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/

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 $|y| \leq 1$
- Analytic in $\mathbb{C} \times \mathbb{D}$, continuous in $\mathbb{C} \times \bar{\mathbb{D}}$
- $F(\cdot, y)$ is entire for each $y \in \bar{\mathbb{D}}$
- 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 $Z_G(q, v) = \sum_{A \subseteq E} q^{k(A)} \prod_{e \in A} v_e$
  
  where $k(A) = \# \text{ connected components in } (V, A)$
- Connected-spanning-subgraph polynomial $C_G(v) = \lim_{q \to 0} q^{-1} Z_G(q, v)$
- 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 \textit{convergent} if $|1 + v| \leq 1$
  
  [see also Flajolet–Salvy–Schaeffer (2004)]
Elementary analytic properties of $F(x, y) = \sum_{n=0}^{\infty} \frac{x^n}{n!} y^{n(n-1)/2}$

- **$y = 0$**: $F(x, 0) = 1 + x$

- **$0 < |y| < 1$**: $F(\cdot, y)$ 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 $\alpha > 0$

- **$y = 1$**: $F(x, 1) = e^x$

- **$|y| = 1$ with $y \neq 1$**: $F(\cdot, y)$ 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]

- **$|y| > 1$**: 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
  $$\sum_{n=1}^{\infty} \frac{x^n}{n!} \overline{C}_n(y) = \log F(x, y) = \sum_{k} \log \left( 1 - \frac{x}{x_k(y)} \right)$$
  and hence
  $$\overline{C}_n(y) = -(n - 1)! \sum_{k} x_k(y)^{-n} \quad \text{for all } n \geq 1$$
  (also holds for $n \geq 2$ when $|y| = 1$)

- This is a convergent expansion for $\overline{C}_n(y)$

- In particular, gives large-$n$ asymptotic behavior
  $$\overline{C}_n(y) = -(n - 1)! \ x_0(y)^{-n} \left[ 1 + O(e^{-\epsilon n}) \right]$$
  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 ($\rightarrow$ 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.

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

**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] $\implies$ 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 $0 \leq y < 1$, 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 $0 \leq y < 1$: 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

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

   and more generally

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

   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

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

And let Mathematica run for a weekend . . .

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

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 \(0 \leq y < 1\), 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 \( x_0(y) \):

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

and all the coefficients (so far) beyond the constant term are \textit{nonpositive}!

**Big Conjecture #5.** For each \( k \), the series \(-(k + 1)y^{-k}/x_k(y)\) has all \textit{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 \textit{probabilities} for a positive-integer-valued random variable.

What might such a random variable be???
Could this approach be used to \textit{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 $D_n(y) = \frac{C_n(y)}{(-1)^{n-1}(n-1)!}$ 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 $0 \leq y < 1$, Vivanti–Pringsheim shows that Big Conjecture #6a implies Big Conjecture #3:

For each $n$, $C_n(y)$ has no zeros with $|y| < 1$.

Moreover, Big Conjecture #6b $\implies$ 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 $n = 21$:

$$P_1(k) = 1$$
$$P_2(k) = 2 + 6k + 3k^2$$
$$P_3(k) = 11 + 29k + 63k^2 + 65k^3 + 28k^4 + 4k^5$$
$$P_4(k) = 22 + 146k + 273k^2 + 359k^3 + 355k^4 + 211k^5 + 63k^6 + 7k^7$$

\[ \vdots \]

$$Q_n(k) = (k + 1)^n \prod_{j=2}^{\infty} (k + j)^{\lfloor n/(j^2) \rfloor}$$

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

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 $k$

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

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

\[
\begin{align*}
\hat{P}_1(k) &= 1 \\
\hat{P}_2(k) &= 1 + 6k + 3k^2 \\
\hat{P}_3(k) &= 2 - 10k + 33k^2 + 59k^3 + 28k^4 + 4k^5 \\
\hat{P}_4(k) &= 3 + 71k + 24k^2 + 82k^3 + 236k^4 + 194k^5 + 63k^6 + 7k^7 \\
\end{align*}
\]

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

- $\hat{P}_n(k)$ does not have nonnegative coefficients (except for $n = 1, 2, 4$)
- $\hat{P}_n(k) \geq 0$ for all real $k \geq 0$ for $n = 1, 2, 3, 4, 5, 7, 8$ but not in general
- But ... $\hat{P}_n(k) \geq 0$ 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
\[
\frac{x_0(y)}{x_1(y)} = \frac{1}{2} y + \frac{1}{6} y^2 + \frac{5}{72} y^3 + \frac{11}{216} y^4 + \frac{29}{1296} y^5 + \ldots
\]
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
  \[
  \frac{x_1(y)}{x_2(y)} = \frac{2}{3} y + \frac{1}{18} y^2 + \frac{17}{216} y^3 + \frac{23}{810} y^4 + \frac{343}{17280} y^5 + \ldots
  \]
  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 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 $\gamma^{-1}$, 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 $e^{-\frac{t^2}{2\gamma^2}}$ 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

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

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

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

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

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

where

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

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 $\gamma$.

Focus for now on (a).
Recall that
\[ h(s) = -\frac{(1 + w)}{2\gamma}s^2 + \frac{w}{\gamma}(e^{is} - 1 - is + \frac{s^2}{2}) \]

Consider for simplicity \( \gamma \) 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 \( \{n \atop m\}_{\geq 3} \). [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 \( \xi \) 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 \( \{n \atop m\}_{\geq 4} \) (at least formally).

  - In the critical regime (\( \xi \) 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 $y^{n(n-1)/2}$]
- $\lim_{N \to \infty} P_N\left(\frac{wx^{1-N}}{N}, w\right) = F(x, w^{-2})$ 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 ($0 \leq w \leq 1$), all zeros are on the unit circle $|x| = 1$
- Laguerre: In antiferromagnetic case ($w \geq 1$), 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

\[
(A_t Q_N)(x) \equiv \sum_{n=0}^{N} a_n x^n e^{tn(N-n)}
\]

Roots of \( A_t Q_N \) 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 \( \text{Re } t > 0 \)???
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 $\lim_{n \to \infty} \nu_n = \infty$.

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

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

which reduces to $\Theta_0$ 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 $\Theta_0$ 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 $\tilde{R}(x, y, q)$ it can be proven that
  
  $$-x_0(y, q) = 1 + \sum_{n=1}^{\infty} \frac{P_n(q)}{Q_n(q)} y^n$$

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

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

I have verified for $n \leq 349$ 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 $\lim_{n \to \infty} \nu_n = \infty$

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

- (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

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

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

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

- 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

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

  and

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

- There is also an alternate form

  $$h(\varphi(y)) = h(0) + \sum_{m=1}^{\infty} \frac{y^m}{m} \left[ \zeta^m h(\zeta) \left[ g(\zeta)^m - \zeta g'(\zeta) g(\zeta)^{m-1} \right] \right]$$
The explicit implicit function formula, continued

• Generalize \( x = g(x)y \) to \( x = G(x, y) \), where
  
  \[- \ G(0, 0) = 0 \text{ and } |(\partial G/\partial x)(0, 0)| < 1 \text{ (analytic-function version)}
  \- \ G(0, 0) = 0 \text{ and } (\partial G/\partial x)(0, 0) = 0 \text{ (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

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

  \[
  = \sum_{m=1}^{\infty} [\zeta^{m-1}][G(\zeta, y)^m - \zeta \frac{\partial G(\zeta, y)}{\partial \zeta} G(\zeta, y)^{m-1}]
  \]

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

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

  \[
  = H(0, y) + \sum_{m=1}^{\infty} [\zeta^{m}]H(\zeta, y) \left[ G(\zeta, y)^m - \zeta \frac{\partial G(\zeta, y)}{\partial \zeta} G(\zeta, y)^{m-1} \right]
  \]

• 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”.

27
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
  $$G(z, y) = \sum_{n=0}^{\infty} (-1)^n \hat{a}_n(y) (1 + z)^n$$

  and
  $$\hat{a}_n(y) = \begin{cases} a_n(y) - 1 & \text{for } n = 0, 1 \\ a_n(y) & \text{for } n \geq 2 \end{cases}$$

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

  More generally, for any formal power series $H(z, y)$, we have
  $$H(\xi_0(y) - 1, y) = H(0, y) + \sum_{m=1}^{\infty} \frac{1}{m} \left[ \zeta^{m-1} \frac{\partial H(\zeta, y)}{\partial \zeta} \left( \sum_{n=0}^{\infty} (-1)^n \hat{a}_n(y) (1 + \zeta)^n \right) \right]^m$$
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 \( \xi_0(y) \):

\[
\xi_0(y)^\beta = 1 + \sum_{m=1}^{\infty} \frac{\beta}{m} \sum_{n_1, \ldots, n_m \geq 0} \left( \beta - 1 + \sum_{m-1} n_i \right) \prod_{i=1}^m (-1)^{n_i} \tilde{a}_{n_i}(y)
\]

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

\[
[y^N] \frac{\xi_0(y)^\beta - 1}{\beta} = \sum_{m=1}^{\infty} \frac{1}{m} \sum_{n_1, \ldots, n_m \geq 2} (-1)^{n_i} \left( \beta - 1 + \sum_{m-1} n_i \right) \prod_{i=1}^m a_{n_i} \]

\[
\sum_{i=1}^m \lambda_{n_i} = N
\]

- Can this formula be used for proofs of nonnegativity???

- **Empirically** I know that the RHS is \( \geq 0 \) when \( \lambda_n = n(n-1)/2 \):
  - For \( \beta \geq -2 \) with \( \alpha_n = 1 \) (partial theta function)
  - For \( \beta \geq -1 \) with \( \alpha_n = 1/n! \) (deformed exponential function)
  - For \( \beta \geq -1 \) 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
  \[ a_n = \sum_{k=1}^{n} \frac{k}{n} c_k a_{n-k} \quad \text{for } n \geq 1 \]
  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 $n \geq 2$
  [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
  
  $$a_n(y) = O(y^{\alpha(n-1)}) \text{ for } n \geq 2$$

  for some real $\alpha > 0$. [This is a bit stronger than (a)–(c).]

- Define $\{\tilde{C}_n(y)\}_{n=1}^{\infty}$ by
  
  $$\frac{x \frac{f'(x, y)}{f(x, y)}}{\sum_{n=1}^{\infty} \tilde{C}_n(y) x^n}$$

  where $'$ denotes $\partial/\partial x$.

**Theorem:** We have

$$\tilde{C}_n(y) = (-1)^{n-1} \xi_0(y)^{-n} + O(y^{\alpha n})$$

or equivalently

$$\xi_0(y) = [(-1)^{n-1} \tilde{C}_n(y)]^{-1/n} + O(y^{\alpha n})$$

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

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

**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

$$P(x, y) = \prod_{i=1}^{k(y)} \left(1 - \frac{x}{X_i(y)}\right)$$

with $k(y) \leq N$. 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

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

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
\[
|\tilde{C}_n(y) - (-1)^{n-1} \xi_0(y)^{-n}| \leq (N - 1) \gamma^{-n} |y|^{-\alpha n}
\]
for small enough $|y|$, as claimed. \qed

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

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 $\alpha > 0$. 33
Computational use of Theorem

- Can compute $\xi_0(y)$ through order $y^{N-1}$ by computing $\tilde{C}_N(y)$
- Do this by computing $\tilde{C}_n(y)$ for $1 \leq n \leq N$ using recursion
- Observe that all $\tilde{C}_n(y)$ 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 $\Theta_0$, 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 $\tilde{R}$, 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 \( S_\alpha \) 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 \( S_\alpha \) consists of those \( f \) for which \( f^\alpha \) (resp. \( \log f \)) has all nonnegative coefficients.
  - For \( \alpha < 0 \), the class \( S_\alpha \) consists of those \( f \) for which \( f^\alpha \) has all nonpositive coefficients after the constant term 1.

- Containment relations among the classes \( S_\alpha \) are given by the following fairly easy result:

  **Proposition** (Scott–A.D.S., unpublished):
  Let \( \alpha, \beta \in \mathbb{R} \). Then \( S_\alpha \subseteq S_\beta \) if and only if either
  
  (a) \( \alpha \leq 0 \) and \( \beta \geq \alpha \), 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 $\xi_0(y) \in S_1$:

$$
\xi_0(y) = 1 + \frac{1}{2}y + \frac{1}{2}y^2 + \frac{11}{24}y^3 + \frac{11}{24}y^4 + \frac{7}{16}y^5 + \frac{7}{16}y^6 \\
+ \frac{493}{1152}y^7 + \frac{163}{384}y^8 + \frac{323}{768}y^9 + \frac{1603}{3840}y^{10} + \frac{57283}{138240}y^{11} \\
+ \frac{170921}{114720}y^{12} + \frac{340171}{829440}y^{13} + \frac{22565}{55296}y^{14} \\
+ \ldots + \text{terms through order } y^{899}
$$

and indeed that $\xi_0(y) \in S_{-1}$:

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

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

- Note that $\xi_0(y)$ is analytic on $0 \leq y < 1$ and diverges as $y \uparrow 1$ like $1/[e(1 - y)]$.
- It follows that $\xi_0(y) \notin S_\alpha$ for $\alpha < -1$. 

36
Application to partial theta function $\Theta_0$

It seems that $\xi_0(y) \in S_1$:

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

and indeed that $\xi_0(y) \in S_{-1}$:

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

and indeed that $\xi_0(y) \in S_{-2}$:

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

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 $\xi_0(y) \not\in S_{\alpha}$ for $\alpha < -2$. 
Application to $\tilde{R}(x, y, q) = \sum_{n=0}^{\infty} \frac{x^n y^{n(n-1)/2}}{(1 + q) \cdots (1 + q + \ldots + q^{n-1})}$

- 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

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

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** $\xi_0(y; q) \in S_{-1}$ for all $q > -1$:

![Graph of $\xi_0(y; q)$ for $q > -1$]
Identities for the partial theta function

- Use standard notation for $q$-shifted factorials:

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

\[
(a; q)_\infty = \prod_{j=0}^{\infty} (1 - a q^j) \quad \text{for } |q| < 1
\]

- 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 $\xi_0 \in S_1$ 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:

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

- 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 $\mathcal{F}: \mathbb{Z}[[y]] \to \mathbb{Z}[[y]]$ by

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

- 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, $\lim_{k \to \infty} \xi_0^{(k)}(y) = \xi_0(y)$, 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 $\xi_0 \in S_{-1}$ and $\xi_0 \in S_{-2}$ 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 \(1/(y^{n+1}; y)_{\infty}\):

\[
\Theta_0(x, y) = (y; y)_{\infty} \sum_{n=0}^{\infty} \frac{x^n y^{n(n-1)/2}}{(y; y)_n} \sum_{k=0}^{\infty} \frac{y^{(n+1)k}}{(y; y)_k}
\]

\[
= (y; y)_{\infty} \sum_{k=0}^{\infty} \frac{y^k}{(y; y)_k} \sum_{n=0}^{\infty} \frac{(xy^k)^n y^{n(n-1)/2}}{(y; y)_n}
\]

\[
= (y; y)_{\infty} \sum_{k=0}^{\infty} \frac{y^k}{(y; y)_k} (-xy^k; y)_{\infty} \text{ by Euler’s second identity}
\]

\[
= (y; y)_{\infty} (-x; y)_{\infty} \sum_{k=0}^{\infty} \frac{y^k}{(y; y)_k (-x; y)_k}
\]

- 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

\[
2\phi_1(a, b; c; q, z) = \frac{(b; q)_\infty (az; q)_\infty}{(c; q)_\infty (z; q)_\infty} \frac{2\phi_1(c/b, z; az; q, b)}{2\phi_1(c/a, q; az; q, c/a)}
\]

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

- 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 \((-1)^\ell\).