Approximate substitutions and the normal ordering problem

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Abstract. In this paper, we show that the infinite generalised Stirling matrices associated with boson strings with one annihilation operator are projective limits of approximate substitutions, the latter being characterised by a finite set of algebraic equations.

1. Introduction

The series of papers [1, 2, 3] had two sequels. First one, algebraic, was the construction of a Hopf algebra of Feynman-Bender diagrams [10, 11] arising from the product formula applied to two exponentials. Second one was the construction and description of one parameter groups of infinite matrices [4, 9] and their link with the combinatorics of so called *Sheffer polynomials*. The object of this paper is to continue the investigation of those *one-parameter groups* by highlighting the structure of the group of substitutions.
It is shown here how we can see this group as a projective limit of what will be called *approximate substitution groups.*

First, we consider Boson creation and annihilation operators with the commutation relation

$$[a, a^{\dagger}] \quad = \quad 1 \tag{1}$$

Recall that [1]

- the annihilation operator a, in the second quantization, represents an operator which changes each state $|N\rangle$ of the Fock space (containing $N \geq 1$) particles to another containing $N-1$ particles. One has here

$$a|N\rangle \quad = \quad \sqrt{N}|N-1\rangle \tag{2}$$

- the hermitian conjugate of the annihilation operator is the creation operator $a^\dagger$ which changes each state $|N\rangle$ of the Fock space containing N particles to another containing $N+1$ particles. One has then

$$a^\dagger|N\rangle \quad = \quad \sqrt{N+1}|N+1\rangle \tag{3}$$

Starting from the vacuum $|0\rangle$, we can reach all the normalized states in the Fock space. There are indeed given by:

$$|N\rangle \quad = \quad \frac{(a^\dagger)^N}{\sqrt{N!}}|0\rangle \tag{4}$$

2. Normally ordered form

The noncommutativity of annihilation and creation operators may cause problems in defining an operator function in quantum mechanics. To solve these problems, we have to find some suitable form which allows computing, reduction and equality test. One of the simplest and widely used procedure is the finding of the *normally ordered form* of the boson operators in which all $a^\dagger$ stand to the left of all the factors a [1].

There are two well known procedures defined on the boson expressions: namely $\mathcal{N}$, the *normal ordering* and :: , the *double dot operation*, [4].

2.1. Normal ordering

By normal ordering of a general expression $F(a^\dagger, a)$, we mean $\mathcal{N}[F(a^\dagger, a)]$ which is obtained by moving all the annihilation operators a to the right, using the commutation relation (1).

Example 2.1 *Let $w \in \{a, a^\dagger\}^*$ a word given by $w = aa^\dagger aaa^\dagger a$. The normal ordering of w is*

$$\begin{aligned}
aa^\dagger aaa^\dagger a &= (1+a^\dagger a)a(1+a^\dagger a)a = a^2 + a^\dagger a^3 + aa^\dagger a^2 + a^\dagger a^2 a^\dagger a^2 \\
&= a^2 + a^\dagger a^3 + (1+a^\dagger a)a^2 + a^\dagger a(1+a^\dagger a)a^2 \\
&= a^2 + a^\dagger a^3 + a^2 + a^\dagger a^3 + a^\dagger a^3 + a^\dagger aa^\dagger a^3 \\
&= 2a^2 + 3a^\dagger a^3 + a^\dagger(1+a^\dagger a)a^3 \\
&= 2a^2 + 3a^\dagger a^3 + (a^\dagger)^2 a^4
\end{aligned}$$

Remark 2.2 *Note that all coefficients of the normal ordering of a word (more precisely the coefficients of the decomposition of a word on the basis $\left\{(a^\dagger)^j a^l\right\}$) are positive integers. This suggests that these integers count combinatorial objects [13].*

2.2. Double dot operation

The double dot operation $: F(a^\dagger, a) :$ is a similar procedure using another commutation relation *i.e.* $[a, a^\dagger] = 0$ instead of $[a, a^\dagger] = 1$, *i.e* moving all annihilation operators a to the right as if they were commuting with the creation operators $a^\dagger$.

Remark 2.3 *The double dot operation :: is a linear operator which can be directly defined, for a word $w \in \{a, a^\dagger\}^*$, by:*

$$: w := a^{\dagger(|w|_{a^\dagger})} a^{(|w|_a)}$$

where $|w|_x$ stands for the number of occurences of a symbol x in the word w.

Example 2.4 *We take the same word as above: $w = aa^\dagger aaa^\dagger a$.*
The double dot operation gives

$$: aa^\dagger aaa^\dagger a : \quad = \quad a^\dagger a^\dagger aaaa$$

3. Combinatorics of the normal ordering

The Bell and Stirling numbers have a purely combinatorial origin [8], but in this communication, we will consider them as coefficients of the normal ordering problem [1].
The general word $w \in \{a, a^\dagger\}^*$ with letters in $\{a, a^\dagger\}$, *i.e.* Boson string, can be described by two sequences of non negative integers $\mathbf{r} = (r_1, r_2, \cdots, r_M)$ and $\mathbf{s} = (s_1, s_2, \cdots, s_M)$, so that we define

$$w_{\mathbf{r},\mathbf{s}} \quad = \quad (a^\dagger)^{r_1} a^{s_1} (a^\dagger)^{r_2} a^{s_2} \cdots (a^\dagger)^{r_M} a^{s_M} \tag{5}$$

and $d = \sum_{m=1}^{n} (r_m - s_m), \quad n = 1, \cdots, M$ represents the excess (*i. e.* the difference between the number of creations and the number of annihilations). Then, the normally ordered form of $w^n_{\mathbf{r},\mathbf{s}}$ is given by

$$\mathcal{N}(w^n_{\mathbf{r},\mathbf{s}}) = \begin{cases} (a^\dagger)^{nd} \sum_{k=0}^{\infty} S_{\mathbf{r},\mathbf{s}}(n,k)(a^\dagger)^k a^k, & \text{if } d > 0; \\ \Big(\sum_{k=0}^{\infty} S_{\mathbf{r},\mathbf{s}}(n,k)(a^\dagger)^k a^k\Big)(a^\dagger)^{n|d|}, & \text{otherwise,} \end{cases}$$

where quantities $S_{\mathbf{r},\mathbf{s}}(n,k)$ are generalizations of standard Stirling numbers [2, 3].
The generalized Bell polynomials $B_{\mathbf{r},\mathbf{s}}(n,x)$ and the generalized Bell numbers $B_{\mathbf{r},\mathbf{s}}(n)$ are defined respectively by

$$B_{\mathbf{r},\mathbf{s}}(n,x) \quad = \quad \sum_{k=0}^{\infty} S_{\mathbf{r},\mathbf{s}}(n,k)x^k = \sum_{k=0}^{nr} S_{\mathbf{r},\mathbf{s}}(n,k)x^k \tag{6}$$

$$B_{\mathbf{r},\mathbf{s}}(n,1) \quad = \quad B_{\mathbf{r},\mathbf{s}}(n) = \sum_{k=0}^{\infty} S_{\mathbf{r},\mathbf{s}}(n,k) = \sum_{k=0}^{nr} S_{\mathbf{r},\mathbf{s}}(n,k) \tag{7}$$

Remark 3.1 *Notice that*

$$S_{r,s}(n,k) = \begin{cases} 1, & \text{for } k = nr; \\ 0, & \text{for } k > nr. \end{cases}$$

Example 3.2 *Using a computer algebra program, we get the following matrices.*

- $w = a^\dagger a$, *we get the usual matrix of Stirling numbers of second kind* $S(n,k)$*[8]*

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 3 & 1 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 7 & 6 & 1 & 0 & 0 & \cdots \\ 0 & 1 & 15 & 25 & 10 & 1 & 0 & \cdots \\ 0 & 1 & 31 & 90 & 65 & 15 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & & \ddots \end{pmatrix}$$

- $w = a^\dagger a a^\dagger$, *we have*

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 2 & 4 & 1 & 0 & 0 & 0 & 0 & \cdots \\ 6 & 18 & 9 & 1 & 0 & 0 & 0 & \cdots \\ 24 & 96 & 72 & 16 & 1 & 0 & 0 & \cdots \\ 120 & 600 & 600 & 200 & 25 & 1 & 0 & \cdots \\ 720 & 4320 & 5400 & 2400 & 450 & 36 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & & \ddots \end{pmatrix}$$

- $w = a^\dagger a a a^\dagger a^\dagger$, *one gets*

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 2 & 4 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 12 & 60 & 54 & 14 & 1 & 0 & 0 & 0 & 0 & \cdots \\ 144 & 1296 & 2232 & 1296 & 306 & 30 & 1 & 0 & 0 & \cdots \\ 2880 & 40320 & 109440 & 105120 & 45000 & 9504 & 1016 & 52 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & & \ddots \end{pmatrix}$$

Remark 3.3 *In each case, the matrix $(S_{r,s}[n,k])_{n\geq 0, k\geq 0}$ is of a staircase form and the dimension of the step is the number of a's in the word w. Thus, all the matrices are row-finite and are unitriangular iff the number of its annihilation operators is exactly one. Moreover, the first column is $(1, 0, \cdots, 0, \cdots)$ iff w ends with a (this means that $\mathcal{N}(w^n)$ has no constant term for all $n > 0$) [4, 9].*

A word w with only one annihilation operator can be written in the unique form $w = (a^\dagger)^{r-p} a (a^\dagger)^p$. Then:

- *if $p = 0$, S_w is the matrix of a unipotent substitution.*
- *if $p > 0$, S_w is the matrix of a unipotent substitution with prefunction [9].*

4. Approximate substitutions

We define here the space of transformation matrices and its topology, and then we concentrate on the *Riordan subgroup* [7] (*i.e* transformations which are substitutions with prefactor functions) [4, 9].

Let $\mathbb{C}^{\mathbb{N}}$ be the vector space of all complex sequences, endowed with the Frechet product topology [6, 12]. The algebra $\mathcal{L}(\mathbb{C}^{\mathbb{N}})$ of all continuous operators $\mathbb{C}^{\mathbb{N}} \longrightarrow \mathbb{C}^{\mathbb{N}}$ is the space of row-finite matrices with complex coefficients (a subspace of $\mathbb{C}^{\mathbb{N}\times\mathbb{N}}$). Let M be a matrix of this space. For a sequence $A = (a_n)_{n\geq 0}$, the transformed sequence $B = MA$ is given by $B = (b_n)_{n\geq 0}$ with:

$$b_n = \sum_{k\geq 0} M(n,k) a_k. \tag{8}$$

We will also associate to A (see paragraph (4.2)) its exponential generating function

$$\sum_{n\geq 0} a_n \frac{z^n}{n!}. \tag{9}$$

4.1. Substitutions with prefunctions

We now examine an important class of transformations: the substitutions with prefunctions.

We consider, for a generating function f, the transformation

$$\mathcal{T}_{g,\phi}[f](x) \quad = \quad g(x) f\Big(\phi(x)\Big) \tag{10}$$

where $g(x) = 1 + \sum_{n=1}^{\infty} g_n x^n$ and $\phi(x) = x + \sum_{n=2}^{\infty} \phi_n x^n$ are arbitrary formal power series. The mapping $\mathcal{T}_{g,\phi}$ is a linear application [9], the matrix of this transformation $M_{g,\phi}$ is given by the transforms of the monomials $\frac{x^k}{k!}$ hence

$$\sum_{n\geq 0} M_{g,\phi}(n,k)\frac{x^n}{n!} = \mathcal{T}_{g,\phi}\Big[\frac{x^k}{k!}\Big] = g(x)\frac{\phi(x)^k}{k!} \tag{11}$$

Remark 4.1 *If $f(x) = e^{yx}$, Eq. (11) comes down to the Sheffer condition on the matrix of $\mathcal{T}$. It amounts to the statement that [1]:*

$$\sum_{n,k\geq 0} T(n,k)\frac{x^n}{n!} y^k \quad = \quad g(x) e^{y\phi(x)} \tag{12}$$

where $T \in \mathcal{L}(\mathbb{C}^{\mathbb{N}})$ is a matrix with non-zero two first columns.

4.2. Approximate substitutions

In this section, we define approximate substitutions matrices and give a way to determine whether an unipotent (lower triangular with all diagonal elements equal to 1) matrix is a matrix of an approximate substitution.

Definition 4.2 *Let $M \in \mathbb{C}^{[0\cdots n]\times[0\cdots n]}$ be a unipotent matrix, $M = M[i,k]_{0\leq i,k\leq n} = (a_{ik})_{0\leq i,k\leq n}$; is called matrix of approximate substitution if it satisfies the following condition:*

$$c_k \quad = \quad \left[c_0 \frac{\left(\frac{c_1}{c_0}\right)^k}{k!}\right]_n, \qquad \textit{for all} \qquad 0 \leq k \leq n \tag{13}$$

where

$$c_k = \sum_{i=0}^{n} M[i,k]\frac{x^i}{i!}$$

$$M = \begin{pmatrix} 1 & 0 & 0 & \cdots & \cdots & \cdots & \cdots \\ a_{1,0} & 1 & 0 & \cdots & \cdots & \cdots & \cdots \\ a_{2,0} & a_{2,1} & 1 & 0 & \cdots & \cdots & \cdots \\ a_{3,0} & a_{3,1} & \cdots & 1 & 0 & \cdots & \cdots \\ a_{4,0} & a_{4,1} & \cdots & a_{4,k} & \cdots & \cdots & \cdots \\ a_{5,0} & a_{5,1} & \cdots & a_{5,k} & \cdots & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$c_0 \quad c_1 \qquad\qquad c_k$

Thus c_k represents the exponential generating series (here a polynomial) of the k^{th} column (hence c_0, c_1 are respectively the exponential generating series of the 1^{st} and the 2^{nd} column) and $\Big[\ \ \Big]_n$ is the truncation, at order n, of a series.

We consider now the set of matrices with complex coefficients noted by $\mathbb{C}^{\mathbb{N}\times\mathbb{N}}$ [5] and let $\mathbb{C}^{[0\cdots n]\times[0\cdots n]}$ be the set of all matrices of size $(n+1)\times(n+1)$. Let also r_n be the truncation of the matrices taking the upper left principal submatrix of dimension $(n+1)$, hence $r_n(M) = \Big(M[i,k]\Big)_{0\le i,k\le n}$. Thus, we get a linear mapping

$$r_n : \mathbb{C}^{\mathbb{N}\times\mathbb{N}} \longrightarrow \mathbb{C}^{[0\cdots n]\times[0\cdots n]}$$

It is clear that r_n is not a morphism for the (partially defined) multiplication (*i.e.* $r_n(AB) \neq r_n(A)r_n(B)$ in general).
We consider now $\mathcal{LT}(\mathbb{N},\mathbb{C})$ the algebra of lower triangular matrices and $\mathcal{LT}([0\cdots n],\mathbb{C})$ the matrices of size $([0\cdots n]\times[0\cdots n])$ obtained by the truncation τ_n. Then

$$\tau_n : \mathcal{LT}(\mathbb{N},\mathbb{C}) \longrightarrow \mathcal{LT}([0\cdots n],\mathbb{C})$$

and, this time, τ_n preserves multiplication (τ_n is a morphism). One has the diagram

$$\begin{tikzcd}
\mathbb{C}^{\mathbb{N}\times\mathbb{N}} \arrow[r, "r_n"] & \mathbb{C}^{[0\cdots n]\times[0\cdots n]} \\
\mathcal{LT}(\mathbb{N},\mathbb{C}) \arrow[u, "\mathcal{J}_1"] \arrow[r, "\tau_n"] & \mathcal{LT}([0\cdots n],\mathbb{C}) \arrow[u, "\mathcal{J}_2"']
\end{tikzcd}$$

where $\mathcal{J}_1$ and $\mathcal{J}_2$ are two canonical injections.

Remark 4.3 *We can write*

$$\mathcal{LT}(\mathbb{N},\mathbb{C}) \ = \varprojlim \ (\mathcal{LT}([0\cdots n],\mathbb{C})) \tag{14}$$

which means that $\mathcal{LT}([0\cdots n],\mathbb{C})$ is the projective limit of $\mathcal{LT}(\mathbb{N},\mathbb{C})$

4.3. Random generation

Our motivation, in this section, consists in approximating the matrices of infinite substitutions by finite matrices of (approximate) substitutions. We are then interested in the probabilistic study of these matrices. To this end, we randomly generate unipotent (unitriangular) matrices and we observe the number of occurrences of matrices of substitutions.
The construction of unipotent matrices is done as follows:

(i) Create an identity matrix.
(ii) Fill randomly the lower part of the identity matrix (strictly under the diagonal) using numbers which follow a uniform law in $[0,1]$.
(iii) Multiply those numbers by the range previously chosen.
(iv) Test if the built unipotent matrix satisfies Eq.(13).

We start by giving some examples of our experiment which are summarized in the table below:

Size	Numbers of drawing	Range of variables	Probability
$[3 \times 3]$	300	$[1 \cdots 10]$	1
		$[1 \cdots 100]$	1
		$[1 \cdots 10000]$	1
$[4 \times 4]$	275	$[1 \cdots 10]$	0.0473
		$[1 \cdots 100]$	0.0001
		$[1 \cdots 10000]$	0^+
$[10 \times 10]$	1500	$[1 \cdots 10]$	0.0327
		$[1 \cdots 100]$	0^+
		$[1 \cdots 10000]$	0^+

According to the results obtained, we observe that the substitutions matrices are not very frequent. However, in meeting certain conditions such as size, the number of drawings and the range of the variables, we can obtain positive probabilities that these matrices appear.
Let us note that the smaller the size of the matrix the more probable one obtains a matrix of substitution in a reasonable number of drawings.
We also notice that, if we vary the range of variables, and this in an increasing way and by keeping unchanged the number of drawings and size, the probability tends to zero. We also notice that the unipotent matrices of size 3 are all matrices of approximate substitutions. This is easy to see because the exponential generating series of the 3^{rd} column will always have the form $c_k = \frac{x^2}{2!}$.
Thus, we can say that the test actually starts from the matrices of size higher or equal to 4.

Result 4.4 *Let r represent the cardinality of the range of variables and $n \times n$ be the size of the matrix.*
According to the results obtained; we can say that the probability p_n of appearance of the matrices of substitutions depends on r and n and we have the following upper bound:

$$p_n \leq \frac{r^{2n-3}}{r^{\frac{n(n-1)}{2}}} \tag{15}$$

which shows that

$$p_n \longrightarrow 0 \qquad as \qquad n \longrightarrow \infty \tag{16}$$

Conjecture 4.5 *One can conjecture that the effect of the range selection vanishes when n tends to infinity. More precisely:*

$$p_n \sim \frac{r^{2n-3}}{r^{\frac{n(n-1)}{2}}} \tag{17}$$

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