Q-grammars and wall polyominoes

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Abstract

We use a variant of the q-grammar method to write functional equations for the generating functions of a subclass of vertically convex polyominoes and directed walks, according to some particular parameters, which include the area. The form of these equations, and some simple singularity computations, are used to prove that the area of wall polyominoes of perimeter $2n$ has the Airy distribution as a limit law.

1 Introduction

Polyomino and self-avoiding walk enumeration is a long-studied subject in both combinatorics and statistical mechanics. Counting unrestricted polyominoes is an extremely hard problem, and only very rough estimates are known. However, various easier subclasses have been studied and exact or approximate enumeration information is known about them.

Many different methods have been used to count column-convex polyominoes, either according to their area or perimeter. One very natural idea is to cut them into a succession of columns; then, examining the rules that govern the way columns are "glued" together yields equations for their enumerating sequences or generating functions [15, 1]. The context-free method, which is the basis for our Q-grammar method, uses bijections between classes of combinatorial objects and *context-free languages* generated by *unambiguous grammars* (also called *algebraic languages*). These languages have algebraic generating functions, and much information can be derived from the equations they satisfy, even when the equations cannot be solved explicitly.

Section 2 of this paper briefly describes the Q-grammar method, an extension of an idea by Delest and Fédou [2] : using attribute grammars, as used in computer science for compilation, to obtain functional equations for some enumerative problems. Section 3 deals with asymptotics of multivariate generating functions, and describes the Airy distribution, which is a recurrent limit law in many dicrete or continuous problems; we also state (see [4] for aproof) a general theorem giving limit Airy distributions in a wide variety of situations. Finally, in Section 4 we show how these ideas can be applied to a simple class of column-convex polyominoes, known as *wall polyominoes* or *bar-graph polygons.*

2 Q-grammar methods

We start from a bijective coding of a class of polyominoes with words of an algebraic language. The length of a word, or the number of occurrences of a given letter in a word, is supposed to correspond to the *perimeter* of the polyomino. By writing an unambiguous grammar generating the language, we immediately obtain an algebraic equation for the generating function of our class of polyominoes (or, if the grammar uses more than one nonterminal symbol, a set of algebraic equations with several unknown functions, one of which is the wanted generating function).

In this situation, we are interested in enumeration of polyominoes according to more than one parameter, say, perimeter and area. In most cases, the bivariate generating function $F(t;q)$, where variable t corresponds to the perimeter and variable q corresponds to the area, is not algebraic. Thus, directly aiming at an equation using the grammar method is doomed to fail. However, in some cases a functional equation can be found, involving a variable substitution σ defined by $(\sigma F)(t;q) = F(tq;q)$.

As an example, it is well known [3] that *parallelogram polyominoes* of perimeter $2n+2$ can be coded with the *Dyck words* of length $2n$. The Dyck words, or parenthese words, are words using letters a and b, generated by the grammar

$$D \;\rightarrow\; \epsilon; \qquad D \;\rightarrow\; aDbD.$$

This grammar gives the following equation for the generating function of Dyck words, where x counts half the length of words :

$$D(x) = 1 + xD(x)^2.$$

In this coding, the *width* (number of columns) of a polyomino is the *number of peaks* ($x\overline{x}$ factors) of the corresponding word, and its *area*, which is also the sum of the heights of all columns, is the sum of heights of these peaks. The first step is to count the Dyck words by their length and number of peaks; this can be done using another grammar (for nonempty Dyck words) :

$$\begin{cases} F \;\rightarrow\; ab & F \;\rightarrow aFb \\ F \;\rightarrow\; abF & F \;\rightarrow aFbF \end{cases}$$

This translates into the following equation (x counts the width of polyominoes, or number of peaks of words; y counts the height of polyominoes – minus 1 – or half the number of letters in the word which are not in peaks) :

$$F(x,y) = x + xF(x,y) + yF(x,y) + yF(x,y)^2. \tag{1}$$

When taking into account the *area* of parallelogram polyominoes, we obtain the following refinement (q counts the area of polyominoes) :

$$F(x,y;q) = xq + xqF + y\sigma(F) + yF.\sigma(F), \tag{2}$$

where the variable substitution σ is defined by $\sigma(F)(x,y;q) = F(xq,y;q)$.

The $y\sigma(F)$ term reflects the fact that all peaks in word awb are one higher than they were in word w, so that the area is increased by the number of peaks, which is counted by variable x in the generating function; each term in the equation has a similar interpretation.

Using this kind of variable substitutions in the equations given by algebraic grammars, constitutes what can be called the Q-grammar method. In the sequel, the parameters counted by the variables in the original algebraic equation, are called *rank 1* parameters. Parameters counted by additional variables which are substituted into rank 1 variables, such as the area above, are called *rank 2* parameters. Rank 3 and higher parameters and variables appear when one uses substitutions into rank 2 and higher variables : if we use substitution σ_2, defined by $\sigma_2(F)(x;q;r) = F(xq;qr;r)$, then variable r is a rank 3 variable.

The following lemma is proved in [5]; it bounds the order of magnitude of parameters according to their rank :

Lemma 1. *For any rank k parameter p, there exists some constant C such that, for any nonempty word w in the language, $p(w) \leq C.|w|^k$.*

If, furthermore, the grammar used to generate the language has a strongly connected dependency graph, then for any rank k parameter, there exists some constant $C' > 0$ and an infinite sequence of words $(w_n)_{n\geq 0}$ in the language, such that, for each $n \geq 0$, $p(w_n) \geq C'.|w_n|^k$.

In other words, a rank 2 parameter always takes values that are, at most, quadratic in the length of the coding words; A rank 3 parameter takes values at most cubic, and so on. In most cases, this provides an upper bound to the rank a given parameter may have : when the perimeter of a polyomino corresponds to the length of the coding words, the area will not appear as a rank 3 parameter, and should be a rank 2 parameter - if it is at all possible to write variable substitution equations for the area.

All of these parameters can be interpreted as counting certain configurations in the derivation trees for the words generated by the grammar. A rank k parameter will be interpreted as counting certain k-tuples of nodes in the derivation trees; see [5] for details. In the case of rank 2 parameters, the interpretation is quite similar to the internal path length in derivation trees - depending on the exact rank 2 parameter, only certain nodes and a certain portion of their depths will be taken into account.

3 Asymptotics and moment evaluation

Exact solving of the variable substitution equations provided by the Q-grammar method is usually a difficult problem, and no general methods are known. A linearization method can be found in [13] for equations involving only one substitution. However, the expressions obtained via this method are complex and deriving information about the coefficients from them is not obvious.

Sometimes it is sufficient to obtain information about the *moments* of some of the parameters; recall that the k-th moment of a parameter (considered as a random variable) is the expected value of the k-th power of parameter $p(w)$, when w is chosen uniformly at random among all objects of size n. These moments can be obtained through differentiation and coefficient extraction.

Moment computations in simple cases indicate that rank 2 parameters tend to have a mean value and a standard deviation of order $n^{3/2}$ (when the average is taken over all objects of size n). Furthermore, the ratio of these two quantities seems to always have the same limit as n tends to infinity. In more complex situations where the combinatorial objects studied are easy to generate randomly, such as binary or ternary trees, simulations involving various kinds of rank 2 parameters support this fact. This suggests that some universal limit law may be present.

This limit law is known to exist, and is identified as the *Airy distribution* in several situations which can be described as rank 2 parameters, namely, the study of path length in simple families of trees [14] and other related objects [9].

In [4], we prove that this limit law holds under much more general condition. Assuming the *algebraic* generating function using only rank 1 parameters as enumeration variable has a *finite* dominant singularity, and using technical assumptions on some derivatives at the dominant singularity, then *each* rank 2 parameter will have, up to a multiplicative constant, the *same* limit distribution, which is the Airy distribution. A multiplicative scaling factor of $K.n^{3/2}$ must be applied; this can be compared to the maximum magnitude of n^2 for rank 2 parameters. The constant K can be easily obtained explicitly when the dominant singularity is known.

The proof follows a "pumping moments" principle. The main terms in an asymptotic expansion of various derivatives of the generating functions are determined inductively, and the limit moments are shown to satisfy a recurrence relation that uniquely determines the moments of the Airy distribution. A similar recurrence can be shown to hold for moments of a parameter with a higher rank, under very similar conditions. However, we have not been able to prove that this moment sequence uniquely determines a limit distribution.

3.1 The Airy distribution

The Airy distribution appears in various situations in combinatorics and probability theory. It was proved by Louchard [10, 11] to represent the area under a Brownian excursion, and by Takács [14] to appear as the limit distribution for the average height of nodes in families of rooted trees. More recently, Flajolet, Poblete and Viola [9] proved that it also appears in the analysis of linear probing hashing, as the limit law for the construction cost of an almost full table.

We will follow [9] for the definition of this distribution, and recall here only the minimum facts about this distribution.

The Airy distribution is the law of a positive random variable X, and is uniquely determined by its moments,

$$\mu^{(k)} = \mathbf{E}\left[X^k\right] = \frac{2\sqrt{\pi}}{\Gamma(\frac{3k-1}{2})}\Omega_k.$$

The (Ω_k) sequence starts with $\Omega_0 = -1$ and can be defined for $k \geq 1$ by the recurrence

$$2\Omega_k = (3k-4)k\Omega_{k-1} + \sum_{i=1}^{k-1}\binom{k}{i}\Omega_i\Omega_{k-i}, \tag{3}$$

or, equivalently, by a differential equation for its exponential generating function $f(t) = \sum_{k\geq 0}\Omega_k t^k/k!$:

$$3t^2 f'(t) - tf(t) + f(t)^2 - 1 = 0.$$

The resolution of this Riccati equation leads to Bessel functions and the Airy function.

The first few values for Ω_k are $-1, 1/2, 5/4, 45/4\dots$ ($2^k\Omega_k$ is always an integer). The first few moments of the Airy distribution are 1, $\sqrt{\pi}$, $10/3$, and $15\sqrt{\pi}/4\dots$ The appearance of the distinctive limit ratio $\sqrt{10/3-\pi}$ between mean value and standard deviation in a discrete problem, can usually be used as a hint that the Airy distribution will appear as a limit law.

3.2 The main theorem

The general result can be expressed as follows :

Theorem 2. *Let $F(x,q)$ be the ordinary generating function for a set of combinatorial object $\mathcal{F}$, with respect to parameters s (counted by x) and p (counted by q). In other words, we have*

$$F(x,q) = \sum_{w\in\mathcal{F}} x^{s(w)} q^{p(w)}.$$

Assume that the following conditions are met :

- *F satisfies a functional equation,*

  $$F(x,q) = \tilde{P}(x,q,F(x,q),\sigma_1(F)(x,q),\dots,\sigma_k(F)(x,q)), \tag{4}$$

  where $\tilde{P} = \tilde{P}(x,q,f,g_1,\dots,g_k)$ is a polynomial with coefficients in $\mathbb{Z}$ (or possibly some polynomial ring $\mathbb{Z}[y]$, in which case y is to be taken as a parameter), with total degree in variables $f, g_1, \dots, g_k$ at least 2, and each operator σ_i is defined by

  $$\sigma_i(F)(x,q) = F(xq^i, q);$$

- *the formal power series $F(x,1)$ is well defined;*

- *$F(x,1)$ has a unique dominant singularity (i.e., a unique singularity of minimal module) x_0, and takes a finite value f_0 at x_0.*

Let P be the polynomial obtained when setting $q=1$ in equation 4 :

$$F(x,1) = P(x,F(x,1)) = \tilde{P}(x,1,F(x,1),F(x,1),\dots,F(x,1)). \tag{5}$$

Define the constants α, β and γ as follows :

$$\left\{\begin{array}{lcl} \alpha & = & x_0\frac{\partial P}{\partial x}(x_0,f_0); \\ \beta & = & \frac{\partial^2 P}{\partial f^2}(x_0,f_0); \\ \gamma & = & \sum_{i=1}^{k}\frac{\partial \tilde{P}}{\partial g_i}(x_0,1,f_0,\dots,f_0). \end{array}\right.$$

Let also X_n be a discrete random variable with distribution given by the distribution of exponents of q in $[x^n]F(x,q)$:

$$\mathbf{Pr}(X_n = k) = \frac{[x^n q^k]F(x,q)}{[x^n]F(x,1)}.$$

Then, if α, and β are strictly positive, the singularity of $F(x,1)$ is of the square root type; i.e., $F(x,1) - f_0 \sim -C\sqrt{1 - x/x_0}$ for some constant $C > 0$ when x is near x_0. Furthermore, if $\gamma > 0$, the random variables

$$Y_n = \frac{X_n\sqrt{2\alpha\beta}}{\gamma n^{3/2}},$$

have the Airy distribution as a limit law.

One important thing to note here is that Equation (4) is only used to compute γ; all other parameters depend only on the algebraic equation (5).

Another important remark is that the various conditions of Theorem 2 reduce to the existence of a unique dominant singularity at (x_0, f_0) for $F(x,1)$ when Equation $\tilde{P}$ has only positive coefficients. This is true when Equation (4) comes from the Q-grammar method.

4 Wall polyominoes and directed positive walks

We will now give an example of application of the Q-grammar method on polyominoes by examining wall polyominoes, to which Theorem 2 can be applied. Neither the equations on wall polyominoes nor the decomposition we use to obtain them are new; they appear in [13] and, independently, in [7].

4.1 Definitions and algebraic equations

A *wall polyomino*, as defined by Feretić [7, 8], is a vertically convex polyomino in which all columns have their lowest cell at the same level; these same polyominoes are called *bar-graph polygons* in [13]. Such a polyomino is entirely determined by its *upper path*, starting at the upper left corner of the bottom cell in the leftmost column and ending at the upper right corner of the bottom cell in the rightmost column. For the sake of simplicity, we will not count the base line of cells, so that a wall polyomino can be seen as a collection of columns of cells, each with non-negative height.

Such a path, starting at the origin, is composed of a succession of North, East and South steps, with the following conditions :

1. an East step always appear between a North step and a South step;

2. the path never goes below the $y = 0$ line;

3. the path ends on the $y = 0$ line.

These paths can be bijectively coded with words using the 3 letters x, y, $\overline{y}$: x corresponds to an East step, y corresponds to a North step, and $\overline{y}$ corresponds to a South step. The language W of nonempty words coding wall polyominoes is algebraic, and is generated by the following unambiguous grammar :

$$\left\{ \begin{array}{lllllll} W & \to & x & \qquad & W & \to & xW \\ W & \to & yW\overline{y} & & W & \to & yW\overline{y}x \\ W & \to & yW\overline{y}xW & & & & \end{array} \right.$$

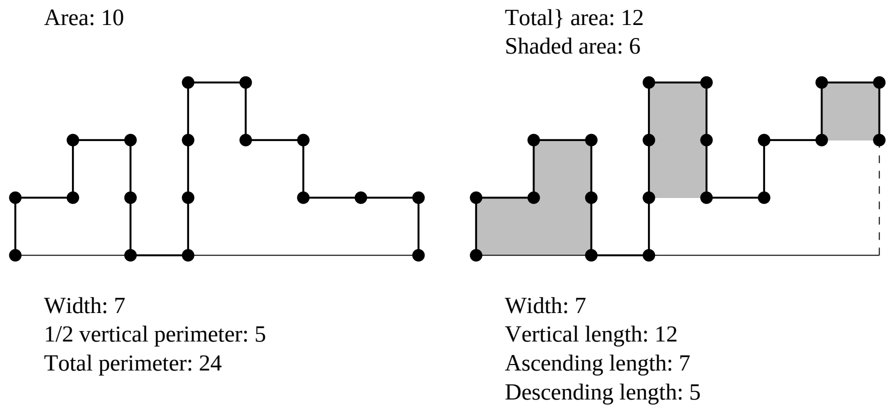

Figure 1: Wall polyominoes and directed positive walks

A *directed positive walk* is a self-avoiding walk starting at the origin, using only North, East and South steps, which is constrained to remain in the $y \geq 0$ region. In other words, it is defined by the same conditions as a wall polyomino, except that condition 3 is removed.

Figure 1 shows examples of both types of objects, together with some of the parameters that can be described using the Q-grammar method.

Using the same coding as above, the words coding (possibly empty) directed positive walks are exactly the left factors of words in the language W. Looking for the *longest* left factor of a word in W' that is also a word in W, leads to an unambiguous grammar generating W'. This grammar is obtained from the one for W by adding the following rules (the axiom is W') :

$$\begin{cases} W' \rightarrow \epsilon & W' \rightarrow yW' \\ W' \rightarrow W & W' \rightarrow WxyW' \\ W' \rightarrow xyW' & \end{cases}$$

This grammar can also be described more graphically, using the *object grammar* [6] formalism; see figure 2

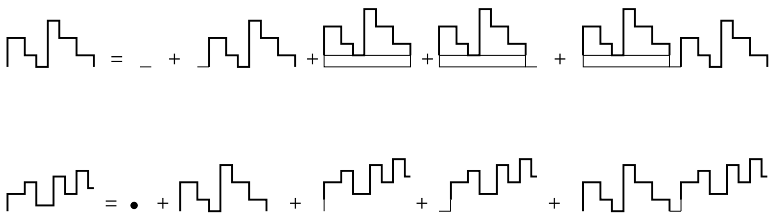

Figure 2: Object grammar definitions

The grammar gives the following equations for the generating functions $W(x,y,\overline{y})$ and $W'(x,y,\overline{y})$:

$$\begin{cases} W(x,y,\overline{y}) &= x + (x + y\overline{y} + xy\overline{y})W(x,y,\overline{y}) + xy\overline{y}W(x,y,\overline{y})^2; \\ W'(x,y,\overline{y}) &= 1 + W(x,y\overline{y}) + (y+xy)W'(x,y,\overline{y}) \\ &+ \; xyW(x,y\overline{y})W'(x,y,\overline{y}). \end{cases}$$

In these equations, variable x counts half the horizontal perimeter of polyominoes, or the width of walks; y counts half the vertical perimeter for polyominoes, or the "ascending" vertical length for walks; and $\overline{y}$ counts the "descending" vertical length for walks. Variable $\overline{y}$ is not needed in the equation for W, since it always appear with the same exponent as variable y. It is only included for use with the equation for W'. For a generating function counting walks by their total vertical length, $\overline{y}$ should be replaced with y; for a generating function counting walks by their total length, all three variables should be replaced with x.

The equation for W is quadratic, and so can be explicitly solved. Once W is known, W' can be expressed as a rational function in W and its variables.

$$\begin{cases} W(x,y) &= \dfrac{1-x-y-xy-\sqrt{(1-y)^2-2x(1-y^2)+x^2(1-y)^2}}{2xy} \\ W'(x,y,\overline{y}) &= \dfrac{1+W(x,y\overline{y})}{1-y-xy-xyW(x,y\overline{y})} \end{cases}$$

These equations appear in [7, 8], and, together with Equation 6 below, in [13]; the decomposition used to obtain the equations here is very similar to the *object grammar* method in all cases.

For asymptotic enumeration purposes, the important thing is the singularities of the generating functions. Here, the generating function $W(x, y)$ has (for $x > 0$ and $y > 0$) a singularity of the square root type along the line

$$y = \left(\frac{1-x}{1+x}\right)^2.$$

This singularity structure also appears in [12], where wall polyominoes are called *solid-on-solid walks.*

The generating function $W'(x, y)$ has a singularity of the inverse square root type along the same line. Thus, we will be able to apply Theorem 2 to wall polyominoes, but not to directed positive walks.

4.2 Rank 2 parameters

The obvious candidate for a rank 2 parameter on wall polyominoes is the area. Using the decomposition given by the grammar, we can write the following q-substitution equation for the generating function with respect to width (counted by x), vertical half-perimeter (counted by y), and area :

$$W = x + x.W + y\sigma(W) + xy\sigma(W) + xyW\sigma(W), \tag{6}$$

with $\sigma(W)(x, y, q) = W(xq, y, q)$.

For directed positive walks, we can define two types of areas. The *total area* is the total area under the walk. The *shaded area* is the part of the total area which lies under the walk, but also to the left of some descending step in the walk; see Figure 1 for an example. These two areas are the same for a walk ending on the $y = 0$ line (which is in fact a wall polyomino).

The equation for $W'(x, y, \overline{y}, q)$, when q counts the *total* area, is

$$W' = 1 + W + y\sigma(W') + xy\sigma(W') + xyW.\sigma(W').$$

If q is to count only the *shaded* area, the equation for W' remains algebraic in x, y and W (though the one for W is not) :

$$W' = 1 + W + yW' + xyW' + xyW.W'.$$

In both cases, the equation for W is the one given above, with the same definition for σ.

We can then apply Theorem 2 to the generating function W, using y as a parameter. This corresponds to examining the area of random wall polyominoes of width n. Each polyomino of width n and vertical perimeter $2k$ is given a probability of being drawn that is proportional to y^k. Then, we know by Theorem 2 that the area, when scaled down by a factor of $n^{3/2}\gamma/\sqrt{2\alpha\beta}$, is asymptotically Airy distributed.

The values of α, β and γ depend on y; since the singularity occurs for $y = ((1-x)/(1+x))^2$, it is natural to set $t = \sqrt{y}$, which yields in turn :

$$\begin{aligned} x_0 &= \tfrac{1-t}{1+t}, \\ w_0 &= 1/t, \\ \gamma &= t, \\ \sqrt{2\alpha\beta} &= 2(1-t)\sqrt{t}. \end{aligned}$$

Overall, the scaling factor which must be applied to the area to obtain the Airy limit is

$$\frac{n^{3/2}\gamma}{\sqrt{2\alpha\beta}} = \frac{n^{3/2}y^{1/4}}{2(1-\sqrt{y})}.$$

It would be a nice development to obtain the same information when the polyominoes are only counted by their perimeter, i.e., when all polyominoes of perimeter $2n$ have the same probability. However, our methods do not apply directly in this case : we would need to set $x = t$, $y = t$, $\overline{y} = t$, and so would no longer have Equation (6) or any similar equation.

In the case of directed positive walks, the situation is not as nice : since the algebraic generating function does not take a finite value at its dominant singularity, Theorem 2 definitely does not apply. An analogue of this theorem for generating functions with an inverse square root singularity would be needed.

4.3 Rank 3 parameters

We can get rank 3 parameters on wall polyominoes and directed positive walks by looking at the *moment of inertia*, that is, a weighted sum where each cell in the polyomino has a contribution equal to its height. Equivalently, a collumn of height k contributes for $1 + 2 + \cdots + k = \binom{k+1}{2}$. With such a definition, the equation for $W(x, y, q, r)$, where r will count the moment of inertia and q still counts the area, is still

$$W = x + xW + y\sigma(W) + xy\sigma(W) + xyW\sigma(W),$$

but σ is now defined by $\sigma(W)(x, y, q, r) = W(xqr, y, qr, r)$; when $r = 1$, we go back to the (x, y, q) variables, with exactly the same equation.

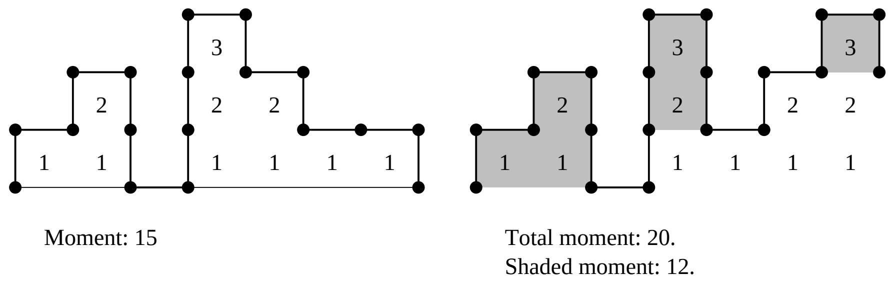

Figure 3: Moments of inertia for wall polyominoes and directed walks

For directed positive walks, two different moments of inertia can be defined : a *total* moment, which counts the sum of heights of all cells that were counted in the total area; and a *shaded* moment, which only counts the height of cells in the shaded area. The equation for the total moment is the same as that for the total area; only the substitution changes :

$$\begin{cases} W &= x + xW + y\overline{y}\sigma(W) + xy\overline{y}\sigma(W) + xy\overline{y}W\sigma(W) \\ W' &= 1 + W + y\sigma(W') + xy\sigma(W') + xyW.\sigma(W'), \end{cases}$$

with $\sigma(W)(x, y, \overline{y}, q, r) = W(xqr, y, \overline{y}, qr, r)$. However, for the shaded moment, the equation for W' is slightly different, and involves two different substitutions :

$$\begin{cases} W &= x + xW + xy\overline{y}\sigma(W) + xy\overline{y}\sigma(W) + xy\overline{y}W\sigma(W), \\ W' &= 1 + W + y\sigma_2(W') + xy\sigma_2(W') + xyW\sigma_2(W'), \end{cases}$$

The substitution operators σ and σ_2 are defined by

$$\begin{cases} \sigma(W)(x, y, \overline{y}, q, r) &= W(xqr, y, \overline{y}, qr, r), \\ \sigma_2(W)(x, y, \overline{y}, q, r) &= W(x, y, \overline{y}, qr, r). \end{cases}$$

We did not state an equivalent of Theorem 2 for parameters of rank 3 and higher. Following the same ideas, we can prove that these parameters, when scaled down by a factor of order n^2 (compare to their maximum order n^3), have moments that satisfy a specific recurrence. Numerical experiments using simple objects suggest that rank 3 parameters do have a universal limit distribution, which is not the Airy distribution. However, we were not able to prove that the moments determine a unique limit law.

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