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 $n \ge 2$; 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

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

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

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 $n \ge 2$

(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 $\log f(x,y)$.
- \bullet 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

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

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

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

The explicit implicit function formula, continued

- Generalize x = g(x)y to x = G(x, y), where
 - -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

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

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

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

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

- \bullet First versions are slightly more convenient but require R to contain the rationals as a subring.
- \bullet 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 φ 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

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

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 $\xi_0(y)$:

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

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

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

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 $\xi_0(y)$:

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

• 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

$$[y^{N}] \frac{\xi_{0}(y)^{\beta} - 1}{\beta} = \sum_{m=1}^{\infty} \frac{1}{m} \sum_{\substack{n_{1}, \dots, n_{m} \geq 2 \\ \sum_{i=1}^{m} \lambda_{n_{i}} = N}} (-1)^{\sum n_{i}} {\beta - 1 + \sum n_{i} \choose m - 1} \prod_{i=1}^{m} \alpha_{n_{i}}$$

- 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 $\beta \geq -2$ 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 with $\beta \geq -1$
- How can we see these facts from this formula???? [open combinatorial problem]

Tools II: Variants of the exponential formula

- \bullet 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

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

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

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

- 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

 $a_n(y) = O(y^{\alpha(n-1)})$ 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

$$\widetilde{c}_n = na_n - \sum_{k=1}^{n-1} \widetilde{c}_k a_{n-k}$$

- Take the power -1/n to extract $\xi_0(y)$ through order $y^{\lceil \alpha n \rceil 1}$
- This abstracts the recursive method shown 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 $|y| \le \rho$.

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

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

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

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

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

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

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 $\mathbb{Z}[\boldsymbol{a}]$.

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 $\tilde{c}_n(y)$ 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 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 S_{α} 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}_{α} consists of those f for which f^{α} (resp. $\log f$) has all nonnegative coefficients.
 - For $\alpha < 0$, the class S_{α} consists of those f for which f^{α} has all *nonpositive* coefficients after the constant term 1.
- Containment relations among the classes S_{α} 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) $\alpha \leq 0$ 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 $\xi_0(y) \in \mathcal{S}_1$:

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

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

$$\xi_{0}(y)^{-1} = 1 - \frac{1}{2}y - \frac{1}{4}y^{2} - \frac{1}{12}y^{3} - \frac{1}{16}y^{4} - \frac{1}{48}y^{5} - \frac{7}{288}y^{6} - \frac{1}{96}y^{7} - \frac{7}{768}y^{8} - \frac{49}{6912}y^{9} - \frac{113}{23040}y^{10} - \frac{17}{4608}y^{11} - \frac{293}{92160}y^{12} - \frac{737}{276480}y^{13} - \frac{3107}{1658880}y^{14} - \dots - \text{ terms through order } y^{899}$$

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

- Note that $\xi_0(y)$ is analytic on $0 \le y < 1$ 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 $\xi_0(y) \in \mathcal{S}_1$:

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

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

$$\xi_0(y)^{-1} = 1 - y - y^2 - y^3 - 2y^4 - 4y^5 - 10y^6 - 25y^7 - 66y^8$$

-178 $y^9 - 490y^{10} - \dots - \text{terms through order } y^{6999}$

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

$$\xi_0(y)^{-2} = 1 - 2y - y^2 - y^4 - 2y^5 - 7y^6 - 18y^7 - 50y^8$$

-138 $y^9 - 386y^{10} - \dots - \text{terms through order } y^{6999}$

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 $\xi_0(y) \notin \mathcal{S}_{\alpha}$ 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

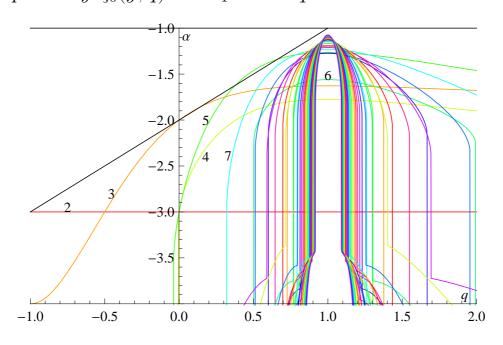
$$\xi_0(y;q) = 1 + \sum_{n=1}^{\infty} \frac{P_n(q)}{Q_n(q)} y^n$$

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:



Can any of this be proven???

- It seems that $\widetilde{R}(x, y, q)$ is the right unification of Θ_0 and F.
- But thus far my proofs are only for q = 0 (i.e. Θ_0). Coming next week!
- Can anything be generalized to $q \neq 0$???
- Open problem: For q = 0, prove $\xi_0(y) \in \mathcal{S}_1$ or \mathcal{S}_{-1} (or even \mathcal{S}_{-2}) directly from the explicit implicit function formula.
- If this works, it might be generalizable to $q \neq 0$.