**Square-Ice Enumeration**

*Alain Lascoux*

Starting with plane partitions possessing certain type of symmetries, many combinatorial objects came to the fore, the enumeration of which was the subject of intensive studies during the last twenty years, with of course, seminal contributions of George Andrews [Axx] .

Thanks to a detour through two-dimensional ice models, algebraic computations cristallised to the description of a certain determinant of Cauchy type. Dividing this determinant by some straightforward factors, one is reduced to studying a symmetric polynomial in two sets of variables. We show in section 2 how to separate the variables with the help of divided differences, and obtain the desired symmetric function as a product of two rectangular matrices, each of them involving only one set of variables (Theorem q). In the same run, we reduce the dimension by 1 and factorize the determinant associated to the Bethe model of a 1-dimensional gas of bosons (Theorem $\gamma$).

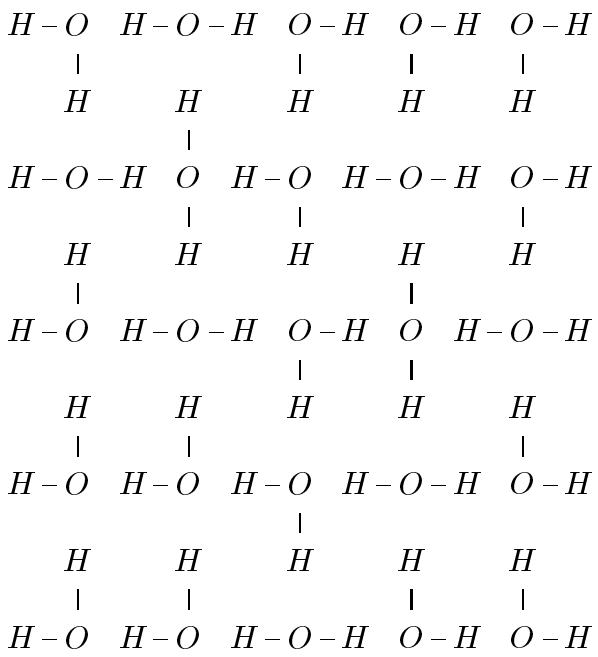
We first evoke some different combinatorial objects related to the algebraic computations of section 2.

**A combinatorial promenade**

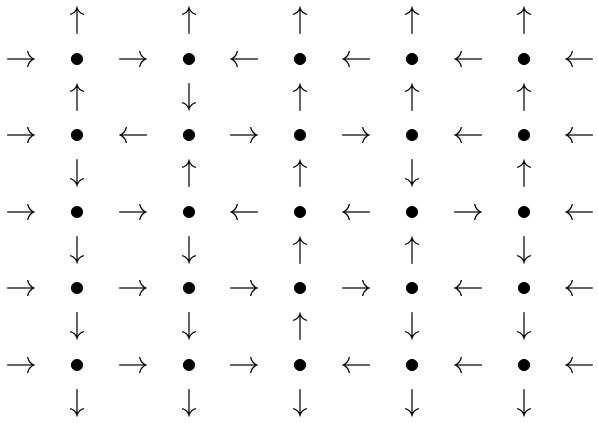
The following figures appear in a forthcoming book by Bressoud [Br]. The elementary pieces are the different models of planar frozen water molecules

$$H-O-H \qquad \begin{matrix} H \\ | \\ O \\ | \\ H \end{matrix} \qquad \begin{matrix} H-O \\ | \\ H \end{matrix} \qquad \begin{matrix} H \\ | \\ H-O \end{matrix} \qquad \begin{matrix} O-H \\ | \\ H \end{matrix} \qquad \begin{matrix} H \\ | \\ O-H \end{matrix}$$

placed on a square grid



Keeping the oxygens, and replacing each hydrogen atom by an arrow pointing toward the oxygen to which it is attached, transforms the preceding figure into the oriented graph



(one has added a top and bottom row of arrows, so that each vertex has two incoming arrows, and two outgoing ones. Now the ice is electrically balanced).

Instead of drawing arrows, one can write the numbers 0,1 or -1 on the vertices of the preceding grid, according to the orientations of the arrows, the precise coding of each of the six possible water molecules being: 1 for the horizontal molecules, $-1$ for the vertical ones, and 0 for the others.

A matrix thereby obtained has the property that non zero entries alternate in each row and column, always starting and finishing with a 1 (*alternating sign matrix*); continuing with the same example we get

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}.$$

Now, interpreting the alternating sign matrix as a history, according to Viennot's paradigm (the entry $+1$ (resp. $-1$) in row $i$, column $j$, means that the letter $i$ appears (resp. disappears) at time $j$), we get a staircase (for bats) Young tableau if we write the letters which are present at time $j$ in decreasing order

| *time* | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| | 2 | 3 | 5 | 5 | 5 |
| | | 1 | 3 | 4 | 4 |
| | | | 1 | 2 | 3 |
| | | | | 1 | 2 |
| | | | | | 1 |

The foregoing tableaux satisfy the usual conditions of being weakly increasing in rows, and strictly decreasing in columns, but also the condition that diagonals are weakly decreasing ; conversely any such "monotonous triangle" (we shall simply say *triangle*) corresponds to an alternating sign matrix, as well as to some ice state.

Enumerating triangles, or more general planar partitions has been studied by Andrews [Axx], Mills, Robbins, Rumsey [MRR1], [MRR2], the story being told by Bressoud in his book [Br].

The previous model is also related with the "Ehresmann-Bruhat order" on the symmetric group (cf. [LS2]). It stems from the remark that the set of triangles of a given order is a lattice (in fact a distributive lattice): the supremum (boxwise) of two triangles is still a triangle. Now, it is easy to see that the generators of the lattice are exactly those triangles having exactly one entry with the property that the triangle remains monotonous if that entry is reduced by 1.

For example,

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | 5 | 6 | 6 | 6 | 6 | 7 |
| | 1 | $V$ | 5 | 5 | 5 | 6 |
| | | 1 | 2 | 3 | 4 | 5 |
| | | | 1 | 2 | 3 | 4 |
| | | | | 1 | 2 | 3 |
| | | | | | 1 | 2 |
| | | | | | | 1 |

is such a generator (the special entry, which is allowed to decrease, is denoted by $V$ and yields a monotonous triangle for $V = 4$).

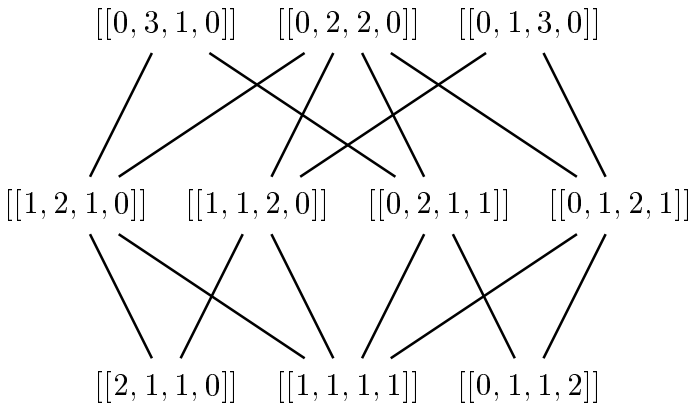
Now, the alternating sign matrix corresponding to such a triangle is a *bigrassmannian permutation* matrix : The bigrassmannian permutations are exactly those permutations obtained from the identity permutation by cutting it into four blocks, and exchanging the two middle blocks. For instance, flipping 234 and 56

$$[1 \mid 234 \mid 56 \mid 7] \mapsto [1 \mid 56 \mid 234 \mid 7]$$

yields the bigrassmannian permutation associated with the previous triangle.

Of course, such permutations can be coded by the successive lengths of the blocks, the two middle blocks being non empty ( in the preceeding case, the sequence of lengths is $1, 2, 3, 1$, and the permutation will be denoted by $[[1, 2, 3, 1]]$).

Taking the boxwise order on triangles into account, one gets the following ordered set for the generators of the lattice of triangles of dimension 4




Antichains in the preceeding set (i.e. $k$-uples of non comparable bigrassmannian permutations) are by definition in bijection with elements of the lattice of triangles of size $n$, or alternating sign matrices of order $n$, or square ice configurations with $n^2$ molecules.

The reader may be willing to derive the 42 alternating sign matrices of order 4 from the above figure; there are, indeed, 42 antichains in this poset.

For other connections, see [La] and for more information about the Ehresmann-Bruhat order on finite Coxeter groups, see [GK].

The problem of enumerating alternating sign matrices, due to Mills, Robbins, and Rumsey [MRR1], [MRR2] has resisted many attempts, till

Zeilberger [Z1] gave a solution with the collaboration of his computer, the control of eighty eight of his friends (he has a lot more), and many references to the Bible. Shorter proofs were given by Kuperberg [Ku] and [Z2] again, after realizing that the partition function of square ice models had already been obtained by Korepin, Bogoliubov and Izergin [KBI] : it is expressed as a determinant generalizing Cauchy determinant.

We are now ready to enumerate square ice models.

**Cauchy type determinants**

Given two sets of variables $X = \{x\}$, $Y = \{y\}$, of the same cardinality Cauchy introduced two matrices (we do not burden variables with indices, because they play a symmetrical role; however, to write matrices one chooses an arbitrary total order on the $x$'s$\in X$ and the $y$'s $\in Y$)

$$M_0 = \left[\frac{1}{1-xy}\right]_{x\in X, y\in Y} \qquad \text{and} \qquad M_1 = \left[\frac{1}{x-y}\right]_{x\in X, y\in Y} .$$

From them one can extract a scalar product on symmetric functions, as well as several pairs of adjoint bases, the most conspicuous one being the self-adjoint basis of Schur functions.

Pulling out from $\det(M_1)$ the Vandermonde determinants $\Delta(X)$, $\Delta(Y)$ and the product $\prod_{x\in X, y\in Y}(1/(x-y))$, one is left with a symmetric polynomial

$$F_1(X,Y) = \det(M_1)\frac{\prod(x-y)}{\Delta(X)\,\Delta(Y)} . \tag{1}$$

One easily checks that $F_1$ is equal to 1, and this fact, in a sense, could summarize the first chapter of Macdonald's book [Ma].

Borchardt [Bo] went one step further, and considered

$$M_2 := \left[\frac{1}{(x-y)^2}\right] .$$

He proved that

$$\det(M_2) = \det(M_1)\ \mathrm{Perm}(M_1) ,$$

where

$$\mathrm{Perm}(M_1) = \sum_{\mu\in\mathfrak{S}(X)} \left(\frac{1}{(x_1-y_1)\cdots(x_n-y_n)}\right)^{\mu}$$

is the usual *permanent*, the summation being over all the permutations of the $x$'s. Therefore the symmetric function

$$F_2(X,Y) = det(M_2)\frac{\prod(x-y)^2}{\Delta(X)\,\Delta(Y)} \tag{2}$$

is expressed by a summation over the symmetric group.

Now, thanks to some giants, the shoulders of which Zeilberger [Z2] escalated to provide a short alternating-sign-matrices enumeration, we know that we must polarize squares, the simplest versions being

$$(x-y)^2 \longrightarrow (x-y)(qx-y) \qquad (ice)$$

$$(x-y)^2 \longrightarrow (x-y)(x-y+\gamma) \qquad (Bethe)$$

with $q$ and $\gamma$ some fixed constants independent of the $x$'s and $y$'s.

Introducing another set of variables $Z = \{z\}$ of the same cardinality as $X$ and $Y$, one can more generally polarize as follows

$$(x_i - y_j) \longrightarrow (x_i - y_j)\,(z_i - y_j)\ .$$

We intend to describe the symmetric polynomial

$$F_Z(X,Y) := \det\left(\left[\frac{1}{(x_i-y_j)(z_i-y_j)}\right]\right)\frac{\prod(x-y)\,\prod(z-y)}{\Delta(X)\,\Delta(Y)} \qquad (3)$$

in the two cases of physical interest

$$z_i = qx_i \qquad \text{or} \qquad z_i = x_i + \gamma$$

We shall need divided differences $\partial_i$ involving pairs of variables $x_i$, $z_i$

$$\partial_i :\ f \mapsto \frac{f - f^{\sigma_i}}{x_i - z_i}\ ,$$

where $\sigma_i$ is the transposition exchanging $x_i$ and $z_i$.

We also need *complete functions* $S_k(A-B)$ of differences of sets of variables (*alphabets*) that can be defined by the following generating function :

$$\sum_0^\infty u^k\, S_k(A-B) := \frac{\prod_{b\in B}(1-ub)}{\prod_{a\in A}(1-ua)}\ .$$

We shall write $x_i + z_i$ for the alphabet $A = \{x_i, z_i\}$ and $S_{\alpha,\beta}(A-B, C-D)$ for the two-row Schur function

$$S_{\alpha,\beta}(A-B,C-D) := \begin{vmatrix} S_\alpha(A-B) & S_{\alpha+1}(A-B) \\ S_{\beta-1}(C-D) & S_\beta(C-D) \end{vmatrix}$$

In particular, $z_i^k\ \prod_{y\in Y}(x_i - y)$ can be written as $S_{n,k}(x_i - Y, x_i + z_i)$.

However, the image of $\prod_{y\in Y}(1-y)/(1-x_i)$ under $\partial_i$ is

$$\prod_{y\in Y}(1-y)/(1-x_i)(1-z_i)\ .$$

In other words, $\partial_i$ sends $S_j(x_i-Y)$ onto $S_{j-1}(x_i+z_i-Y)$ for any $j\in\mathbb{Z}$. Hence the image of $S_{n,k}(x_i-Y,x_i+z_i)$ under $\partial_i$ is

$$S_{n-1,k}(x_i+z_i-Y,x_i+z_i)=\begin{vmatrix} S_{n-1}(x_i+z_i-Y) & S_n(x_i+z_i-Y)\\ S_{k-1}(x_i+z_i) & S_k(x_i+z_i)\end{vmatrix} \quad (4)$$

that can be developped by linearity in $Y$ into

$$=\sum_{h=-1}^{n-1} S_{h,k}(x_i+z_i,x_i+z_i)\,S_{n-1-h}(-Y) \quad (5)$$

$$=\sum_{h=k}^{n-1} S_{h,k}(x_i+z_i)\,S_{n-1-h}(-Y)-\sum_{h=0}^{k-1} S_{k-1,h}(x_i+z_i)\,S_{n-h}(-Y) \quad (6)$$

On the other hand, the image of the Cauchy determinant $|1/(z-y)|$ under the product $\partial_1,\ldots,\partial_n$ is the determinant of

$$M_Z:=\left[\frac{1}{(x_i-y_j)\,(z_i-y_j)}\right]\ ,$$

since each $\partial_i$ acts on row $i$ only.

Write $R(X,Y)$ for the product of differences $\prod(x-y)$. The Cauchy determinant $|1/(z-y)|$ is equal to

$$\frac{\Delta(Y)}{R(X,Y)\,R(Z,Y)}\Delta(Z)\,R(X,Y)=\frac{\Delta(Y)}{R(X,Y)\,R(Z,Y)}\ \det(M_3)\ , \quad (7)$$

with

$$M_3:=[S_{n,j-1}(x_i-Y,x_i+z_i)]$$

Now, the factor $\Delta(Y)\,(R(X,Y)\,R(Z,Y))^{-1}$ commutes with the product of the $\partial_i$, since it is symmetrical in the $x_i$ and $z_i$. According to (4), the image of $\det(M_3)$ is therefore equal to the determinant of

$$M_4:=[S_{n-1,j-1}(x_i+z_i-Y,x_i+z_i)]\ . \quad (8)$$

Expansion (5) exactly tells that the matrix $M_4$ factorizes into a product of a matrix of two-part Schur functions in $(x_i+z_i)$, and a matrix of $\Lambda_i:=S_{1^i}(Y)$ or zeroes.

For example, for n=2, one has

$$\begin{pmatrix} s_0(x_1+z_1) & s_1(x_1+z_1) & s_{1,1}(x_1+z_1) \\ s_0(x_2+z_2) & s_1(x_2+z_2) & s_{1,1}(x_2+z_2) \end{pmatrix} \begin{pmatrix} -\Lambda_1 & -\Lambda_2 \\ \Lambda_0 & 0 \\ 0 & \Lambda_0 \end{pmatrix}$$

For n=3,

$$\begin{pmatrix} 1 & s_1(x_1+z_1) & s_2(x_1+z_1) & s_{1,1}(x_1+z_1) & s_{2,1}(x_1+z_1) & s_{2,2}(x_1+z_1) \\ 1 & s_1(x_2+z_2) & s_2(x_2+z_2) & s_{1,1}(x_2+z_2) & s_{2,1}(x_2+z_2) & s_{2,2}(x_2+z_2) \\ 1 & s_1(x_3+z_3) & s_2(x_3+z_3) & s_{1,1}(x_3+z_3) & s_{2,1}(x_3+z_3) & s_{2,2}(x_3+z_3) \end{pmatrix}$$

$$\times \quad \begin{pmatrix} \Lambda_2 & \Lambda_3 & 0 \\ -\Lambda_1 & 0 & \Lambda_3 \\ \Lambda_0 & 0 & 0 \\ 0 & -\Lambda_1 & -\Lambda_2 \\ 0 & \Lambda_0 & 0 \\ 0 & 0 & \Lambda_0 \end{pmatrix}$$

Finally, for n=4, writing $s_\lambda$ for the Schur functions of $x_i + z_i$, $i = 1, \ldots, 4$, the factorization is

$$[s_0, s_1, s_2, s_3, s_{11}, s_{21}, s_{22}, s_{31}, s_{32}, s_{33}] \begin{pmatrix} -\Lambda_3 & -\Lambda_4 & 0 & 0 \\ \Lambda_2 & 0 & -\Lambda_4 & 0 \\ -\Lambda_1 & 0 & 0 & -\Lambda_4 \\ \Lambda_0 & 0 & 0 & 0 \\ 0 & \Lambda_2 & \Lambda_3 & 0 \\ 0 & -\Lambda_1 & 0 & \Lambda_3 \\ 0 & 0 & -\Lambda_1 & -\Lambda_2 \\ 0 & \Lambda_0 & 0 & 0 \\ 0 & 0 & \Lambda_0 & 0 \\ 0 & 0 & 0 & \Lambda_0 \end{pmatrix}$$

Any specialization $z_i = g(x_i)$, $g$ being an arbitrary function of one variable, will allow to factor out a matrix of determinant $\Delta(X)$ from the left matrix, and thus will allow to explicit the symmetric function $F_Z(X, Y)$.

In that case, $S_{\alpha,\beta}(x_i + z_i)$ becomes a polynomial $f(x_i; \alpha, \beta)$ of degree $n(\alpha, \beta)$ that can be formally written $S_{n(\alpha,\beta)}(x_i - A_{\alpha,\beta})$, for some alphabet $A_{\alpha,\beta}$ of cardinality $n(\alpha, \beta)$ (= the "alphabet of zeroes" of the polynomial $f(x_i; \alpha, \beta)$ ).

Now, for any integer $k$, one has the expansion

$$\begin{aligned} S_k(x_i - A_{\alpha,\beta}) &= S_k((x_i - X) + (X - A_{\alpha,\beta})) \\ &= \sum_{0 \le j \le n-1} S_{k-j}(x_i - X)\, S_j(X - A_{\alpha,\beta}) \ . \end{aligned}$$

Therefore, from the matrix $\left[S_{n(\alpha,\beta)}(x_i - A_{\alpha,\beta})\right]$, one can extract the left factor $[S_{j-1}(x_i - X)]_{1\leq j,i\leq n}$ (the determinant of which is $\Delta(X)$) and one is left with matrix

$$\left[S_{n(\alpha,\beta)-i+1}(X - A_{\alpha,\beta})\right]_{n-1\geq\alpha\geq\beta\geq 0;1\leq i\leq n} \tag{9}$$

Let us be more precise in the case of Bethe's function ( we refer to [Ga] for many other expressions of this function). For $z = x + \gamma$, the Schur function $S_{\alpha,\beta}(x + z)$ specializes to

$$\begin{aligned}\frac{1}{\gamma}\begin{vmatrix} (x+\gamma)^{\alpha+1} & (x+\gamma)^{\beta} \\ x^{\alpha+1} & x^{\beta}\end{vmatrix} &= (x+\gamma)^{\beta}\sum_{i=0}^{\alpha-\beta} x^{\alpha-i}\gamma^{i}\binom{\alpha+1-\beta}{i+1} \\ &= \sum_{0}^{\alpha}\gamma^{i}x^{\alpha+\beta-i}\left(\binom{\alpha+1}{i} - \binom{i}{\alpha+1-i}\right)\end{aligned} \tag{10}$$

Let us write the preceding polynomial as

$$\sum_{0\leq i\leq\alpha+\beta} c^{i}_{\alpha,\beta}\gamma^{i}x^{\alpha+\beta-i}$$

and for any alphabet $X$, and any partition of length $\leq 2$, define

$$S^{k}_{\alpha,\beta}(X) := \sum_{0\leq i\leq\alpha+\beta} c^{i}_{\alpha,\beta}\gamma^{i}S_{\alpha+\beta-i-k}(X)\ . \tag{11}$$

Write $\chi(a = b)$ for the Boolean function which tests equality. The combination of (8) and (10) produces the following factorization.

**Theorem** $\gamma$ **.** *Let $X$ and $Y$ be two alphabets of cardinality $n$, $\gamma$ an extra parameter. Then the symmetric function*

$$F^{\gamma}(X,Y) := \left|\frac{1}{(x-y)(x-y+\gamma)}\right|_{x\in X,y\in Y}\frac{\prod(x-y)(x-y+\gamma)}{\Delta(X)\,\Delta(Y)} \tag{12}$$

*is the determinant of the product of matrices*

$$\left[S^{i-1}_{\alpha,\beta}(X)\right]^{n-1\geq\alpha\geq\beta\geq 0}_{1\leq i\leq n}\left[\chi(\beta{=}j{-}1)S_{n-1-\alpha}(-Y) - \chi(\alpha{=}j{-}2)S_{n-\beta}(-Y)\right]^{1\leq j\leq n}_{n-1\geq\alpha\geq\beta\geq 0}\ .$$

The following factorizations and Bethe functions are readily computed by ACE [AV], the output being randomly distributed by Maple. Writing $\Lambda_i$ for $(-1)^i S_i(-Y)$, and $s_i$ for $S_i(X)$, we get:

$$\begin{pmatrix} 1 & \gamma+2s_1 & \gamma s_1+s_2 \\ 0 & 2 & \gamma+s_1 \end{pmatrix} \begin{pmatrix} -\Lambda_1 & -\Lambda_2 \\ \Lambda_0 & 0 \\ 0 & \Lambda_0 \end{pmatrix} =$$

$$(2\Lambda_2+g^2-g\Lambda_1)+(g-\Lambda_1)s_1+2s_{1,1}\ ;$$

$$\begin{pmatrix} 1 & \gamma+2s_1 & \gamma^2+3\gamma s_1+3s_2 & \gamma s_1+s_2 & \gamma^2 s_1+3\gamma s_2+2s_3 & \gamma^2 s_2+2\gamma s_3+s_4 \\ 0 & 2 & 3\gamma+3s_1 & \gamma+s_1 & \gamma^2+3\gamma s_1+2s_2 & \gamma^2 s_1+2\gamma s_2+s_3 \\ 0 & 0 & 3 & 1 & 3\gamma+2s_1 & \gamma^2+2\gamma s_1+s_2 \end{pmatrix}$$

$$\times \quad \begin{pmatrix} \Lambda_2 & \Lambda_3 & 0 \\ -\Lambda_1 & 0 & \Lambda_3 \\ \Lambda_0 & 0 & 0 \\ 0 & -\Lambda_1 & -\Lambda_2 \\ 0 & \Lambda_0 & 0 \\ 0 & 0 & \Lambda_0 \end{pmatrix} =$$

$6s_{2,2,2}+(\gamma^6-2\Lambda_1\gamma^5+4\Lambda_1\Lambda_3\gamma^2+2{\Lambda_2}^2\gamma^2+3\gamma^4\Lambda_2+{\Lambda_1}^2\gamma^4+6{\Lambda_3}^2-6\Lambda_3\Lambda_2\gamma-3\Lambda_1\Lambda_2\gamma^3-3\Lambda_3\gamma^3)+(-4\Lambda_3\gamma^2-4\Lambda_1\gamma^4+2{\Lambda_2}^2\gamma+4\Lambda_1\Lambda_3\gamma-4\Lambda_1\gamma^2\Lambda_2+2\gamma^5-4\Lambda_2\Lambda_3+2{\Lambda_1}^2\gamma^3+4\Lambda_2\gamma^3)s_1+(\gamma^4+{\Lambda_1}^2\gamma^2-\Lambda_1\Lambda_2\gamma+2\Lambda_1\Lambda_3+\Lambda_2\gamma^2-2\Lambda_1\gamma^3-3\Lambda_3\gamma)s_2+(-4\Lambda_1+6\gamma)s_{2,2,1}+(3\gamma^3-3\Lambda_3-\Lambda_1\Lambda_2-4\Lambda_1\gamma^2+3\Lambda_2\gamma+{\Lambda_1}^2\gamma)s_{2,1}+(2{\Lambda_2}^2+2{\Lambda_1}^2\gamma^2-4\Lambda_1\Lambda_2\gamma-6\Lambda_1\gamma^3+4\gamma^4+6\Lambda_2\gamma^2)s_{1,1}+(12\Lambda_3-8\Lambda_1\gamma^2+6\gamma^3-4\Lambda_1\Lambda_2+4{\Lambda_1}^2\gamma)s_{1,1,1}+(2\Lambda_2+2\gamma^2-2\Lambda_1\gamma)s_{2,2}+(2{\Lambda_1}^2+6\gamma^2-6\Lambda_1\gamma)s_{2,1,1}$

On the other hand, when the $z_i$ specialize to $qx_i$, one has a more convenient factorization into smaller matrices. Indeed,

$$S_{\alpha,\beta}(x+qx)=x^{\alpha+\beta}(q^\beta+q^{\beta+1}+\cdots+q^\alpha)=x^{\alpha+\beta}q^\beta\,[\alpha-\beta+1]_q\ , \quad (13)$$

with $[k]_q := 1+q+\cdots+q^{k-1}$. Combining these values with expansion (6), one gets the following property.

**Theorem q .** *Let $X$ and $Y$ be two alphabets of cardinality $n$, $q$ an extra parameter. Then the symmetric function*

$$F_q(X,Y) := \left|\frac{1}{(x-y)(qx-y)}\right|_{x\in X, y\in Y} \frac{\prod(x-y)(qx-y)}{\Delta(X)\,\Delta(Y)} \qquad (14)$$

*is the determinant of the product of*

$$[S_{j-i}(X)]_{1\le i\le n,1\le j\le 2n-1}\ \left[\frac{q^{j-k+1}-q^{k-1}}{q-1}\,S_{n-j+k-1}(-Y)\right]_{1\le j\le 2n-1,1\le k\le n}$$

*The coefficient of any Schur function $S_\lambda(X)$, $\lambda_1\ge\cdots\ge\lambda_n\ge 0$, in the expansion of $F_q(X,Y)$ is equal to the minor on rows $\lambda_n+1,\dots,\lambda_1+n$, columns $1,\dots,n$ of the matrix in $Y$.*

For example, for $n=2$, $F_q(X,Y)$ is the determinant of the product

$$\begin{pmatrix} S_0 & S_1 & S_2\\ 0 & S_0 & S_1\end{pmatrix}\cdot\begin{pmatrix} -\Lambda_1 & -\Lambda_2\\ 1+q & 0\\ 0 & q\end{pmatrix}=(1+q)\Lambda_2-q(x_1+x_2)\Lambda_1+(q+q^2)\,x_1x_2$$

still writing $S_k$ for $S_k(X)$, and $\Lambda_i$ for $(-1)^iS_i(-Y)$, i.e. for the $i$-th elementary symmetric function of $Y$.

For $n=3,4,5$, writing $[k]$ for the $q$-integer $[k]_q$, ACE [AV] produces the right matrix

$$\begin{pmatrix} \Lambda_2 & \Lambda_3 & 0\\ -[2]\Lambda_1 & 0 & [2]\Lambda_3\\ [3] & -q\Lambda_1 & -q\Lambda_2\\ 0 & q[2] & 0\\ 0 & 0 & q^2\end{pmatrix}\quad,\quad\begin{pmatrix} -\Lambda_3 & -\Lambda_4 & 0 & 0\\ [2]\Lambda_2 & 0 & -[2]\Lambda_4 & 0\\ -[3]\Lambda_1 & q\Lambda_2 & q\Lambda_3 & -[3]\Lambda_4\\ [4] & q[2]\Lambda_1 & 0 & q[2]\Lambda_3\\ 0 & q[3] & -q^2\Lambda_1 & -q^2\Lambda_2\\ 0 & 0 & q^2[2] & 0\\ 0 & 0 & 0 & q^3\end{pmatrix}$$

$$\begin{pmatrix} \Lambda_4 & \Lambda_5 & 0 & 0 & 0\\ -[2]\Lambda_3 & 0 & [2]\Lambda_5 & 0 & 0\\ [3]\Lambda_2 & -q\Lambda_3 & -q\Lambda_4 & [3]\Lambda_5 & 0\\ -[3]\Lambda_1 & q[2]\Lambda_2 & 0 & -q[2]\Lambda_4 & [4]\Lambda_5\\ [5] & -q[3]\Lambda_1 & q^2\Lambda_2 & q^2\Lambda_3 & -q[3]\Lambda_4\\ 0 & q[4] & -q^2[2]\Lambda_1 & 0 & q^2[2]\Lambda_3\\ 0 & 0 & q^2[3] & -q^3\Lambda_1 & -q^3\Lambda_2\\ 0 & 0 & 0 & q^3[2] & 0\\ 0 & 0 & 0 & 0 & q^4\end{pmatrix}$$

and the expansion of $F_q(X,Y)$, for $n=3$, is (writing, for each Schur function of $X$, its coefficient in $Y$ as a sum of Schur functions in $Y$)
$s_0(X):(q+1)(q^2+q+1)(s_{111111}+s_{21111}+s_{222}+s_{2211})$
$s_1(X):-q(q+1)^2(s_{11111}+s_{221}+s_{2111})$
$s_2(X):q^2(s_{1111}+s_{211})(q+1)$

$s_{11}(X) : q^2(s_{1111} + s_{22} + s_{211})(q+1)$
$s_{21}(X) : -q^2(qs_{21} + 2qs_{111} + s_{111}q^2 + s_{111})$
$s_{22}(X) : q^3 s_{11}(q+1)$
$s_{111}(X) : q(q+1)^2(s_{111}q^2 - qs_{21} + s_{111})$
$s_{211}(X) : (q+1)q^3(s_2 + s_{11})$
$s_{221}(X) : -s_1 q^3(q+1)^2$
$s_{222}(X) : sq^3(q+1)(q^2+q+1)$
Lastly, for $n = 4$ one has the following expansion of the function $F_q(X, Y)$ (that it is impossible to obtain directly from the expansion of (3), the object being to large for Maple):
$s_0(X) : (q^2+1)(q^2+q+1)(q+1)^2(s_{1\ldots1} + 2s_{21\ldots1} + 3s_{2211\ldots1} + 5s_{22221\ldots1} + 4s_{2221\ldots1} + 3s_{2222211} + s_{31\ldots1} + 2s_{321\ldots1} + 4s_{3222111} + 3s_{3221\ldots1} + s_{222222} + 2s_{322221} + s_{331\ldots1} + 3s_{332211} + 2s_{3321\ldots1} + s_{3333} + 2s_{33321} + s_{33222} + s_{333111})$
$s_1(X) : -q(q+1)(q^2+q+1)^2(2s_{21\ldots1} + s_{1\ldots111} + 2s_{222221} + s_{31\ldots11} + 2s_{321\ldots1} + 4s_{2221\ldots1} + 3s_{221\ldots1} + 4s_{2222111} + 3s_{3221\ldots1} + 3s_{322211} + s_{3332} + s_{33311} + s_{331\ldots1} + 2s_{33221} + 2s_{332111} + s_{32222})$
$s_2(X) : q^2(q^2+q+1)(q+1)^2(s_{1\ldots11} + 2s_{21\ldots11} + 3s_{221\ldots1} + 3s_{222211} + 3s_{2221\ldots1} + s_{22222} + s_{31\ldots1} + 2s_{321\ldots1} + 2s_{32221} + 2s_{322111} + s_{331\ldots1} + s_{3322} + s_{33211})$
$s_3(X) : -q^3(q+1)(q^2+q+1)(s_{1\ldots1} + 2s_{21\ldots1} + 2s_{221\ldots1} + 2s_{22221} + 2s_{222111} + s_{31\ldots1} + s_{321\ldots1} + s_{3222} + s_{32211})$
$s_{11}(X) : q^2(q+1)^2(q^2 s_{33211} + q^2 s_{322111} + q^2 s_{3331} + q^2 s_{2221\ldots1} + qs_{3331} + 3qs_{221\ldots1} + 3qs_{222211} + 4qs_{2221\ldots1} + 2qs_{21\ldots11} + qs_{1\ldots11} + qs_{331\ldots1} + qs_{3322} + 2qs_{33211} + qs_{22222} + qs_{31\ldots1} + 2qs_{321\ldots1} + 2qs_{32221} + 3qs_{322111} + s_{33211} + s_{322111} + s_{3331} + s_{2221\ldots1})$
$s_{21}(X) : -q^3(q+1)^3(s_{1\ldots1} + 2s_{2111\ldots1} + 3s_{222111} + 3s_{221\ldots1} + 2s_{22221} + s_{31\ldots1} + 2s_{32211} + 2s_{321\ldots1} + s_{3222} + s_{3321} + s_{33111})$
$s_{31}(X) : q^3(q+1)^2(q^2 s_{1\ldots11} + q^2 s_{21\ldots1} + q^2 s_{221\ldots1} + q^2 s_{2222} + q^2 s_{22211} + qs_{1\ldots11} + 2qs_{21\ldots1} + 2qs_{221\ldots1} + qs_{2222} + 2qs_{22211} + qs_{31\ldots1} + qs_{32111} + qs_{3221} + s_{1\ldots11} + s_{21\ldots111} + s_{221\ldots1} + s_{2222} + s_{22211})$
$s_{22}(X) : q^4(q+1)^2(s_{1\ldots11} + 2s_{2111111} + 3s_{221\ldots1} + s_{2222} + 2s_{22211} + 2s_{32111} + s_{3311} + s_{31\ldots1} + s_{3221})$
$s_{32}(X) : -q^4(q+1)(q^2 s_{1\ldots1} + q^2 s_{21\ldots1} + q^2 s_{22111} + q^2 s_{2221} + qs_{31111} + qs_{3211} + 3qs_{22111} + 2qs_{2221} + 2qs_{1\ldots1} + 3qs_{21\ldots1} + s_{1\ldots1} + s_{21\ldots1} + s_{22111} + s_{2221})$
$s_{33}(X) : q^5(q+1)^2(s_{1\ldots1} + s_{21\ldots1} + s_{2211})$
$s_{111}(X) : q^2(q+1)(-q^2 s_{333} - 2q^2 s_{3321} - q^2 s_{33111} + qs_{1\ldots1} + 2qs_{21\ldots1} + qs_{222111} + 2qs_{221\ldots1} + 2qs_{22221} + qs_{31\ldots1} + qs_{321111} - qs_{333} - qs_{3321} + qs_{3222} + q^2 s_{3222} - q^2 s_{32211} + q^2 s_{1\ldots1111} + 2q^2 s_{21\ldots1} + q^2 s_{221\ldots1} + 2q^2 s_{22221} + q^2 s_{31\ldots1} + 2q^4 s_{21\ldots1} + 2q^4 s_{222111} + 2q^4 s_{221\ldots1} + 2q^4 s_{22221} + q^4 s_{31\ldots1} + q^4 s_{32211} + q^4 s_{1\ldots11} + q^4 s_{321\ldots1} + q^4 s_{3222} + q^3 s_{1\ldots1} + 2q^3 s_{21\ldots1} + q^3 s_{222111} + 2q^3 s_{221\ldots1} + 2q^3 s_{22221} + q^3 s_{31\ldots1} + q^3 s_{321\ldots1} - q^3 s_{333} - q^3 s_{3321} + q^3 s_{3222} + s_{31\ldots1} + s_{321\ldots1} + s_{3222} + s_{32211} + 2s_{221\ldots1} + 2s_{22221} + 2s_{222111} + s_{1\ldots1} + 2s_{21\ldots1})$

$s_{211}(X) : -q^2(q+1)^2(qs_{21\ldots1}-2q^2s_{3221}+qs_{221\ldots1}+qs_{2222}-q^2s_{332}+qs_{1\ldots11}-q^2s_{3311}-q^2s_{31\ldots1}-2q^2s_{32111}-q^2s_{22211}+qs_{22211}+q^2s_{1\ldots11}-q^2s_{221\ldots1}+q^2s_{2222}+q^3s_{22211}+q^3s_{1\ldots11}+q^3s_{21\ldots1}+q^3s_{221\ldots1}+q^3s_{2222}+q^4s_{2222}+s_{1\ldots11}+s_{21\ldots1}+s_{221\ldots1}+s_{2222}+s_{22211}+q^4s_{22211}+q^4s_{1\ldots11}+q^4s_{221111}+q^4s_{21\ldots1})$
$s_{311}(X) : -q^4(q+1)(q^2s_{22111}+q^2s_{2221}+q^2s_{1\ldots1}+q^2s_{21\ldots1}+2qs_{2221}+qs_{3211}+qs_{31\ldots1}+2qs_{22111}+2qs_{21\ldots1}+qs_{1\ldots1}+qs_{322}+s_{22111}+s_{2221}+s_{1\ldots1}+s_{21\ldots1})$
$s_{221}(X) : -(q+1)q^3(-q^4s_{1\ldots1}-q^4s_{21\ldots1}-q^4s_{22111}-q^4s_{2221}+q^3s_{3211}-q^3s_{1\ldots1}+q^3s_{31\ldots1}-q^3s_{2221}-q^2s_{1\ldots1}+2q^2s_{22111}+q^2s_{322}+q^2s_{21\ldots1}+2q^2s_{31\ldots1}+3q^2s_{3211}+q^2s_{331}+qs_{3211}-qs_{1\ldots1}+qs_{31\ldots1}-qs_{2221}-s_{1\ldots1}-s_{21\ldots1}-s_{22111}-s_{2221})$
$s_{321}(X) : q^5(2s_{1\ldots1}+2q^2s_{1\ldots1}+3q^2s_{21\ldots1}+q^2s_{222}+2q^2s_{2211}+5qs_{21\ldots1}+3qs_{1\ldots1}+qs_{321}+2qs_{222}+4qs_{2211}+2qs_{3111}+s_{3111}+2s_{2211}+q^2s_{3111}+3s_{21\ldots1}+s_{222})$
$s_{331}(X) : -q^5(q+1)(q^2s_{1\ldots1}+q^2s_{2111}+2qs_{1\ldots1}+qs_{221}+2qs_{2111}+s_{1\ldots1}+s_{2111})$
$s_{222}(X) : -q^4(q+1)^2(q^2s_{222}-qs_{3111}-qs_{321}-qs_{2211}-qs_{21\ldots1}+s_{222})$
$s_{322}(X) : -q^5(q+1)(q^2s_{1\ldots1}+q^2s_{2111}+qs_{11\ldots1}+2qs_{2111}+qs_{311}+qs_{221}+s_{1\ldots1}+s_{2111})$
$s_{332}(X) : q^5(q+1)^2(q^2s_{1\ldots1}+qs_{1\ldots1}+qs_{211}+s_{1\ldots1})$
$s_{333}(X) : -s_{111}q^6(q+1)(q^2+q+1)$
$s_{1\ldots1}(X) : q(q+1)^2(q^2s_{332}+s_{1\ldots11}+s_{21\ldots1}+s_{221\ldots1}+s_{2222}+s_{22211}-2q^4s_{32111}-2q^4s_{31\ldots1}+q^4s_{332}-q^4s_{3221}+2q^2s_{1\ldots1}+2q^2s_{2222}+q^2s_{22211}-q^5s_{32111}-q^5s_{31\ldots1}-q^5s_{3221}+q^6s_{1\ldots1}+q^6s_{2111111}+q^6s_{221\ldots1}+q^6s_{2222}+q^6s_{22211}+q^3s_{22211}-q^3s_{32111}-2q^3s_{31\ldots1}+q^3s_{332}-q^3s_{3221}+2q^3s_{2222}+q^3s_{3311}+q^4s_{22211}+q^5s_{1\ldots1}+q^5s_{2222}+2q^3s_{1\ldots1}+q^3s_{221\ldots1}+2q^4s_{1\ldots1}+2q^4s_{2222}+qs_{1\ldots1}+qs_{2222}-2q^2s_{31\ldots1}-2q^2s_{32111}-q^2s_{3221}-qs_{31\ldots1}-qs_{32111}-qs_{3221})$
$s_{2111}(X) : q^3(q+1)^3(2q^2s_{21\ldots1}+q^2s_{1\ldots1}+q^2s_{31\ldots1}+2q^2s_{22111}+q^2s_{3211}+q^2s_{2221}-qs_{322}-qs_{331}-qs_{3211}-qs_{2221}-qs_{22111}+2s_{21\ldots1}+s_{1\ldots1}+s_{31\ldots1}+2s_{22111}+s_{3211}+s_{2221})$
$s_{3111}(X) : -q^4(q+1)^2(q^2s_{21\ldots1}+q^2s_{3111}-qs_{321}-qs_{222}-qs_{2211}+s_{21\ldots1}+s_{3111})$
$s_{2211}(X) : -q^3(q+1)^2(q^4s_{2211}+q^4s_{1\ldots11}+q^4s_{21\ldots1}+2q^3s_{2211}+2q^3s_{21111}+2q^3s_{1\ldots1}+q^2s_{21\ldots1}+2q^2s_{1\ldots1}-q^2s_{3111}-q^2s_{33}-2q^2s_{321}-q^2s_{222}+2qs_{2211}+2qs_{21\ldots1}+2qs_{1\ldots1}+s_{2211}+s_{111\ldots1}+s_{21\ldots1})$
$s_{3211}(X) : q^4(q+1)(q^4s_{1\ldots1}+q^4s_{2111}+q^3s_{1\ldots1}-q^3s_{221}+q^3s_{2111}-q^2s_{32}+q^2s_{1\ldots1}-q^2s_{311}-3q^2s_{221}+qs_{1\ldots1}-qs_{221}+qs_{2111}+s_{11111}+s_{2111})$
$s_{3311}(X) : q^6(q+1)^2(s_{1\ldots1}+s_{22}+s_{211})$
$s_{2221}(X) : q^4(q+1)^3(q^2s_{1\ldots1}+q^2s_{221}+q^2s_{2111}-qs_{311}-qs_{32}-qs_{221}-qs_{2111}+s_{1\ldots1}+s_{221}+s_{2111})$
$s_{3221}(X) : -q^4(q+1)^2(s_{1\ldots1}q^4+q^3s_{1\ldots1}-q^2s_{31}+q^2s_{1\ldots1}-q^2s_{22}-2q^2s_{211}+qs_{1\ldots1}+s_{1\ldots1})$
$s_{3321}(X) : -q^6(q+1)^3(s_{21}+s_{111})$

$s_{3331}(X) : s_{11}q^6(q^2+q+1)(q+1)^2$
$s_{2222}(X) : q^3(q+1)^2(q^6 s_{1\ldots1} + s_{1\ldots1}q^5 - q^5 s_{211} + 2s_{1\ldots1}q^4 - q^4 s_{211} + q^4 s_{31} - q^3 s_{211} + q^3 s_{31} + q^3 s_{22} + 2q^3 s_{1\ldots1} + 2q^2 s_{1\ldots1} - q^2 s_{211} + q^2 s_{31} + q s_{1\ldots1} - q s_{211} + s_{1\ldots1})$
$s_{3222}(X) : q^5(q+1)(q^4 s_{111} - q^3 s_3 + q^3 s_{111} - q^3 s_{21} - q^2 s_3 - 2q^2 s_{21} + q^2 s_{111} - q s_3 + q s_{111} - q s_{21} + s_{111})$
$s_{3322}(X) : q^6(q+1)^2(s_2 q^2 + q s_2 + q s_{11} + s_2)$
$s_{3332}(X) : -s_1 q^6(q+1)(q^2+q+1)^2$
$s_{3333}(X) : q^6(q^2+q+1)(q^2+1)(q+1)^2$

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C.N.R.S., Institut Gaspard Monge
Université de Marne-la-Vallée,
5 Bd Descartes, Champs sur Marne,
77454 Marne La Vallée Cedex 2 FRANCE
Alain.Lascoux@univ-mlv.fr
http://phalanstere.univ-mlv.fr/∼al