# Computing scaling functions for two-dimensional vesicle models

## from generating functions to coalescing saddle points

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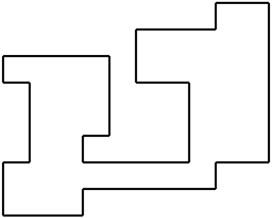
# Topic Outline

1. Motivation
   - Vesicle Generating Function
   - Singularity Diagram
   - Scaling Function
2. From Lattice Walks to Basic Hypergeometric Series
   - $q$-Deformed Algebraic Equations
   - $q$-Difference Equations
   - Basic Hypergeometric Series
3. Asymptotic Analysis
   - Contour Integral Representation
   - Saddle Point Analysis
   - Generalisation
4. Outlook

# Outline

# Vesicle Generating Function

- 3-dim vesicle (bubble) with surface and volume
- 2-dim lattice model: polygons on the square lattice



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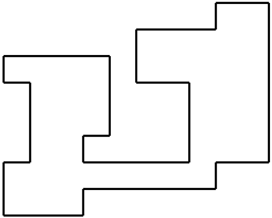


$c_{m,n}$ number of polygons with area $m$ and perimeter $2n$

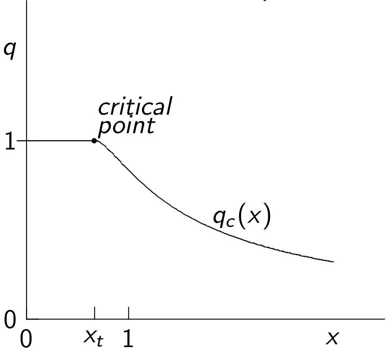
$$G(x,q) = \sum_{n,m} c_{m,n} x^n q^m \qquad \text{generating function}$$

Wanted:

- an explicit formula for $G(x,q)$
- singularity structure, e.g. $q_c(x)$

# Singularity Diagram

Folklore: universal behaviour near a “critical point”



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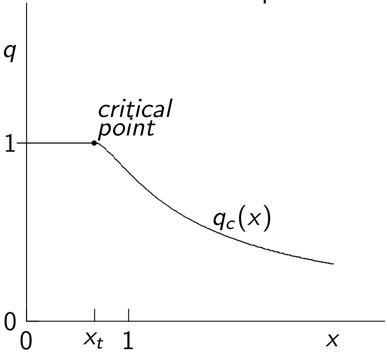


- scaling function $f$ with crossover exponent $\phi$:

$$G^{sing}(x,q) \sim (1-q)^{-\gamma_t} f\left([1-q]^{-\phi}[x_t - x]\right)$$

as $q \to 1$ and $x \to x_t$ with $z = [1-q]^{-\phi}[x_t - x]$ fixed

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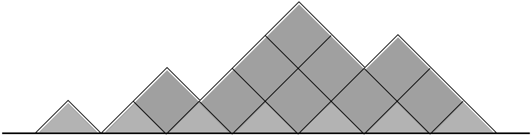
- $q$-Analogue of the Painlevé II equation (Witte)

# Outline

# Example 1: Dyck Paths



$2n = 14$ steps enclosing an area of size $m = 9$

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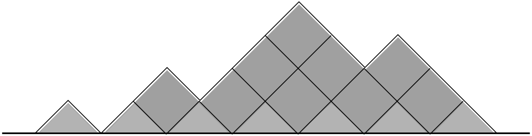


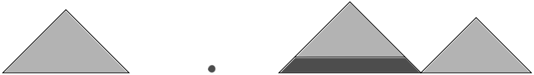
$2n = 14$ steps enclosing an area of size $m = 9$

$$G(t,q) = \sum_{m,n} c_{m,n} t^n q^m$$

$t$ counts pairs of up/down steps, $q$ counts enclosed area

# Example 1: Dyck Paths

- A functional equation



$$G(t,q) \quad = \quad 1 \quad + \quad tG(qt,q)G(t,q)$$

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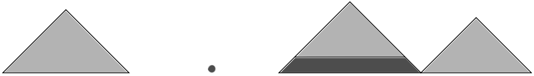


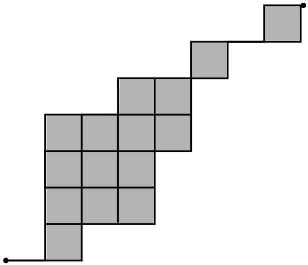
$$G(t,q) \quad = \quad 1 \quad + \quad tG(qt,q)G(t,q)$$

- $C(t) = G(t,1)$ satisfies $C(t) = 1 + tC(t)^2$

$$C(t) = \frac{1-\sqrt{1-4t}}{2t} = \sum_{n=0}^{\infty} \frac{t^n}{n+1}\binom{2n}{n}$$

Generating function of Catalan numbers

# Example 2: A Pair of Directed Walks



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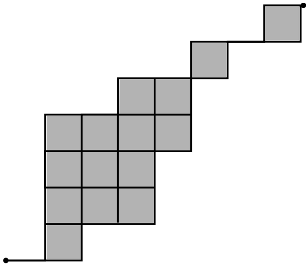

Two directed walks not allowed to cross

$$G(x,y,q)=\sum_{m,n_x,n_y} c_{m,n_x,n_y} x^{n_x} y^{n_y} q^m$$

$x$ and $y$ count pairs of east and north steps, $q$ counts enclosed area

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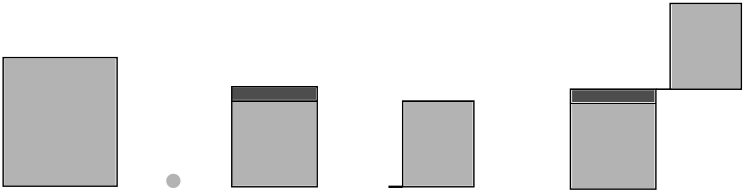

$$G(x,y,q) = 1 + yG(qx,y,q) + xG(x,y,q) + yG(qx,y,q)xG(x,y,q)$$

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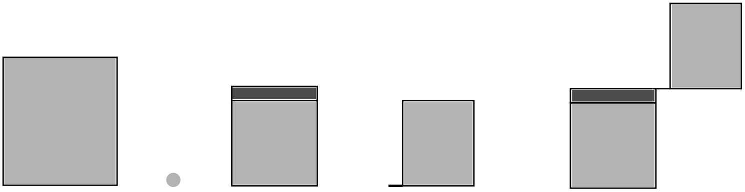

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- $G(t,t,1) = 1 + tC(t)$ Catalan generating function

# Example 3: Partially Directed Walks Above $y = x$

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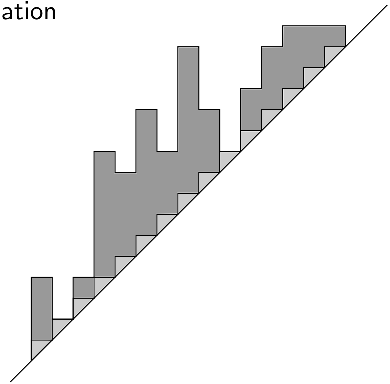

$$G(x,y,q) = 1 + yG(qx,y,q)xG(x,y,q) + y(G(qx,y,q) - 1)y$$

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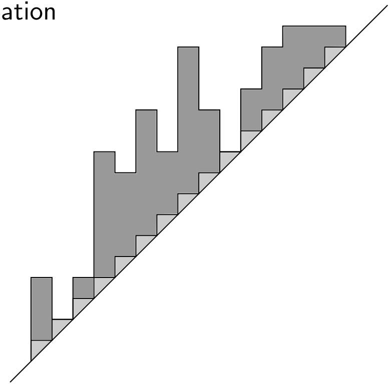

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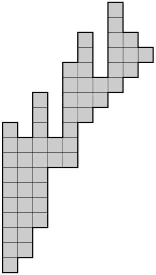
- $G(x,y,1) = C\left(\frac{xy}{1-y^2}\right)$ Catalan generating function

# Example 4: Directed Column-Convex Polygons

- Lattice polygon
  - partially directed upper perimeter
  - fully directed lower perimeter



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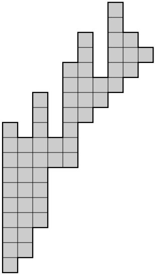

- Lattice polygon
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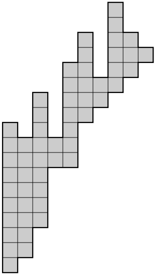
  - fully directed lower perimeter
- A functional equation

$$
\begin{aligned}
0 &= G(q^2x)G(qx)G(x) \\
&+ yG(q^2x)G(qx) + yG(q^2x)G(x) - (1+q)G(qx)G(x) \\
&+ y^2G(q^2x) - y(1+q)G(qx) + q(1+qx(y-1))G(x) \\
&+ yq^2x(y-1)
\end{aligned}
$$

# Example 4: Directed Column-Convex Polygons



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\end{aligned}$$

- $q = 1$ gives a cubic equation for $G(x, y, 1)$

## Summary of the Examples

Different $q$-deformations of Catalan-type generating functions:

- Dyck paths

$$G(t) = 1 + tG(t)G(qt)$$

- Pair of directed walks

$$G(x) = (1 + xG(x))(1 + yG(qx))$$

- Partially directed walks above the diagonal

$$G(x) = 1 + xyG(x)G(qx) + y^2(G(qx) - 1)$$

and also of higher-order algebraic generating functions:

- e.g. directed column-convex polygons

# Example 1: Solving $G(t) = 1 + tG(t)G(qt)$

An aside:

- $G(t)$ admits a nice continued fraction expansion

$$G(t) = \cfrac{1}{1 - \cfrac{t}{1 - \cfrac{qt}{1 - \cfrac{q^2 t}{1 - \dots}}}}$$

- Connections with orthogonal polynomials, combinatorics of weighted lattice paths, ...

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- Connections with orthogonal polynomials, combinatorics of weighted lattice paths, ...
- However, useless for finer asymptotic analysis of $q \to 1$.

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$$H(t) = \sum_{n=0}^{\infty} \frac{q^{n^2-n}(-t)^n}{(q;q)_n} = {}_0\phi_1(-;0;q,-t)$$

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[${}_0\phi_1(-;0;q,-qt)$ a $q$-Airy function (Ismail)]

# Example 2: Solving $G(x) = (1 + xG(x))(1 + yG(qx))$

Again:

- Linearise the functional equation using

$$G(x) = \frac{1}{x}\left(\frac{H(qx)}{H(x)} - 1\right)$$

- Obtain a linear $q$-difference equation

$$q(H(qx) - H(x)) = qxH(qx) + y(H(q^2x) - H(qx))$$

- Explicit solution

$$H(t) = \sum_{n=0}^{\infty} \frac{q^{\binom{n}{2}}(-x)^n}{(y;q)_n(q;q)_n} = {}_1\phi_1(0; y; q, x)$$

# Example 3: $G(x) = 1 + xyG(x)G(qx) + y^2(G(qx) - 1)$

One more time:

- Linearise the functional equation using

$$G(x) = \frac{y}{x}\left(\frac{H(qx)}{H(x)} - 1\right)$$

- Obtain a linear $q$-difference equation

$$q(H(qx) - H(x)) = qx(1/y - y)H(qx) + y^2(H(q^2x) - H(qx))$$

- Explicit solution

$$H(t) = \sum_{n=0}^{\infty} \frac{(-x(1-y^2)/y)^n}{(y^2;q)_n(q;q)_n} = {}_2\phi_1(0,0;y^2;q,-x(1-y^2)/y)$$

# Example 4: Directed Column-Convex Polygons

Surprisingly, this trick works also here:

- Linearise the functional equation using

$$G(x) = y\left(\frac{H(qx)}{H(x)} - 1\right)$$

- Obtain a linear $q$-difference equation

$$y^2H(q^3x) - y(q+y+1)H(q^2x) + (y+q+qy+q^2x(y-1))H(qx) - qH(x) = 0$$

- Explicit solution

$$H(t) = \sum_{n=0}^{\infty} \frac{q^{\binom{n}{2}}(-qx(1-y))^n}{(y;q)_n(qy;q)_n(q;q)_n} = {}_2\phi_2(0,0;y,qy;q,qx(1-y))$$

# Summary:

Different $q$-deformations of Catalan-type generating functions:

- Dyck paths

$$G(t,q) = \frac{{}_0\phi_1(-;0;q,-qt)}{{}_0\phi_1(-;0;q,-t)}$$

- Pair of directed walks

$$G(x,y,q) = \frac{1}{x}\left(\frac{{}_1\phi_1(0;y;q,qx)}{{}_1\phi_1(0;y;q,x)} - 1\right)$$

- Partially directed walks above the diagonal

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- Directed column-convex polygons

$$G(x,y,q) = y\left(\frac{{}_2\phi_2(0,0;y,qy;q,qqx(1-y))}{{}_2\phi_2(0,0;y,qy;q,qx(1-y))} - 1\right)$$

# Outline

# A Puzzle

- The full generating function is a quotient of $q$-series, e.g.

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

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- However, for $q = 1$ we have a simple algebraic generating function

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*How can one understand the limit $q \to 1$?*

# A Standard Trick For Evaluating Alternating Series

- Write an alternating series as a contour integral

$$\sum_{n=0}^{\infty}(-x)^n c_n = \frac{1}{2\pi i}\oint_{\mathcal{C}} x^s c(s)\frac{\pi}{\sin(\pi s)}ds$$

$\mathcal{C}$ runs counterclockwise around the zeros of $\sin(\pi s)$

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- For example,

$$\exp(-x) = \sum_{n=0}^{\infty}\frac{(-x)^n}{n!} = \frac{1}{2\pi i}\int_{-c-i\infty}^{-c+i\infty} x^s\Gamma(-s)ds$$

where $c > 0$ (here, we have used $\Gamma(s)\Gamma(1-s) = \pi/\sin(\pi s)$)

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*Find suitable $q$-version for this trick*

# Contour Integral Representation

Use that

$$\mathrm{Res}\left[(z;q)_\infty^{-1}; z=q^{-n}\right] = -\frac{(-1)^n q^{\binom{n}{2}}}{(q;q)_n (q;q)_\infty} \qquad n = 0, 1, 2, \ldots$$

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to prove that

**Lemma**

*For complex $t$ with $|\arg(t)| < \pi$ and $0 < q < 1$ we have for $0 < \rho < 1$*

$$\sum_{n=0}^{\infty} \frac{q^{n^2-n}(-t)^n}{(q;q)_n} = \frac{(q;q)_\infty}{2\pi i} \int_{\rho-i\infty}^{\rho+i\infty} \frac{z^{\frac{1}{2}\log_q z - \log_q t}}{(z;q)_\infty} \sqrt{z}\, dz$$

# Some Asymptotics

Approximate $\log(z;q)_\infty \sim \frac{1}{\log q}\mathrm{Li}_2(z) + \frac{1}{2}\log(1-z)$ to get

## Lemma

*For* $0 < t < 1$ *and with* $\varepsilon = -\log q$

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

$$\frac{(q;q)_\infty}{2\pi i} \int_{\rho-i\infty}^{\rho+i\infty} e^{\frac{1}{\varepsilon}\left[-\frac{1}{2}(\log z)^2 + \log(z)\log(t) + \mathrm{Li}_2(z)\right]} \sqrt{\frac{z}{1-z}}\, dz\, [1 + O(\varepsilon)]$$

*where* $t < \rho < 1$

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*where $t < \rho < 1$*

We find a Laplace-type integral, where the saddles are given by

$$0 = \frac{d}{dz}\left[-\frac{1}{2}(\log z)^2 + \log(z)\log(t) + \mathrm{Li}_2(z)\right]$$

# Saddle Point Analysis

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$$\int_{\mathcal{C}} e^{g(z)/\varepsilon} f(z) dz$$

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*As $t$ approaches $t_t = 1/4$, the saddles coalesce*

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The transformation is one-to-one and analytic in a neighbourhood of $t = 1/4$.

# Finally: Ai(x)

- Substitute $z = z(u)$ into

$$I(\epsilon) = \int_{\mathcal{C}} e^{g(z)/\varepsilon} f(z) dz = \int_{\mathcal{C}'} e^{g(z(u))/\varepsilon} f(z(u)) \frac{dz}{du} du$$

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- Depending on the contour $\mathcal{C}'$, $V(\lambda)$ is expressible using $\mathrm{Ai}(\lambda)$ and $\mathrm{Ai}'(\lambda)$

# Uniform Asymptotics

**Theorem**

*Let* $0 < t < 1$ *and* $\varepsilon = -\log q$. *Then, as* $\varepsilon \to 0^+$,

$$G(t,q) \sim \frac{1}{2}\left(1 - \sqrt{1-4t}\left[-\frac{\mathrm{Ai}'(\alpha\varepsilon^{-2/3})}{\alpha^{1/2}\varepsilon^{-1/3}\mathrm{Ai}(\alpha\varepsilon^{-2/3})}\right]\right)$$

*where* $\alpha = \alpha(t)$ *is an explicitly given function of* $t$. *In particular,*

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- Stronger than scaling limit which keeps $z = (1-4t)\varepsilon^{-2/3}$ fixed

# More Saddle Points

Saddle point coalescence occurs in all four cases:

- Dyck paths, ${}_0\phi_1(-;0;q,-t)$:

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# Contour Integral for Basic Hypergeometric Series

$$ {}_r\phi_s\left(\begin{matrix} a_1,\ldots,a_r \\ b_1,\ldots,b_s \end{matrix};q,t\right) = \sum_{n=0}^{\infty} \frac{(a_1,a_2,\ldots,a_r;q)_n}{(q,b_1,\ldots,b_s;q)_n} \left[(-1)^n q^{\binom{n}{2}}\right]^{1+s-r} t^n $$

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**Lemma**

*For complex $t$ with $|\arg(t)| < \pi$, and $0 < q < 1$ we have for $0 < \rho < 1$*

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## Lemma

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**Proof**: Compute residues at $z=q^{-n}$ for $n\in\mathbb{N}_0$ (and consider a sequence of contours)

# General Saddle Point Equation

- As $\varepsilon = -\log q \to 0$, we again obtain a Laplace-type integral

$$\int e^{g(z)/\varepsilon} f(z) dz$$

where

$$\begin{aligned} g(z) = &\mathrm{Li}_2(a_1/z) + \ldots + \mathrm{Li}_2(a_r/z) + \mathrm{Li}_2(z) + \log z \log t \\ &- \mathrm{Li}_2(b_1/z) - \ldots - \mathrm{Li}_2(b_s/z) - \frac{s-r}{2}(\log z)^2 \end{aligned}$$

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Work in progress ...

# Outline

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- contour integral
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*The End*