The deformed exponential function $$F(x,y) = \sum_{n=0}^{\infty} \frac{x^n}{n!} \, y^{n(n-1)/2}$$ and a plethora of related things

Alan Sokal
New York University / University College London

Marc Kac seminar, Utrecht
10 June 2011

References:

1. Roots of a formal power series $f(x,y) = \sum_{n=0}^{\infty} a_n(y) \, x^n$, with applications to graph enumeration and q-series, Series of 4 lectures at Queen Mary (London), `http://www.maths.qmw.ac.uk/~pjc/csgnotes/sokal/`
2. The leading root of the partial theta function, arXiv:1106.1003 [math.CO].

The entire function $F(x,y) = \sum_{n=0}^{\infty} \frac{x^n}{n!}\, y^{n(n-1)/2}$

- Defined for complex x and y satisfying $|y| \le 1$
- Analytic in $\mathbb{C} \times \mathbb{D}$, continuous in $\mathbb{C} \times \overline{\mathbb{D}}$
- $F(\,\cdot\,, y)$ is entire for each $y \in \overline{\mathbb{D}}$
- Valiron (1938): "from a certain viewpoint the simplest entire function after the exponential function"

Applications:

- Statistical mechanics: Partition function of one-site lattice gas
- Combinatorics: Generating function for Tutte polynomials on K_n (also acyclic digraphs, inversions of trees, ...)
- Functional-differential equation: $F'(x) = F(yx)$ where $' = \partial/\partial x$
- Complex analysis: Whittaker and Goncharov constants

Application to Tutte polynomials of complete graphs

- Finite graph $G = (V, E)$
- Multivariate Tutte polynomial $Z_G(q, \mathbf{v}) = \sum_{A \subseteq E} q^{k(A)} \prod_{e \in A} v_e$

  where $k(A) = \#$ connected components in (V, A)
- Connected-spanning-subgraph polynomial $C_G(\mathbf{v}) = \lim_{q \to 0} q^{-1} Z_G(q, \mathbf{v})$
- Write $Z_G(q, v)$ and $C_G(v)$ if $v_e = v$ for all edges e

  [standard Tutte polynomial is $Z_G(q, v)$ in different variables]

Specialization to complete graphs K_n:

$$Z_n(q, v) = \sum_{m,k} a_{n,m,k} v^m q^k$$

$$C_n(v) = \sum_m c_{n,m} v^m$$

Exponential generating functions:

$$\sum_{n=0}^{\infty} \frac{x^n}{n!} Z_n(q, v) = F(x, 1+v)^q$$

$$\sum_{n=1}^{\infty} \frac{x^n}{n!} C_n(v) = \log F(x, 1+v)$$

[see Tutte (1967) and Scott–A.D.S., arXiv:0803.1477]

- Usually considered as formal power series
- But series are *convergent* if $|1+v| \le 1$

  [see also Flajolet–Salvy–Schaeffer (2004)]

Elementary analytic properties of $F(x,y) = \sum_{n=0}^{\infty} \frac{x^n}{n!} \, y^{n(n-1)/2}$

- $\boldsymbol{y = 0}$: $F(x,0) = 1 + x$

- $\boldsymbol{0 < |y| < 1}$: $F(\,\cdot\,, y)$ is a nonpolynomial entire function of order 0:
$$F(x,y) \;=\; \prod_{k=0}^{\infty} \left(1 \,-\, \frac{x}{x_k(y)}\right)$$
where $\sum |x_k(y)|^{-\alpha} < \infty$ for every $\alpha > 0$

- $\boldsymbol{y = 1}$: $F(x,1) = e^x$

- $\boldsymbol{|y| = 1}$ **with** $\boldsymbol{y \neq 1}$: $F(\,\cdot\,, y)$ is an entire function of order 1 and type 1:
$$F(x,y) \;=\; e^x \prod_{k=0}^{\infty} \left(1 \,-\, \frac{x}{x_k(y)}\right) e^{x/x_k(y)} \;.$$
where $\sum |x_k(y)|^{-\alpha} < \infty$ for every $\alpha > 1$

  [see also Ålander (1914) for y a root of unity; Valiron (1938) and Eremenko–Ostrovskii (2007) for y not a root of unity]

- $\boldsymbol{|y| > 1}$: The series $F(\,\cdot\,, y)$ has radius of convergence 0

Consequences for $C_n(v)$

- Make change of variables $y = 1 + v$:

$$\overline{C}_n(y) \;=\; C_n(y-1)$$

- Then for $|y| < 1$ we have

$$\sum_{n=1}^{\infty} \frac{x^n}{n!} \overline{C}_n(y) \;=\; \log F(x,y) \;=\; \sum_k \log\Bigl(1 - \frac{x}{x_k(y)}\Bigr)$$

and hence

$$\overline{C}_n(y) \;=\; -(n-1)! \sum_k x_k(y)^{-n} \qquad \text{for all } n \ge 1$$

(also holds for $n \ge 2$ when $|y| = 1$)

- This is a *convergent* expansion for $\overline{C}_n(y)$
- In particular, gives large-n asymptotic behavior

$$\overline{C}_n(y) \;=\; -(n-1)!\; x_0(y)^{-n} \bigl[1 + O(e^{-\epsilon n})\bigr]$$

whenever $F(\,\cdot\,, y)$ has a unique root $x_0(y)$ of minimum modulus

Question: What can we say about the roots $x_k(y)$?

Small-y expansion of roots $x_k(y)$

- For small $|y|$, we have $F(x, y) = 1 + x + O(y)$, so we expect a convergent expansion

$$x_0(y) \;=\; -1 \;-\; \sum_{n=1}^{\infty} a_n y^n$$

(easy proof using Rouché: valid for $|y| \lesssim 0.441755$)

- More generally, for each integer $k \geq 0$, write $x = \xi y^{-k}$ and study

$$F_k(\xi, y) \;=\; y^{k(k+1)/2} F(\xi y^{-k}, y) \;=\; \sum_{n=0}^{\infty} \frac{\xi^n}{n!}\, y^{(n-k)(n-k-1)/2}$$

Sum is dominated by terms $n = k$ and $n = k + 1$; gives root

$$x_k(y) \;=\; -(k+1) y^{-k} \left[1 + \sum_{n=1}^{\infty} a_n^{(k)} y^n \right]$$

Rouché argument valid for $|y| \lesssim 0.207875$ uniformly in k:
all roots are simple and given by convergent expansion $x_k(y)$

- Can also use theta function in Rouché (Eremenko)

Might these series converge for all $|y| < 1$?

Two ways that $x_k(y)$ could fail to be analytic for $|y| < 1$:

1. Collision of roots ($\to$ branch point)
2. Root escaping to infinity

Theorem (Eremenko): No root can escape to infinity for y in the open unit disc $\mathbb{D}$.

In fact, for any compact subset $K \subset \mathbb{D}$ and any $\epsilon > 0$, there exists an integer k_0 such that for all $y \in K \setminus \{0\}$ we have:

(a) The function $F(\,\cdot\,, y)$ has exactly k_0 zeros (counting multiplicity) in the disc $|x| < k_0 |y|^{-(k_0 - \frac{1}{2})}$, and

(b) In the region $|x| \geq k_0 |y|^{-(k_0 - \frac{1}{2})}$, the function $F(\,\cdot\,, y)$ has a simple zero within a factor $1 + \epsilon$ of $-(k+1)y^{-k}$ for each $k \geq k_0$, and no other zeros.

- Proof is based on comparison with a theta function (whose roots are known by virtue of Jacobi's product formula)
- *Conjecture* that roots cannot escape to infinity even in the *closed* unit disc except at $y = 1$

Big Conjecture #1. All roots of $F(\,\cdot\,, y)$ are simple for $|y| < 1$. [and also for $|y| = 1$, I suspect]

Consequence of Big Conjecture #1. Each root $x_k(y)$ is analytic in $|y| < 1$.

But I conjecture more ...

Big Conjecture #2. The roots of $F(\,\cdot\,, y)$ are non-crossing *in modulus* for $|y| < 1$:

$$|x_0(y)| \;<\; |x_1(y)| \;<\; |x_2(y)| \;<\; \ldots$$

[and also for $|y| = 1$, I suspect]

Consequence of Big Conjecture #2. The roots are actually separated in modulus by a factor at least $|y|$, i.e.

$$|x_k(y)| \;<\; |y|\,|x_{k+1}(y)| \qquad \text{for all } k \geq 0$$

PROOF. Apply the Schwarz lemma to $x_k(y)/x_{k+1}(y)$.

Consequence for the zeros of $\overline{C}_n(y)$

Recall

$$\overline{C}_n(y) \;=\; -(n-1)! \sum_k x_k(y)^{-n}$$

and use a variant of the Beraha–Kahane–Weiss theorem [A.D.S., arXiv:cond-mat/0012369, Theorem 3.2] $\Longrightarrow$ the limit points of zeros of $\overline{C}_n$ are the values y for which the zero of minimum modulus of $F(\,\cdot\,, y)$ is *nonunique*.

So if $F(\,\cdot\,, y)$ has a *unique* zero of minimum modulus for all $y \in \mathbb{D}$ (a weakened form of Big Conjecture #2), then the zeros of $\overline{C}_n$ do not accumulate anywhere in the open unit disc.

I actually conjecture more (based on computations up to $n \approx 80$):

Big Conjecture #3. For each n, $\overline{C}_n(y)$ has no zeros with $|y| < 1$. [and, I suspect, no zeros with $|y| = 1$ except the point $y = 1$]

What is the evidence for these conjectures?

Evidence #1: Behavior at real y.

Theorem (Laguerre): For $0 \le y < 1$, all the roots of $F(\,\cdot\,, y)$ are simple and negative real.

Corollary: Each root $x_k(y)$ is analytic in a complex neighborhood of the interval $[0, 1)$.

[Real-variables methods give further information about the roots $x_k(y)$ for $0 \le y < 1$: see Langley (2000).]

Now combine this with

Evidence #2: From numerical computation of the series $x_k(y)$ ...

Three methods for computing the series $x_k(y)$

1. Insert $x_k(y) = -(k+1)y^{-k}\left[1+\sum_{n=1}^{\infty} a_n^{(k)} y^n\right]$ and solve term-by-term

2. Use "explicit implicit function theorem" (generalization of Lagrange inversion formula) given in arXiv:0902.0069:

   solve $z = G(z,w)$ with $G(0,0) = 0$ and $\left|\frac{\partial G}{\partial z}(0,0)\right| < 1$ by

$$z \;=\; \varphi(w) \;=\; \sum_{m=1}^{\infty} \frac{1}{m}\,[\zeta^{m-1}] G(\zeta,w)^m$$

   and more generally

$$H(\varphi(w),w) \;=\; H(0,w) \,+\, \sum_{m=1}^{\infty} \frac{1}{m}\,[\zeta^{m-1}] \frac{\partial H(\zeta,w)}{\partial \zeta}\, G(\zeta,w)^m$$

Methods 1 and 2 work *symbolically* in k.

3. Use

$$\overline{C}_n(y) \;=\; -(n-1)! \sum_k x_k(y)^{-n}$$

   together with recursion

$$\overline{C}_n(y) \;=\; y^{n(n-1)/2} \;-\; \sum_{j=1}^{n-1} \binom{n-1}{j-1} \overline{C}_j(y)\, y^{(n-j)(n-j-1)/2}$$

   [cf. Leroux (1988) and Scott–A.D.S., arXiv:0803.1477]
   — can go to very high n, at least for small k

And let MATHEMATICA run for a weekend ...

$$
\begin{aligned}
-x_0(y) \;=\; & 1 + \tfrac{1}{2}y + \tfrac{1}{2}y^2 + \tfrac{11}{24}y^3 + \tfrac{11}{24}y^4 + \tfrac{7}{16}y^5 + \tfrac{7}{16}y^6 \\
& + \tfrac{493}{1152}y^7 + \tfrac{163}{384}y^8 + \tfrac{323}{768}y^9 + \tfrac{1603}{3840}y^{10} + \tfrac{57283}{138240}y^{11} \\
& + \tfrac{170921}{414720}y^{12} + \tfrac{340171}{829440}y^{13} + \tfrac{22565}{55296}y^{14} \\
& + \ldots + \text{terms through order } y^{899}
\end{aligned}
$$

and all the coefficients (so far) are nonnegative!

Big Conjecture #4. For each k, the series $-x_k(y)$ has all nonnegative coefficients.

Combine this with the known analyticity for $0 \le y < 1$, and Vivanti–Pringsheim gives:

Consequence of Big Conjecture #4. Each root $x_k(y)$ is analytic in the open unit disc.

NEED TO DO: Extended computations for $k = 1, 2, \ldots$ and for symbolic k.

But more is true ...

Look at the *reciprocal* of $x_0(y)$:

$$
\begin{aligned}
-\frac{1}{x_0(y)} \;=\; 1 &- \tfrac{1}{2}y - \tfrac{1}{4}y^2 - \tfrac{1}{12}y^3 - \tfrac{1}{16}y^4 - \tfrac{1}{48}y^5 - \tfrac{7}{288}y^6 \\
&- \tfrac{1}{96}y^7 - \tfrac{7}{768}y^8 - \tfrac{49}{6912}y^9 - \tfrac{113}{23040}y^{10} - \tfrac{17}{4608}y^{11} \\
&- \tfrac{293}{92160}y^{12} - \tfrac{737}{276480}y^{13} - \tfrac{3107}{1658880}y^{14} \\
&- \ldots - \text{terms through order } y^{899}
\end{aligned}
$$

and all the coefficients (so far) beyond the constant term are *nonpositive*!

Big Conjecture #5. For each k, the series $-(k+1)y^{-k}/x_k(y)$ has all *nonpositive* coefficients after the constant term 1.

[This implies the preceding conjecture, but is stronger.]

- Relative simplicity of the coefficients of $-1/x_0(y)$ compared to those of $-x_0(y)$ $\longrightarrow$ simpler combinatorial interpretation?
- Note that $x_k(y) \to -\infty$ as $y \uparrow 1$ (this is fairly easy to prove). So $1/x_k(y) \to 0$. Therefore:

Consequence of Big Conjecture #5. For each k, the coefficients (after the constant term) in the series $-(k+1)y^{-k}/x_k(y)$ are the *probabilities* for a positive-integer-valued random variable.

What might such a random variable be???
Could this approach be used to *prove* Big Conjecture #5?

AGAIN NEED TO DO: Extended computations for $k = 1, 2, \ldots$ and for symbolic k.

But I conjecture that even more is true . . .

Define $D_n(y) = \dfrac{\overline{C}_n(y)}{(-1)^{n-1}(n-1)!}$ and recall that $-x_0(y) = \lim_{n\to\infty} D_n(y)^{-1/n}$

Big Conjecture #6. For each n,

(a) the series $D_n(y)^{-1/n}$ has all nonnegative coefficients,

and even more strongly,

(b) the series $D_n(y)^{1/n}$ has all nonpositive coefficients after the constant term 1.

Since $D_n(y) > 0$ for $0 \le y < 1$, Vivanti–Pringsheim shows that Big Conjecture #6a implies Big Conjecture #3:

For each n, $\overline{C}_n(y)$ has no zeros with $|y| < 1$.

Moreover, Big Conjecture #6b $\Longrightarrow$ for each n, the coefficients (after the constant term) in the series $D_n(y)^{1/n}$ are the *probabilities* for a positive-integer-valued random variable.

Such a random variable would generalize the one for $-1/x_0(y)$ in roughly the same way that the binomial generalizes the Poisson.

Roots $x_k(y)$ computed *symbolically* in k

$$x_k(y) \;=\; -(k+1)y^{-k}\left[1+\sum_{n=1}^{\infty}\frac{P_n(k)}{Q_n(k)}\,y^n\right]$$

where I have computed up to $n = 21$:

$$\begin{aligned}
P_1(k) &= 1 \\
P_2(k) &= 2+6k+3k^2 \\
P_3(k) &= 11+29k+63k^2+65k^3+28k^4+4k^5 \\
P_4(k) &= 22+146k+273k^2+359k^3+355k^4+211k^5+63k^6+7k^7 \\
&\vdots \\
Q_n(k) &= (k+1)^n \prod_{j=2}^{\infty}(k+j)^{\lfloor n/\binom{j}{2}\rfloor}
\end{aligned}$$

- $P_n(k)$ has nonnegative coefficients for $n \le 9$ but not for $n = 10, 15, 16, 18, 19, 20, 21$
- $P_n(k) \ge 0$ for all *real* $k \ge 0$ for $n \le 14$ but not for $n = 15, 18, 19, 21$
- But … $P_n(k) \ge 0$ for all *integer* $k \ge 0$ at least for $n \le 21$

which gives evidence that Big Conjecture #4 holds for all k:

For each k, the series $-x_k(y)$ has all nonnegative coefficients.

Reciprocals of roots $x_k(y)$ computed *symbolically* in k

$$\frac{-(k+1)y^{-k}}{x_k(y)} = \left[1 - \sum_{n=1}^{\infty} \frac{\widehat{P}_n(k)}{Q_n(k)}\, y^n\right]$$

where I have computed up to $n = 21$:

$$\begin{aligned}
\widehat{P}_1(k) &= 1 \\
\widehat{P}_2(k) &= 1 + 6k + 3k^2 \\
\widehat{P}_3(k) &= 2 - 10k + 33k^2 + 59k^3 + 28k^4 + 4k^5 \\
\widehat{P}_4(k) &= 3 + 71k + 24k^2 + 82k^3 + 236k^4 + 194k^5 + 63k^6 + 7k^7 \\
&\;\;\vdots
\end{aligned}$$

and $Q_n(k)$ are the same as before

- $\widehat{P}_n(k)$ does not have nonnegative coefficients (except for $n = 1, 2, 4$)
- $\widehat{P}_n(k) \geq 0$ for all *real* $k \geq 0$ for $n = 1, 2, 3, 4, 5, 7, 8$ but not in general
- But … $\widehat{P}_n(k) \geq 0$ for all *integer* $k \geq 0$ at least for $n \leq 21$

which gives evidence that Big Conjecture #5 holds for all k:

> For each k, the series $-(k+1)y^{-k}/x_k(y)$ has all *nonpositive* coefficients after the constant term 1.

Ratios of roots $x_k(y)/x_{k+1}(y)$

The series

$$\frac{x_0(y)}{x_1(y)} = \tfrac{1}{2}y + \tfrac{1}{6}y^2 + \tfrac{5}{72}y^3 + \tfrac{11}{216}y^4 + \tfrac{29}{1296}y^5 + \ldots$$

has nonnegative coefficients at least up to order y^{136}.
(But its reciprocal does not have any fixed signs.)

Big Conjecture #7. The series $x_0(y)/x_1(y)$ has all nonnegative coefficients.

Consequence of Big Conjecture #7. Since $\lim_{y\uparrow 1} x_0(y)/x_1(y) = 1$, Big Conjecture #7 implies that $|x_0(y)| < |x_1(y)|$ for all $y \in \mathbb{D}$ (a special case of Big Conjecture #2 on the separation in modulus of roots).

- But unfortunately … the series

  $$\frac{x_1(y)}{x_2(y)} = \tfrac{2}{3}y + \tfrac{1}{18}y^2 + \tfrac{17}{216}y^3 + \tfrac{23}{810}y^4 + \tfrac{343}{17280}y^5 + \ldots$$

  has a negative coefficient at order y^{13}. This doesn't contradict the conjecture that $|x_1(y)/x_2(y)| < 1$ in the unit disc, but it does rule out the simplest method of proof.

- Symbolic computation of $x_k(y)/x_{k+1}(y)$ shows that, up to order y^{22}, the *only* cases of a negative coefficient for *integer* $k \geq 0$ are the coefficient of y^{13} for $k = 1, 2, 3$; y^{17} for $k = 2$; and y^{19}, y^{21} for $k = 2, 3, 4$.

- The series $y^{-k}x_0(y)/x_k(y)$ has nonnegative coefficients for all integer $k \geq 0$ through at least order y^{21}.

Asymptotics of roots as $y \to 1$

Write $y = e^{-\gamma}$ with $\operatorname{Re}\gamma > 0$.
Want to study $\gamma \to 0$ (non-tangentially in the right half-plane).

I *believe* I will be able to prove that

$$-x_k(e^{-\gamma}) \;\approx\; \frac{1}{e}\gamma^{-1} \;+\; c_k\gamma^{-1/3} \;+\; \ldots$$

for suitable constants $c_0 < c_1 < c_2 < \ldots$. But I have not yet worked out all the details.

Overview of method:

1. Develop an asymptotic expansion for $F(x, e^{-\gamma})$ when $\gamma \to 0$ and x is taken to be of order γ^{-1}, because this is the regime where the zeros will be found.
2. Use this expansion for $F(x, e^{-\gamma})$ to deduce an expansion for $x_k(e^{-\gamma})$.

Sketch of step #1: Insert Gaussian integral representation for $e^{-\frac{\gamma}{2}n^2}$ to obtain

$$F(x, e^{-\gamma}) \;=\; (2\pi\gamma)^{-1/2} \int_{-\infty}^{\infty} \exp[g(t)]\, dt$$

with

$$g(t) \;=\; -\frac{t^2}{2\gamma} \;+\; xe^{\gamma/2}e^{it}$$

Saddle-point equation $g'(t) = 0$ is $-ite^{-it} = \gamma e^{\gamma/2} x$, so it makes sense to make the change of variables

$$x \;=\; \gamma^{-1} e^{-\gamma/2} w e^w \;,$$

which puts the saddle point at $t_0 = iw$. (Note that this brings in the Lambert W function, i.e. the inverse function to $w \mapsto we^w$.) We then have

$$F(\gamma^{-1} e^{-\gamma/2} w e^w, e^{-\gamma}) \;=\; (2\pi\gamma)^{-1/2} \int\limits_{-\infty}^{\infty} dt \; \exp\!\left[-\frac{t^2}{2\gamma} \,+\, \frac{we^w}{\gamma} e^{it} \right]$$

Now shift the contour to go through the saddle point (parallel to the real axis) and make the change of variables $t = s + iw$: we have

$$F(\gamma^{-1} e^{-\gamma/2} w e^w, e^{-\gamma}) \;=\; (2\pi\gamma)^{-1/2} \exp\!\left[\frac{w^2}{2\gamma} + \frac{w}{\gamma} \right] \int\limits_{-\infty}^{\infty} ds \; \exp[h(s)]$$

where

$$h(s) \;=\; -\frac{(1+w)}{2\gamma} s^2 \;+\; \frac{w}{\gamma} \Big(e^{is} - 1 - is + \frac{s^2}{2} \Big)$$

and the integration goes along the real s axis.

These formulae should allow computation of asymptotics

(a) $\gamma \to 0$ (in a suitable way) for (suitable values of) fixed w; and

(b) $w \to \infty$ (in a suitable direction) for (suitable values of) fixed γ.

Focus for now on (a).

Recall that

$$h(s) \;=\; -\frac{(1+w)}{2\gamma}s^2 \;+\; \frac{w}{\gamma}\Big(e^{is} - 1 - is + \frac{s^2}{2}\Big)$$

Consider for simplicity γ and x real. There seem to be three regimes:

- **"High temperature":** $w > -1$ (i.e. $we^w > -1/e$).

  Easiest case: $s = 0$ saddle point is Gaussian, and can compute the asymptotics to all orders in terms of 3-associated Stirling subset numbers $\left\{ {n \atop m} \right\}_{\geq 3}$. [Still need to justify this formal calculation by showing that only the $s = 0$ saddle point contributes.]

- **"Low temperature":** $w = -\eta \cot \eta + \eta i$ with $-\pi < \eta < \pi$ (i.e. $we^w < -1/e$).

  Saddle points at $s = 0$ and $s = 2\eta$ contribute; I *think* this is all.

- **"Critical regime":** $w = -(1 + \xi\gamma^{1/3})$ with ξ fixed, which corresponds to

  $$x \;=\; -\frac{1}{e\gamma}\left[1 \;-\; \frac{\xi^2}{2}\gamma^{2/3} \;+\; O(\gamma)\right]$$

  – *At* the "critical point" $\xi = 0$: Dominant behavior at $s = 0$ saddle point is no longer Gaussian (it vanishes) but rather the cubic term $is^3/(6\gamma)$. Can compute the asymptotics to all orders in terms of 4-associated Stirling subset numbers $\left\{ {n \atop m} \right\}_{\geq 4}$ (at least formally).

  – In the critical regime (ξ arbitrary): Expect to have Airy asymptotics as in Flajolet–Salvy–Schaeffer (2004). This is where the roots will lie.

I would appreciate help with the details!!!

The polynomials $P_N(x,w) = \sum_{n=0}^{N} \binom{N}{n} x^n w^{n(N-n)}$

- Partition function of Ising model on complete graph K_N, with $x = e^{2h}$ and $w = e^{-2J}$
- Related to binomial $(1+x)^N$ in same way as our $F(x,y)$ is related to exponential e^x [but we have written $w^{n(N-n)}$ instead of $y^{n(n-1)/2}$]
- $\lim_{N\to\infty} P_N\left(\frac{xw^{1-N}}{N}, w\right) \;=\; F(x, w^{-2}) \quad \text{when } |w| > 1$
- So results about zeros of P_N generalize those about F (just as results about the binomial generalize those about the exponential function)
- Lee–Yang theorem: In ferromagnetic case ($0 \le w \le 1$), all zeros are on the unit circle $|x| = 1$
- Laguerre: In antiferromagnetic case ($w \ge 1$), all zeros are real and negative
- What about "complex antiferromagnetic" case $|w| > 1$??

Big Conjecture #8. For $|w| > 1$, all zeros of $P_N(\,\cdot\,, w)$ are separated in modulus (by at least a factor $|w|^2$).

Taking $N \to \infty$, this implies Big Conjecture #2 about the separation in modulus of the zeros of $F(\,\cdot\,, y)$.

Differential-equation approach to $P_N(x,w) = \sum_{n=0}^{N} \binom{N}{n} x^n w^{n(N-n)}$

On the space of polynomials $Q_N(x) = \sum_{n=0}^{N} a_n x^n$ of degree N with $a_0 \neq 0$, define the semigroup

$$(\mathcal{A}_t Q_N)(x) \;\equiv\; \sum_{n=0}^{N} a_n x^n e^{tn(N-n)}$$

Roots of $\mathcal{A}_t Q_N$ evolve according to an *autonomous* differential equation, which is best expressed in terms of *logarithms* of roots $\zeta_i = \log x_i$:

$$\frac{d\zeta_i}{dt} \;=\; \sum_{j \neq i} f(\zeta_i - \zeta_j)$$

where

$$f(z) \;=\; \coth(z/2)$$

These are first-order ("Aristotelian") equations of motion for a system of n "particles" (in $\mathbb{R}$ or $\mathbb{C}$) with a translation-invariant "force" f.

Moreover, the specific force $f = \coth$ is a Calogero–Moser–Sutherland system, much studied in the theory of integrable systems.

For polynomials Q_N with *real* roots and *real* $t > 0$, this approach gives interesting results on separation of zeros. (In particular, it gives a new proof of Laguerre's theorem.)

Is this approach useful for *complex* t with $\operatorname{Re} t > 0$???
Can it be used to prove Big Conjecture #8?

A more general approach to the leading root $x_0(y)$

- Consider a formal power series

$$f(x,y) \;=\; \sum_{n=0}^{\infty} \alpha_n\, x^n\, y^{n(n-1)/2}$$

normalized to $\alpha_0 = \alpha_1 = 1$, or more generally

$$f(x,y) \;=\; \sum_{n=0}^{\infty} a_n(y)\, x^n$$

where

(a) $a_0(0) = a_1(0) = 1$;
(b) $a_n(0) = 0$ for $n \geq 2$; and
(c) $a_n(y) = O(y^{\nu_n})$ with $\lim\limits_{n\to\infty} \nu_n = \infty$.

It makes sense to study the "leading root" $x_0(y)$ in this generality.

- Example: The "partial theta function"

$$\Theta_0(x,y) \;=\; \sum_{n=0}^{\infty} x^n\, y^{n(n-1)/2}$$

beloved of q-series practitioners (going back at least to Ramanujan).

- More generally, consider

$$\widetilde{R}(x,y,q) \;=\; \sum_{n=0}^{\infty} \frac{x^n\, y^{n(n-1)/2}}{(1+q)(1+q+q^2)\,\cdots\,(1+q+\ldots+q^{n-1})}$$

which reduces to Θ_0 when $q=0$, and to F when $q=1$.

A more general approach, continued ...

- A power series for the leading root $x_0(y)$ can be computed from the power-series expansion of $\log f(x,y)$, generalizing Method 3 above for $F(x,y)$. This is extremely efficient!
- Example: For Θ_0 we have

$$-x_0(y) \;=\; 1+y+2y^2+4y^3+9y^4+21y^5+52y^6+133y^7+351y^8+\ldots$$

  with strictly positive coefficients at least through order y^{6999}.

- More generally, for $\widetilde{R}(x,y,q)$ it can be proven that

$$-x_0(y,q) \;=\; 1 \,+\, \sum_{n=1}^{\infty} \frac{P_n(q)}{Q_n(q)}\, y^n$$

  where

$$Q_n(q) \;=\; \prod_{k=2}^{\infty} (1+q+\ldots+q^{k-1})^{\lfloor n/\binom{k}{2} \rfloor}$$

  and $P_n(q)$ is a self-inversive polynomial with integer coefficients.

  I have verified for $n \le 349$ that $P_n(q)$ has *two* interesting positivity properties:

  (a) $P_n(q)$ has all nonnegative coefficients. Indeed, all the coefficients are strictly positive except $[q^1]\, P_5(q) = 0$.

  (b) $P_n(q) > 0$ for $q > -1$.

Can any of this be proven???

Yes, *some* of it ...

The leading root $x_0(y)$, general theory

- Start from a formal power series

$$f(x,y) \;=\; \sum_{n=0}^{\infty} a_n(y)\, x^n$$

  where

  (a) $a_0(0) = a_1(0) = 1$
  (b) $a_n(0) = 0$ for $n \geq 2$
  (c) $a_n(y) = O(y^{\nu_n})$ with $\lim\limits_{n\to\infty} \nu_n = \infty$

  and coefficients lie in a commutative ring-with-identity-element R.

- By (c), each power of y is multiplied by only *finitely many* powers of x.

- That is, f is a formal power series in y whose coefficients are *polynomials* in x, i.e. $f \in R[x][[y]]$.

- Hence, for *any* formal power series $X(y)$ with coefficients in R [not necessarily with zero constant term], the composition $f(X(y), y)$ makes sense as a formal power series in y.

- Not hard to see (by the implicit function theorem for formal power series or by a direct inductive argument) that there exists a unique formal power series $x_0(y) \in R[[y]]$ satisfying $f(x_0(y), y) = 0$.

- We call $x_0(y)$ the **leading root** of f.

- Since $x_0(y)$ has constant term -1, we will write $x_0(y) = -\xi_0(y)$ where $\xi_0(y) = 1 + O(y)$.

How to compute $\xi_0(y)$?

1. **Elementary method:** Insert $\xi_0(y) = 1 + \sum_{n=1}^{\infty} b_n y^n$ into $f(-\xi_0(y), y) = 0$ and solve term-by-term.

2. Method based on the explicit implicit function formula.

3. Method based on the exponential formula and expansion of $\log f(x, y)$.

- Methods #2 and #3 are computationally very efficient.
- Can they also be used to give *proofs*?

Tools I: The explicit implicit function formula

- See A.D.S., arXiv:0902.0069 or Stanley, vol. 2, Exercise 5.59
- (Almost trivial) generalization of Lagrange inversion formula
- Comes in analytic-function and formal-power-series versions
- Recall Lagrange inversion: If $f(x) = \sum_{n=1}^{\infty} a_n x^n$ with $a_1 \neq 0$ (as either analytic function or formal power series), then

$$f^{-1}(y) \;=\; \sum_{m=1}^{\infty} \frac{y^m}{m} \, [\zeta^{m-1}] \left(\frac{\zeta}{f(\zeta)} \right)^m$$

  where $[\zeta^n] g(\zeta)$ denotes the coefficient of ζ^n in the power series $g(\zeta)$. More generally, if $h(x) = \sum_{n=0}^{\infty} b_n x^n$, we have

$$h(f^{-1}(y)) \;=\; h(0) \,+\, \sum_{m=1}^{\infty} \frac{y^m}{m} \, [\zeta^{m-1}] \, h'(\zeta) \left(\frac{\zeta}{f(\zeta)} \right)^m$$

- Rewrite this in terms of $g(x) = x/f(x)$: then $f(x) = y$ becomes $x = g(x)y$, and its solution $x = \varphi(y) = f^{-1}(y)$ is given by the power series

$$\varphi(y) \;=\; \sum_{m=1}^{\infty} \frac{y^m}{m} \, [\zeta^{m-1}] g(\zeta)^m$$

  and

$$h(\varphi(y)) \;=\; h(0) \,+\, \sum_{m=1}^{\infty} \frac{y^m}{m} \, [\zeta^{m-1}] h'(\zeta) g(\zeta)^m$$

- There is also an alternate form

$$h(\varphi(y)) \;=\; h(0) \,+\, \sum_{m=1}^{\infty} y^m \, [\zeta^m] h(\zeta) \left[g(\zeta)^m \,-\, \zeta g'(\zeta) g(\zeta)^{m-1} \right]$$

The explicit implicit function formula, continued

- Generalize $x = g(x)y$ to $x = G(x, y)$, where
  - $G(0,0) = 0$ and $|(\partial G/\partial x)(0,0)| < 1$ (analytic-function version)
  - $G(0,0) = 0$ and $(\partial G/\partial x)(0,0) = 0$ (formal-power-series version)
- Then there is a unique $\varphi(y)$ with zero constant term satisfying $\varphi(y) = G(\varphi(y), y)$, and it is given by

$$\begin{aligned}\varphi(y) &= \sum_{m=1}^{\infty} \frac{1}{m} [\zeta^{m-1}] G(\zeta, y)^m \\ &= \sum_{m=1}^{\infty} [\zeta^{m-1}] \Big[G(\zeta, y)^m - \zeta \frac{\partial G(\zeta, y)}{\partial \zeta} G(\zeta, y)^{m-1} \Big]\end{aligned}$$

  More generally, for any $H(x, y)$ we have

$$\begin{aligned}H(\varphi(y), y) &= H(0, y) + \sum_{m=1}^{\infty} \frac{1}{m} [\zeta^{m-1}] \frac{\partial H(\zeta, y)}{\partial \zeta} G(\zeta, y)^m \\ &= H(0, y) + \sum_{m=1}^{\infty} [\zeta^{m}] H(\zeta, y) \Big[G(\zeta, y)^m - \zeta \frac{\partial G(\zeta, y)}{\partial \zeta} G(\zeta, y)^{m-1} \Big]\end{aligned}$$

- First versions are slightly more convenient but require R to contain the rationals as a subring.
- Proof imitates standard proof of the Lagrange inversion formula: the variables y simply "go for the ride".
- Alternate interpretation: Solving fixed-point problem for the family of maps $x \mapsto G(x, y)$ parametrized by y. Variables y again "go for the ride".

Application to leading root of $f(x,y)$

- Start from a formal power series $f(x,y) = \sum_{n=0}^{\infty} a_n(y)\, x^n$ satisfying properties (a)–(c) above.
- Write out $f(-\xi_0(y), y) = 0$ and add $\xi_0(y)$ to both sides:

$$\xi_0(y) \;=\; a_0(y) \;-\; [a_1(y) - 1]\xi_0(y) \;+\; \sum_{n=2}^{\infty} a_n(y)\, (-\xi_0(y))^n$$

- Insert $\xi_0(y) = 1 + \varphi(y)$ where $\varphi(y)$ has zero constant term. Then $\varphi(y) = G(\varphi(y), y)$ where

$$G(z,y) \;=\; \sum_{n=0}^{\infty} (-1)^n\, \widehat{a}_n(y)\, (1+z)^n$$

and

$$\widehat{a}_n(y) \;=\; \begin{cases} a_n(y) - 1 & \text{for } n = 0,1 \\ a_n(y) & \text{for } n \ge 2 \end{cases}$$

And $\varphi(y)$ is the *unique* formal power series with zero constant term satisfying this fixed-point equation.

- Since this G satisfies $G(0,0) = 0$ and $(\partial G/\partial z)(0,0) = 0$ [indeed it satisfies the stronger condition $G(z,0) = 0$], we can apply the explicit implicit function formula to obtain an explicit formula for $\xi_0(y)$:

$$\xi_0(y) \;=\; 1 \;+\; \sum_{m=1}^{\infty} \frac{1}{m}\, [\zeta^{m-1}] \left(\sum_{n=0}^{\infty} (-1)^n\, \widehat{a}_n(y)\, (1+\zeta)^n \right)^{m}$$

More generally, for any formal power series $H(z,y)$, we have

$$\begin{aligned} & H(\xi_0(y) - 1, y) \\ &=\; H(0,y) \;+\; \sum_{m=1}^{\infty} \frac{1}{m}\, [\zeta^{m-1}] \frac{\partial H(\zeta,y)}{\partial \zeta} \left(\sum_{n=0}^{\infty} (-1)^n\, \widehat{a}_n(y)\, (1+\zeta)^n \right)^{m} \end{aligned}$$

Application to leading root of $f(x, y)$, continued

- In particular, by taking $H(z, y) = (1 + z)^\beta$ we can obtain an explicit formula for an arbitrary power of $\xi_0(y)$:

$$\xi_0(y)^\beta = 1 + \sum_{m=1}^{\infty} \frac{\beta}{m} \sum_{n_1,\ldots,n_m \ge 0} \binom{\beta - 1 + \sum n_i}{m-1} \prod_{i=1}^{m} (-1)^{n_i} \widehat{a}_{n_i}(y)$$

- Important special case: $a_0(y) = a_1(y) = 1$ and $a_n(y) = \alpha_n \, y^{\lambda_n}$ $(n \ge 2)$ where $\lambda_n \ge 1$ and $\lim_{n\to\infty} \lambda_n = \infty$. Then

$$[y^N] \frac{\xi_0(y)^\beta - 1}{\beta} = \sum_{m=1}^{\infty} \frac{1}{m} \sum_{\substack{n_1, \ldots, n_m \ge 2 \\ \sum_{i=1}^{m} \lambda_{n_i} = N}} (-1)^{\sum n_i} \binom{\beta - 1 + \sum n_i}{m-1} \prod_{i=1}^{m} \alpha_{n_i}$$

- Can this formula be used for proofs of nonnegativity???
- *Empirically* I know that the RHS is ≥ 0 when $\lambda_n = n(n-1)/2$:
  - For $\beta \ge -2$ with $\alpha_n = 1$ (partial theta function)
  - For $\beta \ge -1$ with $\alpha_n = 1/n!$ (deformed exponential function)
  - For $\beta \ge -1$ with $\alpha_n = (1-q)^n/(q;q)_n$ and $q > -1$
- And I can *prove* this (by a *different* method!) for the partial theta function.
- **How can we see these facts from this formula???**
  [open combinatorial problem]

Tools II: Variants of the exponential formula

- Let R be a commutative ring containing the rationals.
- Let $A(x) = \sum_{n=0}^{\infty} a_n \, x^n$ be a formal power series (with coefficients in R) satisfying $a_0 = 1$.
- Now consider $C(x) = \log A(x) = \sum_{n=1}^{\infty} c_n \, x^n$.
- It is well known (and easy to prove) that

$$a_n \;=\; \sum_{k=1}^{n} \frac{k}{n} \, c_k \, a_{n-k} \qquad \text{for } n \ge 1$$

  This allows $\{a_n\}$ to be calculated given $\{c_n\}$, or vice versa.
- Sometimes useful to introduce $\widetilde{C}_n = nc_n$, which are the coefficients in

$$\frac{x \, A'(x)}{A(x)} \;=\; \sum_{n=1}^{\infty} \widetilde{C}_n \, x^n$$

- See Scott–Sokal, arXiv:0803.1477 for generalizations to $A(x)^\lambda$ and applications to the multivariate Tutte polynomial

- Now specialize to $R = R_0[[y]]$ and $A(x,y) = \sum_{n=0}^{\infty} a_n(y) \, x^n$ where $a_0(y) = 1$
- Assume further that $a_1(0) = 1$ and $a_n(0) = 0$ for $n \ge 2$ [conditions (a) and (b) for our $f(x,y)$]
- Then

$$\frac{x \, A'(x,y)}{A(x,y)} \;=\; \sum_{n=1}^{\infty} \widetilde{C}_n(y) \, x^n$$

  where $'$ denotes $\partial/\partial x$ and $\widetilde{C}_n(y)$ has constant term $(-1)^{n-1}$.

Application to leading root of $f(x,y)$

- Start from a formal power series $f(x,y) = 1 + x + \sum_{n=2}^{\infty} a_n(y)\, x^n$ satisfying
$$a_n(y) \;=\; O(y^{\alpha(n-1)}) \qquad \text{for } n \ge 2$$
for some real $\alpha > 0$. [This is a bit stronger than (a)–(c).]

- Define $\{\widetilde{C}_n(y)\}_{n=1}^{\infty}$ by
$$\frac{x\, f'(x,y)}{f(x,y)} \;=\; \sum_{n=1}^{\infty} \widetilde{C}_n(y)\, x^n$$
where $'$ denotes $\partial/\partial x$.

- **Theorem:** We have
$$\widetilde{C}_n(y) \;=\; (-1)^{n-1}\, \xi_0(y)^{-n} \;+\; O(y^{\alpha n})$$
or equivalently
$$\xi_0(y) \;=\; [(-1)^{n-1}\widetilde{C}_n(y)]^{-1/n} \;+\; O(y^{\alpha n})$$

- This theorem provides an extraordinarily efficient method for computing the series $\xi_0(y)$:
  - Compute the $\widetilde{C}_n(y)$ inductively using the recursion
  $$\widetilde{C}_n \;=\; n a_n \;-\; \sum_{k=1}^{n-1} \widetilde{C}_k\, a_{n-k}$$
  - Take the power $-1/n$ to extract $\xi_0(y)$ through order $y^{\lceil \alpha n \rceil - 1}$

- This abstracts the recursive method shown earlier for the special case $F(x,y) \;=\; \displaystyle\sum_{n=0}^{\infty} \frac{x^n}{n!}\, y^{n(n-1)/2}$.

Proof of Theorem (via complex analysis)

- Use complex-analysis argument to prove Theorem when $R = \mathbb{C}$ and f is a polynomial.
- Infer general validity by some abstract nonsense.

Lemma. Fix a real number $\alpha > 0$, and let $P(x, y) = 1 + x + \sum_{n=2}^{N} a_n(y) x^n$ where the $\{a_n(y)\}_{n=2}^{N}$ are polynomials with complex coefficients satisfying $a_n(y) = O(y^{\alpha(n-1)})$. Then there exist numbers $\rho > 0$ and $\gamma > 0$ such that $P(\,\cdot\,, y)$ has precisely one root in the disc $|x| < \gamma |y|^{-\alpha}$ whenever $|y| \le \rho$.

Idea of proof: Apply Rouché's theorem to $f(x) = x$ and $g(x) = 1 + \sum_{n=2}^{N} a_n(y) x^n$ on the circle $|x| = \gamma |y|^{-\alpha}$.

Proof of Theorem when $R = \mathbb{C}$ and f is a polynomial: Write

$$P(x, y) \;=\; \prod_{i=1}^{k(y)} \Bigl(1 - \frac{x}{X_i(y)}\Bigr)$$

with $k(y) \le N$. Therefore

$$\frac{x\, P'(x, y)}{P(x, y)} \;=\; \sum_{i=1}^{k(y)} \frac{-x/X_i(y)}{1 \,-\, x/X_i(y)}$$

and hence

$$\widetilde{C}_n(y) \;=\; -\sum_{i=1}^{k(y)} X_i(y)^{-n} \;.$$

Now, for small enough $|y|$, one of the roots is given by the *convergent* series $-\xi_0(y)$ and is smaller than $\gamma |y|^{-\alpha}$ in magnitude, while the other roots have magnitude $\geq \gamma |y|^{-\alpha}$ by the Lemma. We therefore have

$$\left| \widetilde{C}_n(y) \;-\; (-1)^{n-1} \xi_0(y)^{-n} \right| \;\leq\; (N-1) \gamma^{-n} |y|^{\alpha n}$$

for small enough $|y|$, as claimed. $\square$

Proof of Theorem in general case: Write

$$a_n(y) \;=\; \sum_{m=\lceil \alpha(n-1) \rceil}^{\infty} a_{nm}\, y^m$$

Work in the ring $R = \mathbb{Z}[\boldsymbol{a}]$ where $\boldsymbol{a} = \{a_{nm}\}_{n \geq 2,\, m \geq \lceil \alpha(n-1) \rceil}$ are treated as indeterminates. Then the claim of the Theorem amounts to a series of identities between polynomials in $\boldsymbol{a}$ with integer coefficients. We have verified these identities when evaluated on collections $\boldsymbol{a}$ of complex numbers of which only finitely many are nonzero; and this is enough to prove them as identities in $\mathbb{Z}[\boldsymbol{a}]$. $\square$

There is also a direct formal-power-series proof (due to Ira Gessel) at least in the case $\alpha = 1$. I don't know whether it extends to arbitrary real $\alpha > 0$.

Computational use of Theorem

- Can compute $\xi_0(y)$ through order y^{N-1} by computing $\widetilde{C}_N(y)$
- Do this by computing $\widetilde{C}_n(y)$ for $1 \leq n \leq N$ using recursion
- Observe that all $\widetilde{C}_n(y)$ can be truncated to order y^{N-1}
  [no need to keep the full polynomial of degree $n(n-1)/2$]

- For F, have done $N = 900$
  [$N = 400$ takes a minute, $N = 900$ takes less than 6 hours;
  but $N = 900$ needs 24 GB memory!]

- For Θ_0, have done $N = 7000$
  [$N = 500$ takes a minute, $N = 1500$ takes less than an hour;
  $N = 7000$ took 11 days and 21 GB memory]

- For $\widetilde{R}$, have done $N = 350$
  [$N = 50$ takes a minute, $N = 100$ takes less than an hour;
  $N = 350$ took a month and 10 GB memory]

Some positivity properties of formal power series

- Consider formal power series with real coefficients

$$f(y) \;=\; 1 + \sum_{m=1}^{\infty} a_m \, y^m$$

- For $\alpha \in \mathbb{R}$, define the class $\mathcal{S}_\alpha$ to consist of those f for which

$$\frac{f(y)^\alpha - 1}{\alpha} \;=\; \sum_{m=1}^{\infty} b_m(\alpha) \, y^m$$

  has all nonnegative coefficients (with a suitable limit when $\alpha = 0$).

- In other words:
  - For $\alpha > 0$ (resp. $\alpha = 0$), the class $\mathcal{S}_\alpha$ consists of those f for which f^α (resp. $\log f$) has all nonnegative coefficients.
  - For $\alpha < 0$, the class $\mathcal{S}_\alpha$ consists of those f for which f^α has all *nonpositive* coefficients after the constant term 1.

- Containment relations among the classes $\mathcal{S}_\alpha$ are given by the following fairly easy result:

  Proposition (Scott–A.D.S., unpublished):
  Let $\alpha, \beta \in \mathbb{R}$. Then $\mathcal{S}_\alpha \subseteq \mathcal{S}_\beta$ if and only if either

  (a) $\alpha \le 0$ and $\beta \ge \alpha$, or
  (b) $\alpha > 0$ and $\beta \in \{\alpha, 2\alpha, 3\alpha, \ldots\}$.

  Moreover, the containment is strict whenever $\alpha \neq \beta$.

Application to deformed exponential function F

As mentioned earlier, it seems that $\xi_0(y) \in \mathcal{S}_1$:

$$\begin{aligned}\xi_0(y) \;=\; & 1 + \tfrac{1}{2}y + \tfrac{1}{2}y^2 + \tfrac{11}{24}y^3 + \tfrac{11}{24}y^4 + \tfrac{7}{16}y^5 + \tfrac{7}{16}y^6 \\ & + \tfrac{493}{1152}y^7 + \tfrac{163}{384}y^8 + \tfrac{323}{768}y^9 + \tfrac{1603}{3840}y^{10} + \tfrac{57283}{138240}y^{11} \\ & + \tfrac{170921}{414720}y^{12} + \tfrac{340171}{829440}y^{13} + \tfrac{22565}{55296}y^{14} \\ & + \ldots + \text{terms through order } y^{899}\end{aligned}$$

and indeed that $\xi_0(y) \in \mathcal{S}_{-1}$:

$$\begin{aligned}\xi_0(y)^{-1} \;=\; & 1 - \tfrac{1}{2}y - \tfrac{1}{4}y^2 - \tfrac{1}{12}y^3 - \tfrac{1}{16}y^4 - \tfrac{1}{48}y^5 - \tfrac{7}{288}y^6 \\ & - \tfrac{1}{96}y^7 - \tfrac{7}{768}y^8 - \tfrac{49}{6912}y^9 - \tfrac{113}{23040}y^{10} - \tfrac{17}{4608}y^{11} \\ & - \tfrac{293}{92160}y^{12} - \tfrac{737}{276480}y^{13} - \tfrac{3107}{1658880}y^{14} \\ & - \ldots - \text{terms through order } y^{899}\end{aligned}$$

But I have no proof of either of these conjectures!!!

- Note that $\xi_0(y)$ is analytic on $0 \le y < 1$ and diverges as $y \uparrow 1$ like $1/[e(1-y)]$.
- It follows that $\xi_0(y) \notin \mathcal{S}_\alpha$ for $\alpha < -1$.

Application to partial theta function Θ_0

It seems that $\xi_0(y) \in \mathcal{S}_1$:

$$\begin{aligned} \xi_0(y) &= 1 + y + 2y^2 + 4y^3 + 9y^4 + 21y^5 + 52y^6 + 133y^7 + 351y^8 \\ &\quad +948y^9 + 2610y^{10} + \ldots + \text{terms through order } y^{6999} \end{aligned}$$

and indeed that $\xi_0(y) \in \mathcal{S}_{-1}$:

$$\begin{aligned} \xi_0(y)^{-1} &= 1 - y - y^2 - y^3 - 2y^4 - 4y^5 - 10y^6 - 25y^7 - 66y^8 \\ &\quad -178y^9 - 490y^{10} - \ldots - \text{terms through order } y^{6999} \end{aligned}$$

and indeed that $\xi_0(y) \in \mathcal{S}_{-2}$:

$$\begin{aligned} \xi_0(y)^{-2} &= 1 - 2y - y^2 \qquad - y^4 - 2y^5 - 7y^6 - 18y^7 - 50y^8 \\ &\quad -138y^9 - 386y^{10} - \ldots - \text{terms through order } y^{6999} \end{aligned}$$

Here I *do* have a proof of these properties (see below).

- Note that

$$\frac{\xi_0(y)^\alpha - 1}{\alpha} = y + \frac{\alpha+3}{2}y^2 + \frac{(\alpha+2)(\alpha+7)}{6}y^3 + O(y^4)$$

- So $\xi_0(y) \notin \mathcal{S}_\alpha$ for $\alpha < -2$.

Application to $\widetilde{R}(x, y, q) = \sum_{n=0}^{\infty} \frac{x^n\, y^{n(n-1)/2}}{(1+q)\,\cdots\,(1+q+\ldots+q^{n-1})}$

- Can use explicit implicit function formula to prove that

$$\xi_0(y; q) = 1 + \sum_{n=1}^{\infty} \frac{P_n(q)}{Q_n(q)}\, y^n$$

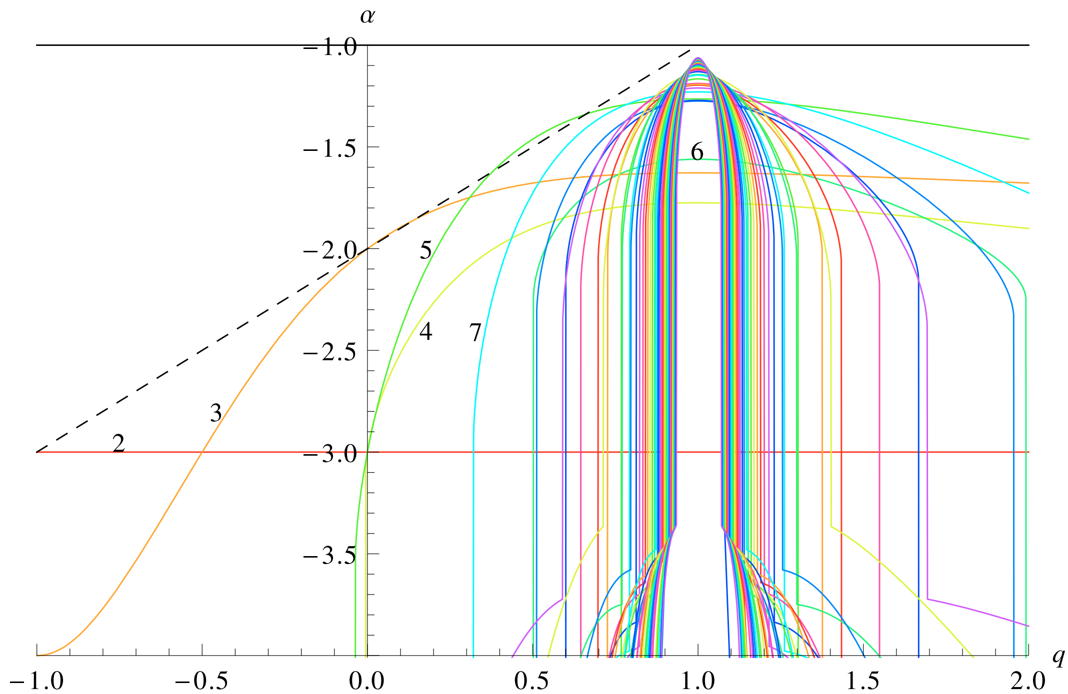
where

$$Q_n(q) = \prod_{k=2}^{\infty} (1+q+\ldots+q^{k-1})^{\lfloor n/\binom{k}{2} \rfloor}$$

and $P_n(q)$ is a self-inversive polynomial in q with integer coefficients.

- *Empirically* $P_n(q)$ has *two* interesting positivity properties:
  (a) $P_n(q)$ has all nonnegative coefficients. Indeed, all the coefficients are strictly positive except $[q^1]\, P_5(q) = 0$.
  (b) $P_n(q) > 0$ for $q > -1$.

- *Empirically* $\xi_0(y; q) \in \mathcal{S}_{-1}$ for all $q > -1$:



Identities for the partial theta function

- Use standard notation for q-shifted factorials:

$$(a;q)_n = \prod_{j=0}^{n-1}(1-aq^j)$$

$$(a;q)_\infty = \prod_{j=0}^{\infty}(1-aq^j) \qquad \text{for } |q|<1$$

- A pair of identities for the partial theta function:

$$\sum_{n=0}^{\infty} x^n\, y^{n(n-1)/2} = (y;y)_\infty\, (-x;y)_\infty \sum_{n=0}^{\infty} \frac{y^n}{(y;y)_n\, (-x;y)_n}$$

$$\sum_{n=0}^{\infty} x^n\, y^{n(n-1)/2} = (-x;y)_\infty \sum_{n=0}^{\infty} \frac{(-x)^n\, y^{n^2}}{(y;y)_n\, (-x;y)_n}$$

as formal power series and as analytic functions on $(x,y) \in \mathbb{C} \times \mathbb{D}$

- Rewrite these as

$$\sum_{n=0}^{\infty} x^n\, y^{n(n-1)/2} = (y;y)_\infty\, (-xy;y)_\infty \left[1 + x + \sum_{n=1}^{\infty} \frac{y^n}{(y;y)_n\, (-xy;y)_{n-1}}\right]$$

$$\sum_{n=0}^{\infty} x^n\, y^{n(n-1)/2} = (-xy;y)_\infty \left[1 + x + \sum_{n=1}^{\infty} \frac{(-x)^n\, y^{n^2}}{(y;y)_n\, (-xy;y)_{n-1}}\right]$$

- The first identity goes back to Heine (1847).
- The second identity can be found in Andrews and Warnaar (2007).

Proof that $\xi_0 \in \mathcal{S}_1$ for the partial theta function

- Let's say we use the first identity:

$$\Theta_0(x,y) \;=\; (y;y)_\infty \, (-xy;y)_\infty \left[1 + x + \sum_{n=1}^{\infty} \frac{y^n}{(y;y)_n \, (-xy;y)_{n-1}} \right]$$

- So $\Theta_0(x,y) = 0$ is equivalent to "brackets = 0".
- Insert $x = -\xi_0(y)$ and bring $\xi_0(y)$ to the LHS:

$$\xi_0(y) \;=\; 1 \,+\, \sum_{n=1}^{\infty} \frac{y^n}{\prod\limits_{j=1}^{n} (1-y^j) \prod\limits_{j=1}^{n-1} [1 - y^j \xi_0(y)]}$$

- This formula can be used iteratively to determine $\xi_0(y)$, and in particular to prove the strict positivity of its coefficients:
- Define the map $\mathcal{F}\colon\ \mathbb{Z}[[y]] \to \mathbb{Z}[[y]]$ by

$$(\mathcal{F}\xi)(y) \;=\; 1 \,+\, \sum_{n=1}^{\infty} \frac{y^n}{\prod\limits_{j=1}^{n} (1-y^j) \prod\limits_{j=1}^{n-1} [1 - y^j \xi(y)]}$$

- Define a sequence $\xi_0^{(0)}, \xi_0^{(1)}, \ldots \in \mathbb{Z}[[y]]$ by $\xi_0^{(0)} = 1$ and $\xi_0^{(k+1)} = \mathcal{F}\xi_0^{(k)}$.
- Then $\xi_0^{(0)} \preceq \xi_0^{(1)} \preceq \ldots \preceq \xi_0$ and $\xi_0^{(k)}(y) \;=\; \xi_0(y) \,+\, O(y^{3k+1})$.
- In particular, $\lim\limits_{k\to\infty} \xi_0^{(k)}(y) = \xi_0(y)$, and $\xi_0(y)$ has strictly positive coefficients.
- Thomas Prellberg has a combinatorial interpretation of $\xi_0(y)$ and $\xi_0^{(k)}(y)$.
- Proofs of $\xi_0 \in \mathcal{S}_{-1}$ and $\xi_0 \in \mathcal{S}_{-2}$ use second identity in a similar way.

Elementary proof of the first identity

- Proof uses nothing more than Euler's first and second identities

$$\frac{1}{(t;q)_\infty} = \sum_{n=0}^{\infty} \frac{t^n}{(q;q)_n}$$

$$(t;q)_\infty = \sum_{n=0}^{\infty} \frac{(-t)^n\, q^{n(n-1)/2}}{(q;q)_n}$$

valid for $(t,q) \in \mathbb{D} \times \mathbb{D}$ and $(t,q) \in \mathbb{C} \times \mathbb{D}$, respectively.

- Write

$$\sum_{n=0}^{\infty} x^n\, y^{n(n-1)/2} = \sum_{n=0}^{\infty} x^n\, y^{n(n-1)/2} \frac{(y;y)_\infty}{(y;y)_n\, (y^{n+1};y)_\infty}$$

- Insert Euler's first identity for $1/(y^{n+1};y)_\infty$:

$$\begin{aligned}
\Theta_0(x,y) &= (y;y)_\infty \sum_{n=0}^{\infty} \frac{x^n\, y^{n(n-1)/2}}{(y;y)_n} \sum_{k=0}^{\infty} \frac{y^{(n+1)k}}{(y;y)_k} \\
&= (y;y)_\infty \sum_{k=0}^{\infty} \frac{y^k}{(y;y)_k} \sum_{n=0}^{\infty} \frac{(xy^k)^n\, y^{n(n-1)/2}}{(y;y)_n} \\
&= (y;y)_\infty \sum_{k=0}^{\infty} \frac{y^k}{(y;y)_k} (-xy^k;y)_\infty \quad \text{by Euler's second identity} \\
&= (y;y)_\infty\, (-x;y)_\infty \sum_{k=0}^{\infty} \frac{y^k}{(y;y)_k\, (-x;y)_k}
\end{aligned}$$

- This identity goes back to Heine (1847), but does not seem to be very well known.
- It can be found in Fine (1988) and Andrews and Warnaar (2007).
- **Did anyone know it between 1847 and 1988???**

Proof of the first and second identities

- A simple limiting case of Heine's first and second transformations

$$
\begin{aligned}
{}_2\phi_1(a,b;c;q,z) &= \frac{(b;q)_\infty\,(az;q)_\infty}{(c;q)_\infty\,(z;q)_\infty}\,{}_2\phi_1(c/b,z;az;q,b) \\
{}_2\phi_1(a,b;c;q,z) &= \frac{(c/a;q)_\infty\,(az;q)_\infty}{(c;q)_\infty\,(z;q)_\infty}\,{}_2\phi_1(abz/c,a;az;q,c/a)
\end{aligned}
$$

  for the basic hypergeometric function

$$
{}_2\phi_1(a,b;c;q,z) = \sum_{n=0}^{\infty} \frac{(a;q)_n\,(b;q)_n}{(q;q)_n\,(c;q)_n}\,z^n
$$

- Just set $b = q$ and $z = -x/a$, then take $a \to \infty$ and $c \to 0$.
- This is how Heine (1847) proved the first identity.
- Heine didn't know his second transformation, which is apparently due to Rogers (1893).
- **Who first wrote the second identity for the partial theta function???**
- Surely it must have been known before Andrews and Warnaar (2007)!?!

Can any of this be generalized?

- Recall our friend

$$\widetilde{R}(x,y,q) \;=\; \sum_{n=0}^{\infty} \frac{x^n\, y^{n(n-1)/2}}{(1+q)\;\cdots\;(1+q+\ldots+q^{n-1})}$$

- Can this proof be extended to cases $q \neq 0$?

- Here is a general identity:

$$\sum_{n=0}^{\infty} \frac{x^n\, y^{n(n-1)/2}}{(q;q)_n} \;=\; \frac{1}{(q;q)_\infty} \sum_{\ell=0}^{\infty} \frac{(-1)^\ell\, q^{\ell(\ell+1)/2}}{(q;q)_\ell}\, \Theta_0(xq^\ell, y)$$

- Can deduce generalizations of the first and second identities for the partial theta function:

$$\sum_{n=0}^{\infty} \frac{x^n\, y^{n(n-1)/2}}{(q;q)_n} \;=\;$$

$$\frac{(y;y)_\infty}{(q;q)_\infty} \sum_{\ell=0}^{\infty} \frac{(-1)^\ell\, q^{\ell(\ell+1)/2}}{(q;q)_\ell}\, (-xq^\ell;y)_\infty \sum_{n=0}^{\infty} \frac{y^n}{(y;y)_n\, (-xq^\ell;y)_n}$$

$$\sum_{n=0}^{\infty} \frac{x^n\, y^{n(n-1)/2}}{(q;q)_n} \;=\;$$

$$\frac{1}{(q;q)_\infty} \sum_{\ell=0}^{\infty} \frac{(-1)^\ell\, q^{\ell(\ell+1)/2}}{(q;q)_\ell}\, (-xq^\ell;y)_\infty \sum_{n=0}^{\infty} \frac{(-xq^\ell)^n\, y^{n^2}}{(y;y)_n\, (-xq^\ell;y)_n}$$

- But I don't know what to do with these formulae, because of the factors $(-1)^\ell$.