{Z}_{\geq 0}$, but with weights taken according to the rule (with $x^{\underline{r}} = x(x-1)\cdots(x-r+1)$)

$$\alpha_j = 1, \qquad \delta_j = (rj)^{\underline{r}}, \qquad \ell_j = 0.$$

An appeal to the continued fraction theorem (as summarized by (78)) applied to these condensed paths completes the proof. $\square$

For $r=2$, we can make use of the computations of Subsection 5.1 relative to the normal ordering of $(X^2+D^2)^n$, to derive the continued fraction identity:

$$\mathcal{L}\left[\frac{1}{\sqrt{\cos(2z)}}\right] = \cfrac{1}{1-\cfrac{1\cdot 2\cdot z^2}{1-\cfrac{3\cdot 4\cdot z^2}{1-\cfrac{5\cdot 6\cdot z^2}{\ddots}}}}. \tag{82}$$

This fraction can otherwise be deduced from expansions due to Stieltjes and Rogers and relative to $\mathcal{L}[\sec^\theta z]$; here, $\theta = \frac{1}{2}$. Rescaling z to $z/\sqrt{2}$ leads to a continued fraction for the OGF of the sequence

$$1,\ 1,\ 7,\ 139,\ 5473,\ 357721,\ 34988647,\ \ldots,$$

which is *OEIS* **A126156**.

It is unclear whether explicit expressions can be distilled out of the expansion of Proposition 15, when $r \geq 3$. The most intriguing questions in this range is to identify the special functions associated to the simplest case $r=3$, namely,

$$\begin{aligned}
\Phi_3(z) &= \cfrac{1}{1-\cfrac{1\cdot 2\cdot 3\cdot z^2}{1-\cfrac{4\cdot 5\cdot 6\cdot z^2}{1-\cfrac{7\cdot 8\cdot 9\cdot z^2}{\ddots}}}} \\
&= 1 + 6\,z^2 + 756\,z^4 + 458136\,z^6 + 765341136\,z^8 + \cdots .
\end{aligned} \tag{83}$$

Note 20. *On cubic continued fractions.* Only a few cubic analogues of Φ_3 are known. One group is related to the Dixonian elliptic functions [24, 25]; for instance, with a coefficient law that alternates, depending on the parity of levels,

$$\int_0^\infty e^{-t}\,\mathrm{sm}(zt)\,dt = \cfrac{z}{1-\cfrac{1\cdot 2^2\cdot z^3}{1-\cfrac{3^2\cdot 4\cdot z^3}{1-\cfrac{4\cdot 5^2\cdot z^3}{\ddots}}}},$$

where the elliptic function $\mathrm{sm}(z)$ is defined as inverse of an Abelian integral:

$$\int_0^{\mathrm{sm}(z)} \frac{dy}{(1-y^3)^{2/3}} = z.$$

Another group, of Stieltjes–Rogers–Ramanujan–Apéry fame, is related to the Hurwitz zeta function,

$$\zeta(3, x+1) = \sum_{k=1}^{\infty} \frac{1}{(x+k)^3},$$

and it contains, for instance (see [8, p. 153]):

$$\zeta(3,x+1) = \cfrac{1}{2x(x+1)+\cfrac{1^3}{1+\cfrac{1^3}{6x(x+1)+\cfrac{2^3}{1+\cfrac{2^3}{10x(x+1)+\cdots}}}}},$$

which is somehow related to Apéry's proof [111] of the irrationality of $\zeta(3)$. .... ■

From the previous examples, it is easily realized that the general scheme giving rise to explicit continued fraction expansions is when $\mathfrak{h}$ is of the form

$$X^rD^s + X^sD^r + \sum h_j X^j D^j.$$

The steps in the cartesain plane are now of the three vectorial types $\binom{r-s}{1}$, $\binom{s-r}{1}$, and $\binom{0}{1}$, which can be collapsed by a linear change of coordinates to the three types that serve to form Motzkin paths—hence continued fractions. The weights are invariably a polynomial function of the altitude (i.e., the index k). In this way, continued fractions with polynomial coefficients of all degrees can be constructed, though both the special functions aspects (the existence of explicit forms) and the combinatorics (bijections with simple "natural" combinatorial structures) remain unclear at this level of generality.

Note 21. *Horzela structures and* $(XD^2 + X^2D)$. Imagine[19] a universe where particles may be subject both to fission (a particle gives rise to two particles) and fusion (two particles merge to give rise to a single particule). The diagrams are those associated with $(XD^2 + X^2D)$, where gates are of type either $\mathbb{Y}$ or its horizontally flipped image. Thus, the graphical representations are a complex network of trees and "inverted" trees. The

[19] This case was suggested to us by Andrzej Horzela (private communication, 2010).

ordinary generating function $H(z)$ of the diagrams with one root (one input) and one surving particle (one output) is then

$$\begin{aligned} H(z) &= \cfrac{1}{1-\cfrac{1^2\cdot 2\cdot z^2}{1-\cfrac{2^2\cdot 3\cdot z^2}{1-\cfrac{3^2\cdot 4\cdot z^2}{\ddots}}}} \\ &= 1+2\,z^2+28\,z^4+1256\,z^6+129904\,z^8+25758368\,z^{10}+\cdots. \end{aligned}$$

Such H-structures are loosely evocative of cellular decompositions (combinatorial maps) of surfaces of arbitrary genus, a subject of active research (see, e.g., [20, 22] and references therein). . . . . ■

Whenever available, continued fractions are associated with a rich set of identities, due most notably to their connection with orthogonal polynomials [41, 94, 115], and they potentially give rise to efficient computational procedures [71].

7.3. **The general binomial case** $(X^a + D^b)$**.** The general correspondence expressed by Proposition 13 (for monomials) is still applicable to the normal ordering of $(X^p + D^q)$. Thus, there exists a transcription in terms of paths in the Weyl graph, where the allowed steps are either rightward moves of amplitude a or leftward moves of amplitude $-b$; the multiplicity of a path, as before, is the product of the starting altitudes of descents.

However, when $a \neq b$, the connection with continued fractions is lost, as the case is no longer reducible to the Dyck paradigm. The simplest instances are $(X^3 + D^2)$ and $(X^4 + D^2)$ (or their duals, $(X^2 + D^3)$ and $(X^2 + D^4)$). These formally correspond to the *anharmonic quantum oscillator* with a *cubic* or *quartic potential*. The extensive quest for explicit solutions in this context indicates the difficulty of finding connections with the most classical special functions. For the record, we tabulate here the following constant terms:

$$\begin{array}{lcl} \mathbf{C.T.}\left[(D^2+X^3)^n\right]\Big|_{n=0,\ldots,10} & : & 1,0,0,0,0,864,0,0,0,0,1157815296 \\ \mathbf{C.T.}\left[(D^2+X^4)^n\right]\Big|_{n=0,\ldots,10} & : & 1,0,0,24,0,0,49536,0,0,828002304,0\,. \end{array} \tag{84}$$

These seem not to be related to existing sequences in the *OEIS*.

Note 22. *Duchon's clubs.* The lattice paths relative to $(X^3 + D^2)$, but when weights of both leftward and rightward steps are set to 1, appears in the literature under the name of "Duchon's numbers", which enumerate the combinatorial class of "Duchon's clubs" [4, 30]. The sequence of nonzero Duchon numbers (δ_{5n}),

$$1, 2, 23, 377, 7229, 151491, 3361598, 77635093,$$

is *OEIS* **A060941**. In the figurative description of [4, p. 53]:

> "A club opens in the evening and closes in the morning. People arrive by pairs and leave in threesomes. What is the possible number of scenarios from dusk to dawn as seen from the club's entry?"

In this simplified situation (multiplicities of steps are disregarded), we are only considering the possible evolutions in time of the club's population. The *ordinary* generating function $\delta(z)$ is then an *algebraic function*, here of degree 10,

$$z\delta^{10} + 5z\delta^9 + 5z\delta^8 - 10z\delta^7 - 15z\delta^6 + 11z\delta^5 + (15z-1)\,\delta^4 + (1-10z)\,\delta^3 - 5z\delta^2 + 5z\delta - z = 0,$$

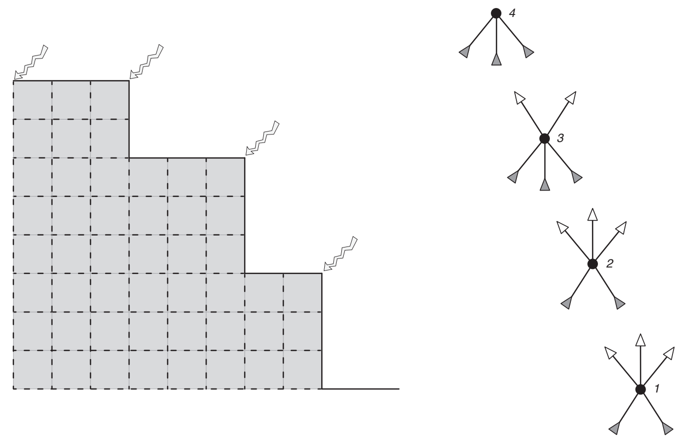


FIGURE 17. The correspondence between the composition of a diagram and its contour,

$$|D^3\,|X^2D^3\,|X^3D^2\,|X^3D^2,$$

interpreted in the discrete plane.

and one has the following explicit expression

$$\delta_{5n} = \sum_{i=0}^{n} \frac{1}{5n+i+1}\binom{5n+i}{n-i}\binom{5n+2i}{i}.$$

It is interesting to note that the case of $(D^2 + X^3)$, or, equivalently $(X^2 + D^3)$, in the first line of (84), corresponds to the situation where, furthermore, we count complete evolutions, in which, additionally, *identities of individuals are taken into account.* .... ■

8. Related frameworks

In this section, we return to the the gates-and-diagram model of creation–annihilation operators of Sections 2–6. We first discuss a model of the reduction to normal form that is expressed in terms of rook placements on a board. This rook model can be derived from first principles (Wick's Theorem, cf Note 1, p. 9, and [112]), but it can also be attached to the basic construction of diagrams and the equivalence asserted by Theorem 1. As we explain in Subsection 8.1, one of the interesting features of the latter approach is the possibility of relating diagrams to the lattice-path methods of the previous section, Section 7: the connection is achieved by a simple "scanning algorithm". Next, in Subsection 8.2, we briefly revisit diagrams within the framework of q-analogue theory, where the q-difference operator Δ replaces the ordinary differential operator D and crossing numbers of (plane embedded) diagrams are shown systematically to produce q-analogues.

8.1. **Rook placements, lattice paths, and diagrams.** We first describe some simple combinatorics that relates diagrams and rook placements on a chessboard. This thread closely follows an insightful article of Varvak [112]; see also [12, 105]. The message here is that one can describe the *complete history* of the construction of diagrams by means of certain kinds of lattice configurations.

We fix a basis $\mathcal{H}$ of gates that, for notational convenience, we take to be unweighted. In other words, we are considering a polynomial with coefficients in $\{0,1\}$,

$$\mathfrak{h} := \sum_{j=1}^{m} X^{r_j} D^{s_j},$$

for a finite set of distinct pairs $(r_j, s_j) \in \mathbb{Z}_{\geq 0} \times \mathbb{Z}_{\geq 0}$. (The general case is easily treated by suitably accommodating weights.) Let g_j represent a generic gate of type $X^{r_j} D^{s_j}$. A diagram δ of size n is determined by the collection $(g_{i_1}, \dots, g_{i_n})$ of its gates, where g_{i_j} is the type of the gate associated to the inner node labelled j, together with the interconnection pattern, which describes the way the outputs of gates are connected with the inputs of some other (later arrived) gates.

As we know (Note 1), a diagram is uniquely associated with a particular reduction of a monomial

$$X^{r_{i_n}} D^{s_{i_n}}\, X^{r_{i_{n-1}}} D^{s_{i_{n-1}}}\, \cdots\, X^{i_{r_1}} D^{s_{i_1}}, \tag{85}$$

using at each stage either of the two rewrite rules $DX \mapsto XD$ or $DX \mapsto 1$. We then define the *contour* of δ as a word over the extended alphabet $\{X, D, |\}$, where "|" serves as a separator and is called a *pin*, as follows:

$$\operatorname{cont}(\delta) := |X^{r_{i_n}} D^{s_{i_n}}\, |\, X^{r_{i_{n-1}}} D^{s_{i_{n-1}}} |\, \cdots\, |X^{i_{r_1}} D^{s_{i_1}}. \tag{86}$$

The contour in this sense is thus an unambiguous representation[20] of the gates that δ is comprised of. Next we represent the contour as a polygonal path in the discrete plane $\mathbb{Z} \times \mathbb{Z}$, with X being interpreted as the vertical unit vector $(0, -1)$ and D being the horizontal unit vector $(1, 0)$. In the discrete plane, this polygonal line determines what is known as a *Ferrers board* [23, 112], see Figure 17, where the pins are represented by arrows.

In order to obtain a bijective encoding of circuits, one need to augment the contour $\operatorname{cont}(\delta)$ so as to encode all the information relative to interconnections of links in the diagram δ. We now consider the Ferrers board whose upper envelope is the contour. Since the order of application of operators in a monomial is from the right, the contour (as of (85) or (86)) is scanned *from the right.* The procedure is as follows (Figure 18):

> In each vertical column (which corresponds to a letter D) do one of two things:
> — either put a single dot (a "rook") in one of the column's cells: a dot in the jth cell from the bottom of the board means that the jth outgoing link (conventionally starting from the right) present in the partial diagram at this stage is connected to the currently active input link of the current gate (this corresponds to the D currently taken into account);
> — or put nothing in the column: this corresponds to a dangling (unattached) D-link.

[20] The pins serve to disambiguate the parsing of a word over the alphabet $\{X, D\}$. They are needed in a few cases; for instance, if $\mathfrak{h}$ contains $(X + X^2)$, since $X^2 = X \cdot X$ can be parsed in two different ways; or in the case of $(X + D + XD)$, since $X^2D^2 = X \cdot XD \cdot D = X \cdot X \cdot D \cdot D$. They are superfluous in cases such as $(X + D)$, $(X^2 + D)$, (X^2D^3), and so on, as considered by Varvak [112].

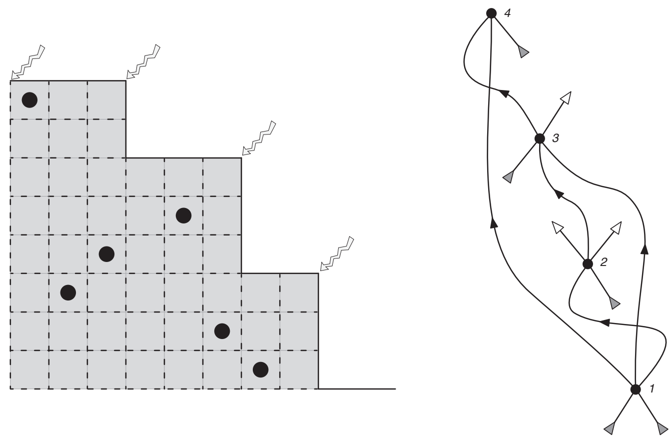


FIGURE 18. The correspondence between a diagram and a rook placement in the square lattice.

A moment's reflection should convince our reader that at most one dot/rook can be placed in each line (since the output of a gate can be "closed" at most once by the input of a later gate), as well as in each column (by construction). This is precisely the rule that constrains the placement of *non-attacking rooks* on a chessboard—here in the case of a board with unconvential right and upper boundaries [100, Ch 7].

We now arrive at a general statement, which is a version adapted to our needs of Varvaks' Theorem 3.1 in [112].

Proposition 16. *The coefficient of X^aD^b in the normal form $\mathfrak{N}(\mathfrak{h}^n)$ is equal to the number of rook placements in Ferrers boards, whose contour is consistent with $\mathfrak{h}^n$, that have $\underline{a}$ rook-free columns and $\underline{b}$ rook-free rows.*

Varvak's proof essentially amounts to an appeal to Wick's Theorem (Note 1, p. 9). The proof given above, without being radically different, amounts to applying to diagrams a *scanning algorithm* whose general scheme is as follows:

> **Scanning algorithm.** Gates are scanned in increasing order of their labels; gate types, encoded by corresponding vectors of $\mathbb{Z} \times \mathbb{Z}$, are generated (these form the steps of a "contour"); additional information (a sequence of numbers) is supplied to specify the interconnection pattern of the new gate with its predecessors.

A variety of encodings are possible, due to the flexibility of the coding conventions, when implementing the scanning algorithm. For instance, regarding the reduction of $(X + D)$, we may associate a northeast step $\binom{1}{1}$ to an X and a southeast step $\binom{1}{-1}$ to a D. The constant term in the normal form of $(X + D)^{2n}$ is then associated with the collection of all Dyck paths of length $2n$, each such path being augmented by a sequence of numbers that serves to encode the interconnection pattern of gates in a particular $\{X, D\}$-diagram. In this specific case, it can be seen that the allowed number sequences are such that an ascent has one possibility whereas a descent has ℓ possibilities, if it corresponds to a step with initial altitude ℓ. The augmented paths produced by the scanning algorithm thus correspond exactly to the weighted Dyck paths considered in Equation (81) and Proposition 14, to be later revisited in Proposition 17 and Figure 21 in relation with q-analogues. Beyond this particular example, *the scanning algorithm generally links circuit-based models and the direct matrix–Weyl graph approach of Section 7.*

8.2. $q-$**analogues and the difference operator.** In this subsection, we propose to discuss briefly the way the theory of gates and diagrams leads in a systematic way to *q-analogues.* The starting point is the *q-difference operator* $\Delta \equiv \Delta_q$ defined by

$$\Delta f(x) = \frac{f(qx) - f(x)}{(q-1)x}. \tag{87}$$

We shall take q to be a real number in $[0, 1]$ and note that, as $q \to 1$, the operator Δ_q becomes the standard derivative operator D. The operators X and Δ satisfy the commutation relation

$$\Delta X - qX\Delta = I, \tag{88}$$

to be compared to (1). A normal form, with all Xs preceding all Δs can always been attained by the rewrite rule analogous to (2):

$$\Delta X \longrightarrow 1 + qX\Delta.$$

(The book by Kac and Cheung [66] provides an undemanding introduction to basic properties of such operators.)

We shall now build in stages a combinatorial interpretation of arbitrary compositions of Δs and Xs. To start with, we observe the effect of Δ on (formal or analytic) power series: if $f(x) = \sum f_n x^n$, then

$$\Delta_q(f)(x) = \sum_{n \geq 0} f_n \frac{1-q^n}{1-q} x^{n-1}. \tag{89}$$

In other words, Δ operates linearly and, on the monomial x^n, its effect is to produce a monomial of degree $(n-1)$:

$$\Delta x^n = [n]x^{n-1}, \qquad \text{where} \quad [n] \equiv [n]_q := \frac{1-q^n}{1-q} = 1 + q + \cdots + q^{n-1}, \tag{90}$$

using classical notations.

Combinatorics of Δx^n***.*** From (90), the operator Δ admits an obvious interpretation: think of the monomial x^n as a row of n occurrences of the variable x; pick up (in all possible ways) one of the x–occurrences and record with a power q^{k-1} the situation where the kth occurrence from the left has been picked up; finally replace the chosen occurrence of x with the neutral element 1 (the identity). (Under this form, it is apparent that the Δ–operator is a deformation of the standard derivative operator: see Note 1.)

A visual image of the action of the Δ operator on an arbitrary monomial can be given in terms of "speed dating clubs" as follows.

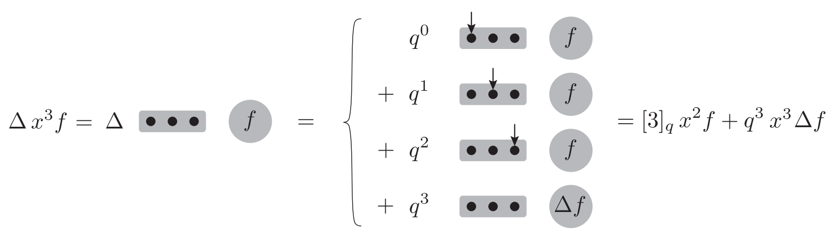
> Imagine a longish hall in which there is a long row of tables. At each table there sits one x–element. A particular operation consists in letting in, at the entrance of the hall, on the *left*, a Δ–element, who will eventually pick up a table. However, for each table that the Δ–element passes by (but does not pick up), he has to pay for a drink (the cost of drinks is recorded by q). Once he settles for a table, the x–element at that table ceases to become available for further drinks and solicitations. What

> the Δ operator does is simply to keep track of all the possible scenarios, when *one* Δ–individual is let in.

For instance, with the example of Note 1:

$$\Delta(xxxx) \;=\; \overbrace{\cancel{x}xxx}^{q^0}+\overbrace{x\cancel{x}xx}^{q^1}+\overbrace{xx\cancel{x}x}^{q^2}+\overbrace{xxx\cancel{x}}^{q^3} \;=\; [4]_q x^3.$$

Combinatorics of $\Delta(x^n f) \equiv \Delta X^n(f)$***.*** In our treatment of operator calculus, an identity $\mathfrak{U} = \mathfrak{V}$ between operators means that, for an arbitrary f (on which the operators act), we have $\mathfrak{U}f = \mathfrak{V}f$. Here, the nature of f is immaterial and, in particular, when dealing with normal forms, quantities such as $\Delta f, \Delta^2 f, \ldots$ are to be considered as non-simplifiable. We can then amend the combinatorial interpretation of the previous paragraph as follows. Imagine now that the longish hall has an exit on the right, leading to a courtyard (biergarten) designated as "f", where Δ elements can accumulate if they haven't picked up an x–element in the hall. This situation is seen to model the action of Δ on $(x^n f)$ or what amounts to the same, the action of ΔX^n on an arbitrary f. Here is an example:



(As a simple exercise, the reader may wish to verify combinatorialy the general identity $\Delta(f \cdot g)(x) = \Delta f(x) \cdot g(x) + f(qx) \cdot \Delta g(x)$.)

Compositions. The interest of this visual image is that it describes well what goes on upon iteration. For instance, we can see that

$$\Delta^n(x^n) = [n] \cdot [n-1] \cdots [2] \cdot [1] \equiv [n]!_q,$$

where the right hand side gives the generating function of permutations counted according to the number of inversions[21]; see Figure 19. This computation is also nothing but the reduction of $\Delta^n X^n(1)$ to normal form.

More generally, given an arbitrary term X and Δ, each possible expansion that it can give rise to, when applied to an arbitrary f, can be described by a succession of operations of adding a table with an x-girl[22] or launching a Δ-boy into the game.

Diagrams. The discussion above leads to a natural extension of the notion of diagram. A quantity $X^r \Delta^s$ will again be represented by a gate in the sense of Section 2, Equation (5). However, when gates are composed to form graphs, a definite convention should be observed.

> All edges are drawn as segments or half-lines parallel to the axes. Each new gate γ, which is added to an existing diagram δ (where the latter involves only smaller labels) is placed on the north-west of the diagram. The inputs of gates γ are drawn horizontally, pointing to the right; the

[21] With our notations, the number of inversions is the number of pairs of values (j, k) such that $j < k$ and the value j is placed on the right of the value k.

[22] The operator X clearly corresponds to placing a new table at the beginning of an existing hall–courtyard configuration.

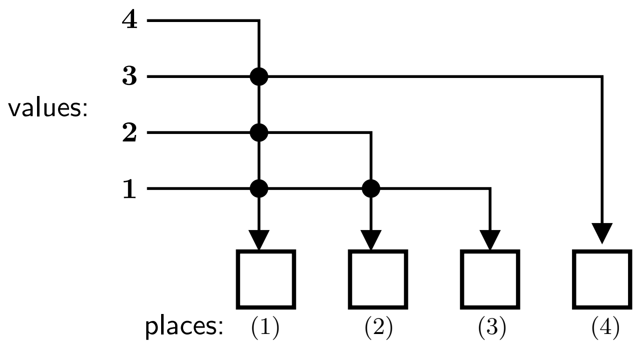


FIGURE 19. A permutation of size 4, such as $\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 3 & 2 & 4 & 1 \end{pmatrix}$, where the first value 1 goes to place 3, and so on, corresponds to a particular expansion of $\Delta^4[x^4]$: it is seen that the number of crossing links equals the number of inversions in the permutation.

outputs are drawn vertically, pointing upwards. Inputs of γ not connected to an output of δ are prolonged as half-lines to the right of the diagram. Outputs of γ not connected to a later gate's input are prolonged upwards as half-lines. See Figure 20.

This convention corresponds to the fact that, in a gate of type (say) $X^2\Delta^3$, the first input corresponds to a first application of Δ, and so on. A diagram represented in this way will be called an *embedded diagram* (Figure 20). The number of pairs of edges that cross is called the *crossing number* of the embedded diagram.

The observations relative to the combinatorics of Δ and the case of permutations then immediately lead to the following statement.

Theorem 2 (Δ–Equivalence Principle)**.** *Consider a polynomial $\mathfrak{h}$ with normal form form*

$$\mathfrak{h} := \sum_{(r,s)\in\mathcal{H}} w_{r,s} X^r \Delta^s. \tag{91}$$

Then the normal ordering of the power $\mathfrak{h}^n$,

$$\mathfrak{N}(\mathfrak{h}^n) = \sum_{n,a,b} c_{n,a,b}(q) X^a \Delta^b, \tag{92}$$

is such that the polynomial $c_{n,a,b}(q)$ coincides with the total weight *of (labelled) embedded diagrams that admit $\mathcal{H}$ as a basis weighted by w, have size n, and are comprised of a outputs and b inputs, where the variable q marks the number of crossings.*

In the case of the reduction of expressions of type $X^{r_1}\Delta^{s_1}\cdots X^{r_n}\Delta^{s_n}$, Méndez and Rodriguez [88] developed an interpretation similar to ours, in terms of crossings. This theme is further explored by Mansour, Schork, and Severini [82] in the context of "Wick's formula". We also refer to the early work of Katriel, Kibler, Solomon, and Duchamp [71, 72, 73] and to the subsequent studies [69, 70, 87, 103] for results relative to the q-Stirling and Bell numbers.

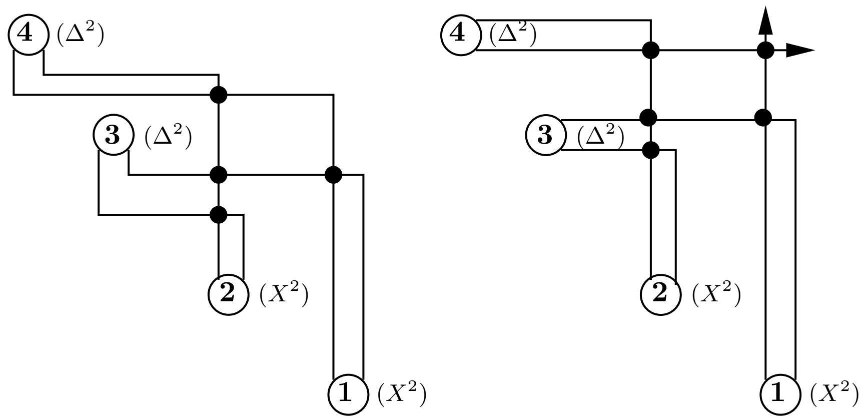


FIGURE 20. *Embedded diagrams* formed with two gates of type X^2 and two gates of type Δ^2: (*left*) a diagram with 4 crossings and $a = b = 0$; (*right*) a diagram with 5 crossings and $a = b = 1$.

The interest of previous developments, where the Δ difference operator replaces the usual derivative D is that they systematically lead to a natural class of q-analogues, which may or may not be classical. The case of Stirling numbers ($(X\Delta)$ and generalizations) being well covered in the literature, we limit ourselves here to examing two cases: $(X + \Delta)^n$, which leads to a q-analogue of the involution numbers (§3.1 above); $(X^2 + \Delta^2)^n$, which is related to alternating permutations (§5.1 above). Our brief treatment will be along the lines of Section 7 dedicated to binomial forms $(X^a + D^b)^n$, with emphasis placed on "constant terms" and continued fraction aspects. We state (cf Proposition 15):

Proposition 17. *Consider the constant term of the normal form of* $(X + \Delta)^n$,

$$I_n(q) := \mathbf{C.T.}\,\mathfrak{N}\left[(X+\Delta)^n\right].$$

Its ordinary generating function satisfies

$$\sum_{n\geq 0} I_n(q)z^n = \cfrac{1}{1 - \cfrac{[1]_q \cdot z^2}{1 - \cfrac{[2]_q \cdot z^2}{1 - \cfrac{[3]_q \cdot z^2}{\ddots}}}}. \tag{93}$$

Furthermore, there exists an explicit form for $I_n(q)$,

$$I_n(q) = \frac{1}{(1-q)^n} \sum_{k=-n}^{n} (-1)^k q^{k(k-1)/2} \binom{2n}{n+k}. \tag{94}$$

Proof. First, the embedded diagrams assocated with the reduction of powers of $(X+\Delta)$ are similar to the ones for permutations (but the distribution of integer labels differs): see Figure 21 and compare with Figure 19. Under this form, it is easily recognized that the embedded diagrams are isomorphic to the arch representatons

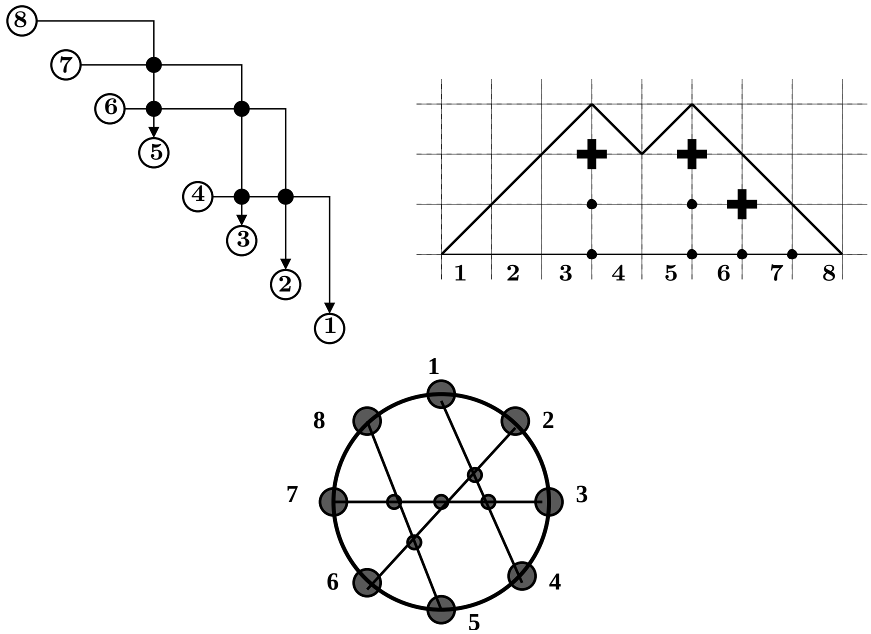


FIGURE 21. Three representations of the involution

$$\sigma = \{\,(1\ 4),\ (2\ 6),\ (3\ 7),\ (5\ 8)\,\}.$$

From top to bottom: (a) the embedded diagram; (b) the associated Hermite history; (c) the chord diagram. The number of crossings equals 5.

of involutions, themselves in bijective correspondence with "Hermite histories"; that is, weighted Dyck paths where a descent from altitude j has multiplicity j.

To see the bijective correspondence[23] with Hermite histories, start from the embedded diagram (Figure 21 (a)). Scan the values from 1 to $n = 2\nu$ and associate an ascent to a value that is smaller in its cycle, a descent otherwise. This gives rise to a Dyck path exemplifed by Figure 21.(b). When a descent from altitude k is produced, say at time τ, there are k possible choices for the 2–cycle that could be closed, the possibilities being enumerated by $[k]_q$. Number conventionally these possibilities according to "age" (oldest first); that is, the open cycle with largest element is numbered 0 the second oldest is numbered 1, and so on. The rank of the possibility chosen appears to be equal to the number of crossings that the cycle ending at τ has with its preceding cycles. Thus, Dyck paths where any ascent is weighted by 1 and a descent from altitude k is weighted by $[k]_q$ are in bijective correspondence with involutions, where each crossing is weighted by q. The expansion (93) now results from the basic theorem of continued fraction combinatorics [41, Th. 1].

The explicit form (94) is none other than the celebrated Touchard–Riordan formula [97, 99, 110] in the enumeration of chord crossings: see Figure 21 (c). $\square$

Similarly, we have:

[23]This correspondence is classical and due to Françon and Viennot (see, e.g., [41, 48] or the accounts in the books [47, p. 333] and [51, §5.2]).

Proposition 18. *The constant terms $I_n^{(2)}(q)$ of the normal form of $(X^2 + \Delta^2)^n$, satisfy*

$$\sum_{n\geq 0} I_n^{(2)}(q) z^{2n} = \cfrac{1}{1 - \cfrac{[1]_q\,[2]_q \cdot z^2}{1 - \cfrac{[3]_q\,[4]_q \cdot z^2}{1 - \cfrac{[5]_q\,[6]_q \cdot z^2}{\ddots}}}}. \tag{95}$$

This is a q-generalization of the continued fraction attached to $1/\sqrt{\cos z}$, for which the authors have not found an explicit form—perhaps some of the methods developed by Josuat-Vergès [61, 62, 63] could be relevant. Also, it would seem interesting to elicit possible connections with q-analogs of expansions of trigonometric functions, as considered by Prodinger [95, 96]. At any rate, we can observe that the continued fraction expansions provided by Propositions 17 and 18 are not devoid of content: they can in particular be employed to derive useful asymptotic information, as is exemplified by several studies [45, 46, 57, 78].

9. Multivariate schemes.

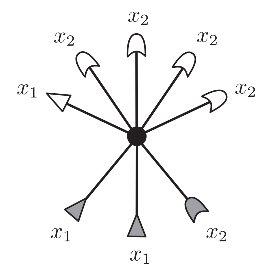
The principles underlying the construction of circuits by means of gates can be extended painlessly to certain multivariate calculi and we provide here brief indications to that effect. Algebraically, we now consider a family of operators $A_1, \dots, A_r, B_1, \dots, B_r$, satisfying the partial commutation relations (expressed in terms of the Lie bracket $[\cdot, \cdot]$):

$$[A_j, B_j] = 1,\ (j = 1, \dots r); \quad [A_j, A_k] = [A_j, B_k] = [B_j, B_k] = 0\ (j \neq k); \tag{96}$$

A faithful model is that of (multivariate) differential algebra where we interpret the operators as acting on functions $f(x_1, \dots, x_r)$, take A_j to be the jth partial derivative, $A_j := \frac{\partial}{\partial x_j}$, and B_j to be multiplication by x_j, that is, $B_j f := x_j f$. We shall adopt this suggestive interpretation and write D_j instead of A_j and X_j instead of B_j. (In concrete examples, we may also name variables and use, for instance, in the case of variables $\{x, y\}$, the notations $\partial_x, \partial_y, X, Y$.) Obviously, any polynomial in the operators X_j, D_j has a normal form in which all the Xs precede all the Ds. Furthermore, we may freely adopt the additional convention that variables obey a standard ordering $x_1 \prec x_2 \prec x_3 \prec \cdots$, so that X_j will be systematically written before X_k if $j < k$, and similarly for D_j and D_k.

The idea is now simply to construct *decorated gates*, which are gates as considered before, with the additional characteristics that each incoming and each outgoing vertex is tagged with a variable name (or its index). We shall also agree that the tags, in left to right order, follow the standard ordering of variables. Thus for instance, the gate associated with $X_1 X_2^4 D_1^2 D_2$ has one inner node connected to three ingoing edges and five outgoing edges:

$X_1 X_2^4 D_1^2 D_2$:



(A tag x_j on an input signifies that derivation is to be effected with respect to the corresponding variable, i.e., ∂_{x_j}, also abbreviated as D_j.) To define diagrams, the rule is now the following: *Outputs of a gate can be connected to inputs of another gate if and only if they have identical variable tags.* Equivalently, the edges of a graph bear various colours (i.e., tags), and when composing an existing diagram with a gate, colours of connecting links must match.

We then have an easy generalization of Theorem 1:

Proposition 19. *The coefficient of*

$$X_1^{a_1} \cdots X_r^{a_r} D_1^{b_1} \cdots D_r^{b_r}$$

in the normal form $\mathfrak{N}(\mathfrak{h}^n)$ is the number (total weight) of (tagged, coloured) graphs built out of gates associated with the monomials of $\mathfrak{h}$, that are comprised of n gates and have a_j outputs of type x_j and b_j inputs of type x_j, for all $j = 1, \ldots, r$.

In the physics literature, multivariate normal form corresponding to (96) are often referred to as “multimode”; see, e.g., [1, 85, 116]. Explicit forms are likely to be quite rare, due to the additional complexity introduced by the need to match colours. We content ourselves with a few examples that are of (some) combinatorial significance.

Note 23. *The combinatorics of $x\partial_y + y\partial_x$ and the Ehrenfest model.* Consider the operator

$$\Gamma := x\frac{\partial}{\partial y} + y\frac{\partial}{\partial x},$$

which serves as a simple illustration of the combinatorial approach to partial differential operators via diagrams. We first state:

Proposition 20. *The operator Γ satisfies the identity*

$$e^{z\Gamma} f(x, y) = f(x \cosh z + y \sinh z, x \sinh z + y \cosh z). \tag{97}$$

Proof. A single application of Γ to $f(x, y)$ picks up the occurrence of a variable, x or y, and either replaces the x with a y, or the y with an x. The diagrams are of the kind constructed in Subsection 4.1 and relative to the normal form of (XD): they consist of line graphs, which are sequences of edges (drawn vertically, as in Figure 7). However, edges are now of one of two colours (x or y), with the additional constraints that the colours along each linear path alternate, as in $xyxy \ldots$ or $yxyx \ldots$.

Now comes the combinatorial reasoning that justifies (97). By linearity, it suffices to consider the action of $e^{z\Gamma}$ on a generic monomial. First, we claim the identities

$$e^{z\Gamma}\, x = (x \cosh z + y \sinh z)\,, \qquad e^{z\Gamma}\, y = (y \cosh z + x \sinh z)\,.$$

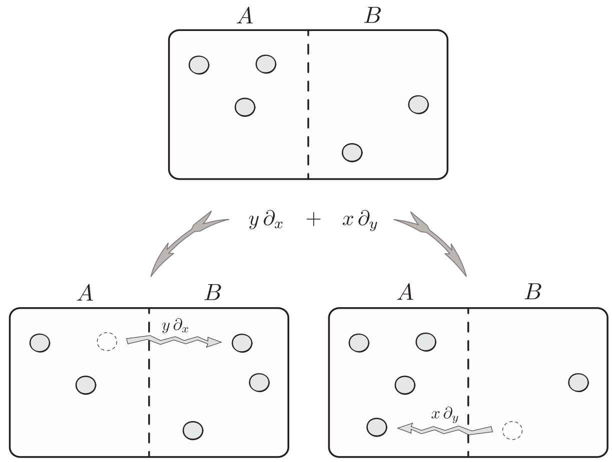


FIGURE 22. Modelling of the Ehrenfest urn by the partial differential operator $x\partial_y + y\partial_x$.

This corresponds to the fact[24] that a connected diagram is a line graph (as in Subsection 4.1), whose input and output are tagged by the same letter (either xx or yy) if the graph has an *even* size, but by different letters (either xy or yx) if the graph has and *odd* size. The formula

$$e^{z\Gamma}\left(x^{a_0}y^{b_0}\right) = (x\cosh z + y\sinh z)^{a_0}\,(y\cosh z + x\sinh z)^{b_0} \tag{98}$$

then results from the general property that the product of EGFs enumerates all possible distributions of labels (marked by z) among components. □

From a combinatorial point of view, what has been done amounts to enumerating ordered partitions into m (possibly empty) blocks, with x and y recording the parity of each block. In the particular case where $b_0 = 0$, $a_0 = m$, and $y = 0$, we obtain the univariate EGF $\cosh^m z$, which enumerates ordered partitions whose blocks are all of even size—this is a well-known (and easy) result.

The analysis above yields as a byproduct a nonstandard analysis of the classical Ehrenfest model [36] (Figure 22), which is defined as follows.

> **Ehrenfest Model.** There are two communicating chambers A, B and m distinguishable particles (say, numbered from 1 to m). At any given instant $1, \ldots, n$, a particle is randomly chosen to change chamber.

The problem consists in determining the probability $P_m(n; a_0, a)$ of having, at time n, a particles in chamber A knowing that there are a_0 particles in that chamber at time 0. (The Ehrenfest Model is a simple statistical model of the diffusion of particles or heat in a heterogenous environment.)

Kac [65] provides a complete solution based on matrix algebra and *ordinary* generating functions. Here, we may simply observe that, by virtue of (98), the probability is

$$P_m(n; a_0, a) = n!m^{-n}[x^a y^b z^n]\,(x\cosh z + y\sinh z)^{a_0}\,(y\cosh z + x\sinh z)^{b_0}\,,$$

[24] Notice the classical expansions

$$\cosh(z) = \sum_{n\equiv 0 \bmod 2} \frac{z^n}{n!}, \qquad \sinh(z) = \sum_{n\equiv 1 \bmod 2} \frac{z^n}{n!}.$$

where $b_0 = m - a_0$ and $b = m - a$. (The factor m^{-n} transforms counts of sample paths into probabilities; the factor $n!$ is due to the fact that we deal with EGFs.) It is then a simple matter to perform coefficient extraction, by successive binomial expansions.

Proposition 21. *The transition probabilities of the Ehrenfest model are given by*

$$P_m(n; a_0, a) = \frac{1}{2^m} \sum_{j=0}^{m} \lambda_{i,j} \lambda_{j,k} \left(1 - \frac{2j}{m}\right)^n,$$

where $\lambda_{i,j} := [z^j](1-z)^i(1+z)^j$.

The derivation just given of the solution to the Ehrenfest model seems to us as "conceptual" as can be. It has strong similarities with the one given by Goulden and Jackson in [52]. It is further developed in several other papers [35, 42, 44] and in the book [47], pp. 118 and 530. . . . . ■

We next discuss a class of bivariate first-order operators, given by Equation (100) below, for which the normal form problem is solvable in finite terms (Proposition 23). Following [42], Figure 23 lists some representative operators for which the connection with urn processes detailed in the Note 24 provides explicit forms. There are also two interesting papers [32, 33] published by Dumont in *Seminaire Lotharingien de Combinatoire* in 1986 and 1996 that deal with combinatorial aspects of powers of special linear partial differential operators: the later one [33] is in particular based on Chen grammars that can be reagarded as a non-probabilistic version of urn processes.

Note 24. *Pólya urn models with two colours.* Here is a specification of this model, also sometimes known as Pólya–Eggenberger model [58, 81].

> **Pólya Urn.** An urn may contain balls of different colours. A fixed set of replacement rules is given (one for each colour). At any discrete instant, a ball is chosen uniformly at random, its colour is inspected, and the corresponding replacement rule is applied.

The modelling capability of the Pólya Urn process is stupendous and the literature on the subject, mostly probabilistic, is immense. Here, we follow the purely combinatorial line of Flajolet *et al.* [42, 43], and only consider models with two colours (say, $\mathcal{X}$ and $\mathcal{Y}$). A model is then determined by a 2×2 matrix with integer entries:

$$\mathbf{M} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}, \qquad \alpha, \beta, \gamma, \delta \in \mathbb{Z}.$$

At any instant, if a ball of the first colour is drawn, then it is placed back into the urn together with α balls of the first colour and β balls of the second colour; similarly, when a ball of the second colour is drawn, with γ balls of the first colour and δ balls of the second colour. A figurative rendition of this replacement rule that we may use occasionally is

$$\mathcal{X} \mapsto \mathcal{X}^\alpha \mathcal{Y}^\beta; \qquad \mathcal{Y} \mapsto \mathcal{X}^\gamma \mathcal{Y}^\delta.$$

(Some authors prefer an additive notation, such as $\mathcal{X} \mapsto \alpha\mathcal{X} + \beta\mathcal{Y}$, which is evocative of chemical reactions.) For instance, the Ehrenfest model of Note 23 is rendered by the following matrix and rule:

$$\mathbf{E} = \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad \left(\mathcal{X} \mapsto \mathcal{X}^{-1}\mathcal{Y}; \quad \mathcal{Y} \mapsto \mathcal{X}\mathcal{Y}^{-1}\right).$$

(Negative diagonal entries α, δ mean that balls are taken out of the urn, rather than added to it). We henceforth restrict attention to balanced urns, which are such that there exists a number s, called the balance, such that

$$s = \alpha + \beta = \gamma + \delta. \tag{99}$$

Name	*operator* (Γ)	*model*
Pólya	$x^2\partial_x + y^2\partial_y$	Models propagation of epidemics or genes (Pólya–Eggenberger). Admits separation of variables and corresponds to shuffles of 1-dimensional histories. References: [42, 58, 80, 81].
Friedman	$xy\partial_x + xy\partial_y$	Friedman's model of "adverse safety campaign". Associated with Eulerian numbers and rises in perms. References: [33, 42, 49, 58, 80, 81].
Ehrenfest	$y\partial_x + x\partial_y$	Ehrenfest model of the diffusion of particles. Associated with ordered set partitions and parity of blocks. References: Note 23 and [42, 47, 58, 81].
Coupon collector	$y\partial_x + y\partial_y$	Models the classical coupon collector problem. Associated with surjections, ordered set partitions, and Sirling$_2$ numbers. References: [42, 47, 58, 81].
Sampling I	$x\partial_x + y\partial_y$	Sampling with replacement. Admits separation of variables. References: [42, 58, 81].
Sampling II	$\partial_x + \partial_y$	Sampling without replacement. Admits separation of variables. References: [42, 58, 81].
Records	$x^2\partial_x + xy\partial_y$	Models records in permutations and is associated with Stirling$_1$ numbers. Describes the growth of the rightmost branch in a binary increasing tree. References: [42].
Bimodal-2	$y^2\partial_x + x^2\partial_y$	Models a (binary) chain reaction with two types of particles: $\mathcal{X} \mapsto \mathcal{Y}^2, \mathcal{Y} \mapsto \mathcal{X}^2$. Corresponds to parity of levels in increasing binary trees and models fringe-balanced trees. Is solved in terms of Dixonian elliptic functions sm, cm. References: [25, 42, 43, 93].
Bimodal-3	$y^3\partial_x + x^3\partial_y$	Models a (ternary) chain reaction with two types of particles: $\mathcal{X} \mapsto \mathcal{Y}^3, \mathcal{Y} \mapsto \mathcal{X}^3$. Corresponds to parity of levels in increasing ternary trees and is solved in terms of lemniscatic elliptic functions sl, cl. References: [42, 43].

FIGURE 23. A list of some first-order bivariate operators (99) associated with solvable urn models and explicit normal forms, together with the main characteristics of the models, after [42].

Given an urn initialized with a_0 balls of the first colour and b_0 balls of the second colour, what is sought[25] is the multivariate generating function $H(x, y, z)$ (of exponential

[25] For balanced urns (only), there is complete equivalence between probabilistic analysis and enumeration of histories [42].

type), such that $n![z^n x^a y^b]\, H(x,y,z)$ is the number of possible evolutions (also known as "histories" or "sample paths") of the urn leading at time n to an urn with colour composition (a,b). Let $t_0 = a_0 + b_0$ be the initial size of the urn. For $s \geq 1$, the total number of evolutions is clearly $t_0(t_0+s)\cdots(t_0+(n-1)s)$, so that $H(1,1,z) = (1-sz)^{-t_0}$.

Let the formal monomial $\mathfrak{m} = x^a y^b$ represent a particular urn comprised of a balls of type $\mathcal{X}$ and b bals of type $\mathcal{Y}$. From our introductory discussion of the combinatorics of derivatives in Note 1, we can see that the effect of all the one-step evolutions of the urn are described by the linear *partial differential operator*

$$\Gamma = x^{\alpha+1} y^{\beta} \frac{\partial}{\partial x} + x^{\gamma} y^{\delta+1} \frac{\partial}{\partial y}, \qquad \alpha+\beta = \gamma+\delta. \tag{100}$$

applied to $\mathfrak{m}$. In the same way, Γ^2 generates all two-step evolutions, and so on. We then have an easy observation [43]:

Proposition 22. *The EGF of histories of a balanced urn with two colours and initial composition* (a_0, b_0) *satisfies*

$$H(x,y,z) = e^{z\Gamma}\,(x^{a_0} y^{b_0}),$$

where Γ *is the operator specified in* (100).

In other words, the solution to the urn problem is equivalent to the reduction to normal form of the powers Γ^n (equivalently, the exponential $e^{z\Gamma}$) of the associated first-order partial differential operator Γ. It is noteworthy that, under the conditions (two-coloured and balanced), this normal ordering problem is solvable. The treatment consists in associating an *ordinary* differential system,

$$\Sigma \ : \quad \left\{ \frac{d}{dt} X(t) = X(t)^{\alpha+1} Y(t)^{\beta}, \quad \frac{d}{dt} Y(t) = X(t)^{\gamma} Y(t)^{\delta+1} \right\}, \tag{101}$$

which admits a first integral that is a polynomial (namely, $Y^p - X^p = 1$, with $p = \gamma - \alpha$) and which can be explicitly related to the multivariate EGF $H(x,y,z)$. We quote from [42, Th. 2].

Proposition 23. *Two-coloured balanced urns and the associated normal form problem for the operator* Γ *in* (100) *are solvable by quadrature*[26]*: in the case*[27] $\alpha < 0$*, one has*

$$\left[e^{z\Gamma}\,(x^{a_0} y^{b_0}) \right]_{y=1} = \Delta^{t_0} S\left(-\alpha z \Delta^s + J(x^{-\alpha}\Delta^{\alpha})\right)^{-\frac{a_0}{\alpha}} C\left(-\alpha z \Delta^s + J(x^{-\alpha}\Delta^{\alpha})\right)^{-\frac{b_0}{\delta}}.$$

The notations are

$$s = \alpha+\beta, \quad p = \beta - \alpha; , \quad t_0 = a_0 + b_0,$$

as well as $\Delta \equiv \Delta(x) = (1-x^p)^{1/p}$*, and* $J(u) := \displaystyle\int_0^u \frac{d\zeta}{(1+\zeta^{-p/\alpha})^{p/\beta}}$*. The function* $S(z)$ *is defined as the inverse of* $J(u)$*, namely,* $S(J(u)) = J(S(u)) = u$*; the function* $C(z)$ *is given by* $C(z) = (1+S(z)^{-p/\alpha})^s$*.*

Though the general formula looks rather formidable, great simplifications occur in many models of pratical interest and the expressions lend themselves to precise asymptotic analysis, as detailed in [42]. . . . . ■

[26] It can be seen that the variable y is redundant, so that the substitution $y \mapsto 1$ entails no loss of generality.

[27] Among negative values, only $\alpha = -1$ is of direct relevance to the normal ordering problem in its standard form, since, in the present study, negative powers of X are excluded. The case $\alpha \geq 0$ seems to give rise to similar developments (B. Morcrette, work in progress, July 2010).

Name	*operator* (Γ)	*model*
Pólya	$w^2\partial_w + x^2\partial_x + y^2\partial_y$	Models propagation of genes. Admits separation of variables and corresponds to shuffles of 1-dimensional histories. References: [42, 58, 81].
C-Ehrenfest	$x\partial_w + y\partial_x + w\partial_y$	Models particles in a cycle of three chambers. Associated with ordered set partitions and congruence properties of block sizes. References: [42].
S-Ehrenfest	$(x+y)\partial_w + (y+w)\partial_x + (w+x)\partial_y$	Models particles in a symmetric set of three chambers. References: [42].
Coupon	$x\partial_w + y\partial_x + y\partial_y$	Models multiple coupon collections. Associated with surjections, ordered set partitions, and generalized Sirling$_2$ numbers. References: [42, 47].
Pelican	$xy\partial_w + yw\partial_x + wx\partial_y$	Models the pelican sacrifice model. Is solved in terms of Jacobian elliptic functions sn, cn. References: [32, 42, 113].

FIGURE 24. Some first-order trivariate operators (99), in variables w, x, y, that are associated with solvable urn models and explicit normal forms, together with the main characteristics of the models, after [42].

Note 25. *First-order differential operators, multitype trees, and the method of characteristics.* The objet of interest here is the operator

$$\Lambda = \sum_{j=1}^{m} \phi_j(X_1, \ldots, X_m) D_j + \rho(X_1, \ldots, X_m).$$

What we do here is to extend the univariate framework of the semilinear case of Section 6 to m variables. The combinatorial model will once more be expressed in terms of increasing trees. We shall write $\mathbf{x}$ for the vector of variables $(x_1, \ldots, x_m)$. We state:

Proposition 24. *The exponential $e^{z\Lambda}$ admits a normal form*

$$e^{z\Lambda} = e^{R(\mathbf{x},z)} \exp\left(\sum_{j=1}^{m} T_j(\mathbf{x}, v_j) \right)_{v_j \mapsto D_j},$$

where the functions T_j and satisfy the ordinary differential system

$$(102)\qquad \begin{cases} \dfrac{\partial}{\partial z} T_1(\mathbf{x}, z) &=& \phi_1(x_1 + T_1(\mathbf{x}, z), \ldots, x_m + T_m(\mathbf{x}, z)), & T_1(\mathbf{x}, 0) = 0 \\ \vdots & \vdots & \vdots & \vdots \\ \dfrac{\partial}{\partial z} T_m(\mathbf{x}, z) &=& \phi_m(x_1 + T_1(\mathbf{x}, z), \ldots, x_m + T_m(\mathbf{x}, z),) & T_m(\mathbf{x}, 0) = 0, \end{cases}$$

and

$$R(\mathbf{x}, z) = \int_0^z \rho(x_1 + T_1(\mathbf{x}, w), \ldots, x_m + T_m(\mathbf{x}, w))\, dw. \tag{103}$$

Proof. Combinatorially, we are now dealing with a collection $\mathcal{T}_1, \ldots, T_m$ of trees of m different types. The multivariate extension of the basic framework of gates, Proposition 19 shows that the $\mathcal{T}_j$ must represent a collection of types of increasing trees satisfying the equations

$$\mathcal{T}_j = \mathcal{Z}^\square \star \phi_j(x_1 + \mathcal{T}_1, \ldots, x_m + \mathcal{T}_m),$$

for $j = 1, \ldots, m$, and $\mathcal{R}$ is a "planted" variety of trees corresponding to

$$\mathcal{R} = \mathcal{Z}^\square \star \rho(x_1 + \mathcal{T}_1, \ldots, x_m + \mathcal{T}_m).$$

(Here, the variables x_j serve to mark the types of leaves.) This gives rise to a set of integral equations,

$$\frac{\partial}{\partial z} T_j(\mathbf{x}, z) = \int_0^z \phi_1(x_1 + T_1(\mathbf{x}, w), \ldots, x_m + T_m(\mathbf{x}, w))\, dw$$

which are cleary equivalent to the differential relations (102), as well as to the expression of R in (103). $\square$

In terms of *partial* differential equations, Proposition 24 concerns the solution $F(\mathbf{x}, z)$ of

$$\frac{\partial}{\partial z} F(\mathbf{x}, z) = \sum_{j=1}^m \phi_j(x_1, \ldots, x_m) \frac{\partial}{\partial x_j} F(\mathbf{x}, z) + \rho(x_1, \ldots, x_m) F(\mathbf{x}, z). \tag{104}$$

What is noticeable is the fact that there is a reduction to a collection of *ordinary* differential equations, of which the Ehrenfest urn of Note 23 provides an explicitly solvable case—the equations are in general non-linear, though, and integrability is far from being granted. This reduction is classically achieved by the well-known method of characteristics [109, §1.15]. We then have: *the method of characteristics, in the special case* (104) *at least, admits a combinatorial model, which is that of multitype increasing trees.*

In the particular case where $\rho = 0$ and the ϕ_j are homogeneous[28] polynomials of total degree s, the solution $F(\mathbf{x}, z)$ provides the enumeration of histories of a balanced urn model with m colours and balance s. This generalizes the results of Note 24 relative to two-colour models. Our equivalence with the combinatorics of increasing trees can then be seen as a parallel to the reduction of urn models to multitype branching processes [2, §9]. . . . . ■

Explicit iteration formulae (normal forms) for first-order operators in more than two variables are somewhat rare: see Figure 24 for some solvable cases associated with balanced urn models, drawn from [42], and the papers by Dumont [32, 33] for some additional examples related to classical combinatorics. Even less is explicit in the case of higher order operators. In the quantum physics literature, the paper of Agrawal and Mehta [1] shows what can be done with the exponential of multivariate quadratic forms in X_j, D_j and it would be of obvious interest to elicit its combinatorial content. Similar comments apply to the works of Heffner and Louisell [56], Louisell [79, pp. 203–207], Marburger [83, 84], and Wilcox [117], to name a few.

[28] In the inhomogeneous case, the probabilistic connection with urn processes is lost and we are plainly enumerating combinatorial tree families, or, what amounts to the same by Subsection 8.1, certain families of weighted lattice paths.

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Appendix A. **Scherk's dissertation of 1823**

In this appendix, we examine the "inaugural dissertation" [102] which Heinrich Ferdinand [Henricus Ferdinandus] Scherk defended in 1823 at the University of Berlin. The dissertation is in Latin, and, as this language may not be easily understood by the younger generation, we offer here a brief account of its contents. In modern terms, Scherk's thesis can be seen as dealing with the reduction to normal form of an expression of the form $(yD)^n$, where various choices for the function $y = y(x)$ are considered. The evocative title of the dissertation is, from its front page:

DE

EVOLVENDA FUNCTIONE

$$\frac{\mathbf{yd.\,yd.\,yd}\ldots\mathbf{yd}\mathcal{X}}{\mathbf{dx^n}}$$

DISQUISITIONES NONNULLAE ANALYTICAE.

That is, *"Some analytic investigations relative to the expansion of the function* $(yD)^n\mathcal{X}$*"*. Throughout this section, the calligraphic $\mathcal{X} = \mathcal{X}(x)$ is taken to represent an arbitrary function, not to be confused[29] with the operator X.

The memoir is comprised of 10 sections (numbered **1** to **10**) and the body of the text consists of 36 pages, It is supplemented by a two page table of values of Stirling numbers, followed by a two page Vita [102, pp. 36-37], where we learn that Scherk was born on October 27, 1797 in the (now Polish) city of Poznań. It concludes with a page containing four assertions (called *"theses"*), apparently of the author's own design, amongst which the second one reads

Calculi, quos dicunt superiores, in Algebra elementari ponendi sunt.

A rough rendition is: *"What is known as the higher calculus is to be placed within the framework of elementary algebra"*. This excellently summarizes the philosophy underlying Scherk's work (as well as ours!).

We are very much indebted to Dr Morteza Mohammad Noori, from the University of Tehran, for drawing our attention to Scherk's thesis. An electronic version can be found under the rich and highly useful GDZ site (Göttinger Digitalisierungszentrum),

`http://gdz.sub.uni-goettingen.de/` ,

from which a large portion of the nineteenth century mathematical literature in German is available. The MacTutor reference site for mathematicians' biographies has an extended bibliographic notice on Scherk, which can be supplemented by the dedicated site hosted by the University of Halle. The url's are:

[29] This is meant to preserve the correspondence with Scherk's original notations.

`http://www-history.mcs.st-and.ac.uk/`
`http://cantor1.mathematik.uni-halle.de/history/scherk/`.

(There we learnt that Scherk's later discovery of the third non-trivial examples of a minimal surface brought him considerable fame. He appears to have been otherwise interested in Bernoulli and secant numbers, as well as in the number of combinations with bounded repetitions.) The Mathematical Genealogy Project indicates that Scherk had 19728 descendants (via his famous student, Ernst Kummer), as of July 2010.

∼∼∼∼∼∼∼∼

§1. Scherk first notes (p. 1) that the series previously considered mostly involve an iterated use of arithmetic operations, especially, multiplication and division. In this category, we find series such as

$$\sum f_n x^n, \qquad \sum_n f_n x(x-1)\cdots(x-n), \qquad \sum_n f_n \frac{1}{x(x+1)\cdots(x+n)},$$

which are of Taylor, Newton-interpolation, and factorial type, respectively—these had all been investigated by his time. Scherk then notes that little is known if the formation law of the general term of a series involves arbitrary differentiation and integration operations. The most general problem, he notes, exceeds by far his own strength. Accordingly, he focuses his attention to the special case

$$\frac{(yd)^n \mathcal{X}}{dx^n},$$

which, in our notations, is $(yD)^n\mathcal{X}$, where $y = y(x)$ and $\mathcal{X} = \mathcal{X}(x)$. He then goes on to explain (p. 2) that his purpose will be to express the general term as a function of the derivatives $\mathcal{X}, \mathcal{X}', \ldots$. In our terminology, this is equivalent to seeking *normal forms*, where all the occurrences of the derivative D appear on the right.

§2. The problem to be considered now is the case $y = x$. A small table (p. 2),

$$\begin{array}{lcl} (xD)\mathcal{X} & = & xD\mathcal{X} \\ (xD)^2\mathcal{X} & = & xD\mathcal{X} + x^2D^2\mathcal{X} \\ (xD)^3\mathcal{X} & = & xD\mathcal{X} + 3x^2D^2\mathcal{X} + x^3D^3\mathcal{X}, \end{array}$$

suggests an interesting law. Indeed, the operator formula (with $D \equiv \frac{d}{dx}$ and X representing as usual multiplication by x; i.e., $Xf(x) := xf(x)$)

$$(XD)^n = \sum_{j=1}^{n} a_j^n X^j D^j \tag{105}$$

serves to define a (yet unknown) array of numbers $\{a_j^n\}$. (Scherk writes $\overset{n}{\underset{j}{a}}$ for what we denote by a_j^n)

By considering $(xD)^n\mathcal{X} = (xD)\,(xD)^{n-1}\mathcal{X}$, one easily obtains the recurrence (p. 3)

$$a_k^n = a_{k-1}^{n-1} + k a_k^{n-1}. \tag{106}$$

Scherk	*definition*	*modern*	*properties*
a_k^n	defined for §2–3 as coefficients in the normal form of $(XD)^n$, cf Eq. (105)	$\left\{ {h+k \atop k} \right\}$	equivalence with Stirling_2 numbers is granted via Eq. (107), assuming as known the alternating sum expression of Stirling_2 numbers
${C'}_k^h$	defined, as in Eq. (108) below, as elementary symmetric function of degree h in the integers $1, 2, \dots, k$; see [102, p. 4]	$\left[{k+1 \atop h+1} \right]$	equivalence via the (now) classical generating function of Stirling_1 numbers
${}'C_k^h$	defined, as in Eq. (109) below, as complete homogeneous symmetric function of degree h in the integers $1, 2, \dots, k$; see [102, p. 5]	$\left\{ {h+k \atop k} \right\}$	equivalence via the (now) classical generating function of Stirling_2 numbers

FIGURE 25. A correspondence table for §1–7: Scherk's notations, his definitions, the corresponding modern notations, and corresponding properties.

Scherk then derives (p. 4) the (by now classical) alternating sum formula

$$a_k^n = \frac{1}{(k-1)!} \sum_{h=0}^{k-1} \binom{k-1}{h-1} (-1)^{k-h} h^{n-1}, \tag{107}$$

his notations being $\Pi(k) = k!$ and $P_y^x = \binom{y}{x} = \frac{y!}{x!\,(y-x)!}$.

Next (bottom of p. 4 and top of page 5), Scherk proceeds to introduce two types of numbers[30] ${C'}_k^h$ and ${}'C_k^h$, s follows.

— The quantity ${C'}_k^h$ is defined as the sum of combinations *without repetitions* of h of the integers $1, 2 \dots, k$; in symbols,

$${C'}_k^h = \sum_{1 \le j_1 < j_2 < \cdots < j_h \le k} j_1 j_2 \cdots j_h. \tag{108}$$

— The quantity ${}'C_k^h$ is similarly defined as a sum of combinations *with repetitions*; in symbols,

$${}'C_k^h = \sum_{1 \le j_1 \le j_2 \le \cdots \le j_h \le k} j_1 j_2 \cdots j_h. \tag{109}$$

Remarks. The definitions of the number arrays ${}'C, C'$ are nowadays easily seen to be equivalent to the generating function expressions

$$\sum_h {C'}_n^h x^h = (x+1) \cdots (x+n), \qquad \sum_h {}'C_n^h x^h = \frac{1}{(1-x)(1-2x)\cdots(1-nx)},$$

where one can recognize variants of Stirling numbers [23].

Scherk then gives (p. 5) two recurrences

$${C'}_k^h = {C'}_{k-1}^h + k{C'}_{k-1}^{h-1}; \qquad {}'C_k^h = {}'C_{k-1}^h + k\,{}'C_k^{h-1}. \tag{110}$$

[30] We continue using more modern notations and write C_k^h for what Scherk denotes by $\mp C_k^h$.

and he concludes (p. 6) from a comparison of the recurrences (106) and (110) that

$$a_{n,k} = {}'C_k^{n-k},$$

which provides the normal form of $(XD)^n$ as (his notations, p. 6):

$$\frac{(xd)^n \mathcal{X}}{dx^n} = \sum_{k=1}^{n} {}'C_k^{n-k} x^k \frac{d^k \mathcal{X}}{dx^k}. \tag{111}$$

We state[31], with modern notations:

Proposition A.1 (Scherk [102, p. 6])**.** *The normal form of $(XD)^n$ is given by*

$$(XD)^n = \sum_{k=1}^{n} \begin{Bmatrix} n \\ k \end{Bmatrix} X^k D^k, \qquad n \geq 1.$$

§3. Scherk continues (pp. 7–8) with various considerations related to setting $\mathcal{X} = -x(1-x)^{k-1}$ followed by the substitution $x = 1$. His goal is to obtain a new proof of the normal form result (111). He also rederives in this framework the relation (107) directly from the definition of the a_k^n.

§4. We now come to another problem, namely, that of the reduction of

$$(e^x D)^n \mathcal{X}.$$

The coefficients[32] b_k^n are determined by the normal form (p. 9):

$$(e^x D)^n \mathcal{X} = e^{nx} \sum_{k=1}^{n} b_k^n D^k \mathcal{X} \tag{112}$$

Scherk then derives a recurrence to be compared to our Equation (110), from which there results (p. 10) that

$$b_k^n = C'^{n-k}_{n-1}.$$

Thus the b_k^n are now recognizable as Stirling numbers of the first kind. We state:

Proposition A.2. *The normal form of $(e^x D)^n$ is given by*

$$(e^x D)^n = e^{nx} \sum_{k=1}^{n} \begin{bmatrix} n \\ k \end{bmatrix} D^k.$$

The section concludes with representations of Stirling_1 numbers in terms of (sort of) generalized harmonic numbers.

§5. This section digresses from the main course of the dissertation (p. 14) and is admittedly only loosely related to the other sections. The problem consists in finding the laws of the derivatives of a composite function. The formula, commonly attributed to Faà di Bruno (born in 1825(!), publication dated 1850), figures explicitly (p. 14); see [23] for a statement. Scherk says:

expressionem quamdam invenimus, qualem frustra in multis libris jam seapius quaesiveramus, quam itaque paucis verbis hic tangere liceat.	*we have discovered a certain formula, which we have very often tried in vain to find in books, so that we feel allowed to devote a few words to its description.*

---

[31] As it was customary in his time, Scherk does not provide typographically marked statements, such as theorems or propositions, but rather plainly quotes his main results *en passant*.

[32] In fact, Scherk also denotes the new coefficients by $a_{n,k}$; we adopt a different convention for clarity.

We refer to the scholarly study of Warren Johnson [59], regarding the history of this formula, which was once considered a basic component of combinatorial analysis. Nowadays, via generating functions, the computation of the nth derivative of a composite function $f(g(z))$ amounts to nothing but the determination of a coefficient,

$$n!\,[z^n]\sum_{j=0}^{n}\frac{f_j}{j!}\left(\sum_{k=1}^{n} g_k\frac{z^k}{k!}\right)^j;$$

i.e., it is a simple avatar of the multinomial formula.

§6. Scherk now considers (p. 15) the *inverse problem*: how to express the derivatives D^nX in terms of the quantities $(xD)^nX$ and $(e^xD)^n\mathcal{X}$. His main formula is (p. 18)

$$(X^nD^n)\mathcal{X} = \sum_{h=0}^{n-1}(-1)^h {C'}^h_{n-1}(xD)^{n-h}\mathcal{X}.$$

and a parallel one serves to express $e^{nx}D^n$ in terms of the powers $(e^xD)^j$, this time by means of the Stirling$_2$ numbers (his $'C$). In rerospect, these two formulae are manifestations of the fact that the matrices of Stirling$_1$ and Stirling$_2$ are inverse of each other. Scherk can then conclude that the coefficients C' serve to make explicit the law of the successive derivatives of $1/(x\log x)$ (p. 18) and $\log\log x$ (p. 19, top):

$$\frac{d^n}{dx^n}\log\log x = \frac{(-1)^{n-1}}{x^n}\left(\sum_{k=0}^{n-1}\begin{bmatrix} n\\ k+1\end{bmatrix}\frac{k\,!}{(\log x)^{k+1}}\right).$$

§7. This section gives two further consequences (p. 20) of previous developments including a formula which expresses the expansion of a function $g(z)$ in terms of $\log z$, when z is near 1.

§8. The purpose is now to come back to the general problem (p. 20) of the reduction of $(yD)^n$. Naturally, large symbolic expressions are available, for small n, involving $y, y', y'', \ldots$ (The notation used in the memoir is $\underset{i}{y} = y^{(i)}$.) A typical formula (p. 20) reads:

$$\frac{(yd)^4\mathcal{X}}{dx^4} = \left(yy'^3 + 4y^2y'y'' + y^3y'''\right)\mathcal{X}' + (7y^2y'^2 + 4y^3y'')\mathcal{X}'' + 6y^3y'\mathcal{X}''' + y^4\mathcal{X}''''.$$

A discussion of the combinatorics of the coefficients occupies the next few pages (pp. 21–27). Naturally, the previously considered cases $y = x$ and $y = e^x$ provide various checks. The corresponding coefficients are denoted by v_n^k (written as usual as $\overset{k}{\underset{n}{v}}$ in the memoir). Scherk deduces various *qualitative* results on the shape of a general expansion: he obtains exact values for the first few coefficients as well as some infinite classes of particular coefficients. He then concludes regarding a possible discovery of the general law: .

Solutio itaque ideo tam difficilis facta est, quod disquisitionem coefficientium numericorum ab inventione singulorum terminorum ipsorum segregare non potuirimus.	*Then, the process has become so untractable that we could not succeed with an investigation of all the numerical coefficients, based on the sole discovery of some individual terms.*

Remarks. The symbolic problem is indeed *difficult*. From the solution described earlier, in our Section 6, we now know the following.

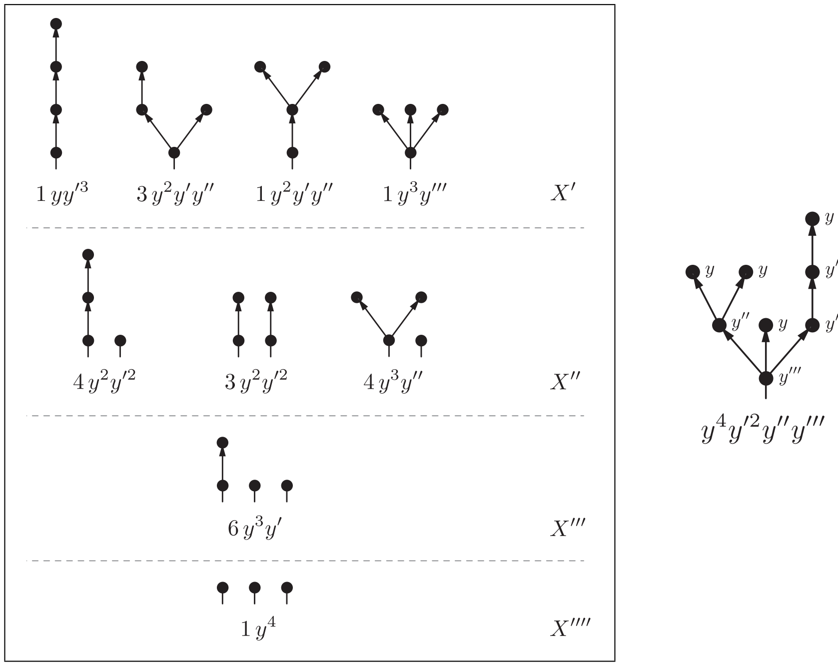

Figure 26. *Left*: An illustration of the correspondence between Scherk's expansion of $(yD)^n\mathcal{X}$ and forests of trees (case $n = 4$). *Right*: the decoration of a particular tree by the derivatives of y

(*i*) The coefficient of $\mathcal{X}^{(r)}$ in $(yD)^n\mathcal{X}$ is obtained from the set of unordered r-forests of (rooted, non plane) increasing trees having a total size of n, by assigning to a vertex of outdegree j a weight equal to $y^{(j)}$; see Figure 26. (Trees are taken "unordered" (i.e., non-plane) owing to the fact that $y(x)$ is here an exponential generating function.)

(*ii*) Symbolically, one should proceed as follows, for an expansion of $(yD)^n\mathcal{X}$:
- — Start from $y(x) = \sum_j y_j x^j/j!$, so that y_j plays the rôle of $y^{(j)}$.
- — Compute $1/y(x)$, which involves a series of multinomial expansions.
- — Integrate the previous expansion, which only involves a substitution $x^n \mapsto x^n/n$ for each n: we get in this way $\Phi := \int y^{-1}$.
- — Take the compositional inverse of the preceding expansion Φ—this, by the Lagrange inversion theorem only involves a further sequence of multinomial expansions. (We determine here the generating function $T(x)$ of increasing trees.)
- — Raise $T(x)$ to the rth power (for the coefficient of $\mathcal{X}^{(r)}$), extract the coefficient of x^n in $\frac{1}{r!}T^r$, and finally multiply this coefficient by $n!$ since we are dealing with exponential generating fuctions.

Barely half a dozen instruction suffice to implement the general procedure in a symbolic manipulation system such as Maple. We can in this way verify, in a fraction of a second, the correctness of the expansion relative to $(yD)^5\mathcal{X}$, in the form given by Scherk (p. 20). For the benefit of the curious reader, here is the outcome of our program in the case of $(yD)^6\mathcal{X}$:

$$\begin{aligned}
&\mathcal{X}_1\left(32\,y_3{y_0}^3{y_1}^2 + 34\,{y_2}^2{y_0}^3y_1 + y_0{y_1}^5 + 26\,y_2{y_0}^2{y_1}^3 + 11\,y_1y_4{y_0}^4 + 15\,y_3{y_0}^4y_2 + y_5{y_0}^5\right)\\
+\,&\mathcal{X}_2\left(34\,{y_0}^4{y_2}^2 + 31\,{y_0}^2{y_1}^4 + 146\,{y_0}^3y_2{y_1}^2 + 57\,{y_0}^4y_1y_3 + 6\,{y_0}^5y_4\right)\\
+\,&\mathcal{X}_3\left(90\,{y_0}^3{y_1}^3 + 120\,{y_0}^4y_1y_2 + 15\,{y_0}^5y_3\right)\\
+\,&\mathcal{X}_4\left(65\,{y_0}^4{y_1}^2 + 20\,{y_0}^5y_2\right) \;+\; 15\,\mathcal{X}_5{y_0}^5y_1 \;+\; \mathcal{X}_6{y_0}^6.
\end{aligned}$$

§9. This section starting p. 27 contains a further combinatorial investigation of the general case, in the light of the special cases considered earlier in §2–4. Near the end, the author offers a brief discussion (pp. 29–30) of the particular reduction of $(x^p D)^n$. What he obtains is, in present day notations (we write $c_{n,k}$ for coefficients, which Scherk once more denotes by a_n^k):

Proposition A.3 (Scherk [102, pp. 30–31])**.** *The normal form of* $(X^p D)^n$ *is given by*

$$(X^p D)^n = X^{n(p-1)} \sum_k c_n^k X^k D^k,$$

where the coefficients c_n^k *satisfy*

$$c_n^k = \sum_{1 \le j_1 \le j_2 \le \cdots \le j_{n-k} \le k} [j_1 p] \cdot [(j_2+1)p-1] \cdot [(j_3+2)p-2] \cdots [(j_{n-k}+n-k-1)p-(n-k-1)].$$

§10. This section (pp. 31–36) contains formulae that the author obtained, not being at the time cognizant of similar works by the Bernoullis and Laplace. They are relative to Bernoulli numbers, hence they will not be discussed further here.

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