Roots $x_k(y)$ 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

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LECTURE #2

Applications of
the explicit implicit function formula
and the exponential formula
The basic set-up

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 \( \lim_{n \to \infty} \nu_n = \infty \).

Examples:

- The “partial theta function”
  \[ \Theta_0(x, y) = \sum_{n=0}^{\infty} x^n y^{n(n-1)/2} \]

- The “deformed exponential function” studied in Lecture #1:
  \[ F(x, y) = \sum_{n=0}^{\infty} \frac{x^n}{n!} y^{n(n-1)/2} \]

- 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 \( q = 1 \).
The leading root $x_0(y)$

- 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

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

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

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

- 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

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

- Generalize \( x = g(x)y \) to \( x = G(x, y) \), where
  \[ \begin{align*}
  - G(0, 0) &= 0 \quad \text{and} \quad |(\partial G/\partial x)(0, 0)| < 1 \quad \text{(analytic-function version)} \\
  - G(0, 0) &= 0 \quad \text{and} \quad (\partial G/\partial x)(0, 0) = 0 \quad \text{(formal-power-series version)}
  \end{align*} \]

- Then there is a unique \( \varphi(y) \) with zero constant term satisfying \( \varphi(y) = G(\varphi(y), y) \), and it is given by
  \[ \varphi(y) = \sum_{m=1}^{\infty} \frac{1}{m} [\zeta^{m-1}] G(\zeta, y)^m \]
  \[ = \sum_{m=1}^{\infty} [\zeta^{m-1}] \left[ G(\zeta, y)^m - \zeta \frac{\partial G(\zeta, y)}{\partial \zeta} G(\zeta, y)^{m-1} \right] \]

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”.

A possible extension [open problem]

- Conditions on $G$ and $\varphi$ in the explicit implicit function formula seem natural:
  - If $G(x, y)$ is a formal power series, it ordinarily makes sense to substitute $x = \varphi(y)$ only when $\varphi(y)$ is a formal power series with zero constant term.
  - Then a solution to the fixed-point equation $\varphi(y) = G(\varphi(y), y)$ with $\varphi(y)$ having zero constant term can exist only if $G(0, 0) = 0$.

- But there is one important case where these conditions can be weakened: namely, if $G(x, y)$ belongs to $R[x][[y]]$, i.e. if the coefficient of each power of $y$ is a polynomial in $x$.
  - In this case it makes sense to substitute for $x$ an arbitrary formal power series $\varphi(y)$, not necessarily with zero constant term.
  - The result $G(\varphi(y), y)$ is a well-defined formal power series in $y$.
  - What can be said about existence and uniqueness of solutions to $\varphi(y) = G(\varphi(y), y)$?
  - And is there an explicit “Lagrange-like” formula for $\varphi(y)$?
  - I suspect that the answer is yes, but I haven’t worked out the details.
  - And it looks like this may be useful in our application.
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 $\xi_0(y)$:

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

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

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

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

• 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 with $\beta \geq -1$

• 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 $\tilde{c}_n = nc_n$, which are the coefficients in
  \[ \frac{x A'(x)}{A(x)} = \sum_{n=1}^{\infty} \tilde{c}_n x^n \]
- 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
  \[ \frac{x A'(x, y)}{A(x, y)} = \sum_{n=1}^{\infty} \tilde{c}_n(y) x^n \]
  where $'$ denotes $\partial/\partial x$ and $\tilde{c}_n(y)$ 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
  
  $$a_n(y) = O(y^{\alpha(n-1)}) \quad \text{for } n \geq 2$$

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

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

  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 in Lecture #1 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

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

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. □

**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 $R = \mathbb{Z}[a]$ where $a = \{a_{nm}\}_{n \geq 2, m \geq \lceil\alpha(n-1)\rceil}$ are treated as indeterminates. Then the claim of the Theorem amounts to a series of identities between polynomials in $a$ 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 $\mathbb{Z}[a]$. □

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 $\alpha > 0$. 

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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 shown last week, it seems that $\xi_0(y) \in S_1$:

$$\xi_0(y) = 1 + \frac{1}{2}y + \frac{1}{2}y^2 + \frac{11}{24}y^3 + \frac{11}{24}y^4 + \frac{7}{16}y^5 + \frac{7}{16}y^6$$

$$+ \frac{493}{1152}y^7 + \frac{163}{384}y^8 + \frac{323}{768}y^9 + \frac{1603}{3840}y^{10} + \frac{57283}{138240}y^{11}$$

$$+ \frac{170921}{414720}y^{12} + \frac{340171}{829440}y^{13} + \frac{22565}{55296}y^{14}$$

$$+ \ldots + \text{terms through order } y^{899}$$

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

$$\xi_0(y)^{-1} = 1 - \frac{1}{2}y - \frac{1}{4}y^2 - \frac{1}{12}y^3 - \frac{1}{16}y^4 - \frac{1}{48}y^5 - \frac{7}{288}y^6$$

$$- \frac{1}{96}y^7 - \frac{7}{768}y^8 - \frac{6912}{512}y^9 - \frac{113}{23040}y^{10} - \frac{17}{4608}y^{11}$$

$$- \frac{293}{92160}y^{12} - \frac{737}{276480}y^{13} - \frac{3107}{1658880}y^{14}$$

$$- \ldots - \text{terms through order } y^{899}$$

**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 $\alpha < -1$.
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 the first two properties (but not the third). Coming next week!

• 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 $\xi_0(y) \notin S_\alpha$ 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

\[ \xi_0(y; q) = 1 + \sum_{n=1}^{\infty} \frac{P_n(q)}{Q_n(q)} \cdot y^n \]

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 \( q > -1 \):
Can any of this be proven???

- It seems that $\tilde{R}(x, y, q)$ is the right unification of $\Theta_0$ and $F$.
- But thus far my proofs are only for $q = 0$ (i.e. $\Theta_0$).
  \textbf{Coming next week!}
- Can anything be generalized to $q \neq 0$??

- \textbf{Open problem:} For $q = 0$, prove $\xi_0(y) \in S_1$ or $S_{-1}$ (or even $S_{-2}$) \textit{directly from the explicit implicit function formula}.
- If this works, it might be generalizable to $q \neq 0$. 