Combinatorial enumeration of two-dimensional vesicles

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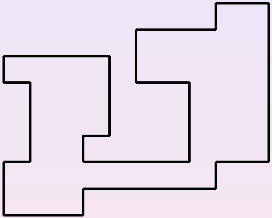
Outline

vesiculum (latin) = bubble

- physical motivation:
  - polygons as models of vesicles (= closed fluctuating membranes)
  - statistical mechanics of vesicles
  - phase transition in the thermodynamic limit
  - tricritical phase diagram
- partially directed vesicles – solvable models
  - non-linear functional equations
  - generating functions
- asymptotic analysis:
  - perturbation expansion $\longrightarrow$ critical exponents
  - contour integral $\longrightarrow$ saddle points $\longrightarrow$ scaling function

Polygon Models of Vesicles

- 3-dim bubble with surface tension and osmotic pressure
- 2-dim lattice model: polygons on the square lattice



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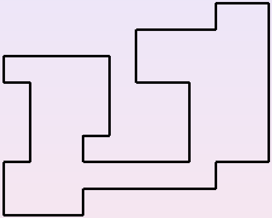

$c_{m,n}$ number of polygons with area m and perimeter $2n$

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

Wanted:

- an explicit formula for $G(x,q)$
- information on the singularity structure of $G(x,q)$

Statistical Mechanics

- system size: area m, thermodynamic limit: $m \to \infty$

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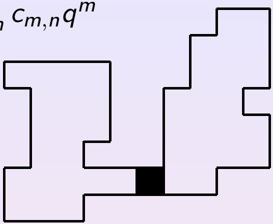
- thermodynamic limit: relation to radius of convergence

$$q_c(x) = \lim_{m\to\infty} (Z_m(x))^{-\frac{1}{m}}$$

Existence of Thermodynamic Limit

Consider $Q_n(q) = \sum_m c_{m,n} q^m$



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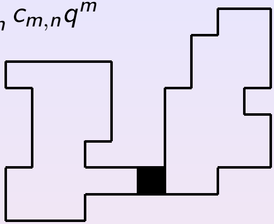

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$$c_{m+1,n_1+n_2} \geq \sum_{m_1+m_2=m} c_{m_1,n_1} c_{m_2,n_2}$$

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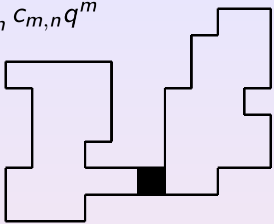

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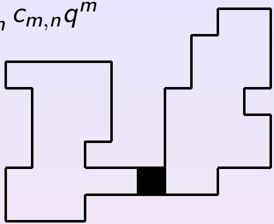

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- $qQ_n(q)$ is sub-multiplicative, which implies existence of

$$x_c(q) = \lim_{n\to\infty} (Q_n(q))^{-\frac{1}{n}}$$

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Jump of $x_c(q)$ *at* $q = 1 \Rightarrow$ *Phase Transition!*

Precise Asymptotics for $q > 1$

Theorem (TP, Owczarek)

Let $Q_n(q)$ be the finite-perimeter partition function of polygons on the square lattice. Then

$$Q_n(q) \sim Q_n^{as}(q) = \frac{1}{(q^{-1};q^{-1})_\infty^4} \sum_{k=-\infty}^{\infty} q^{k(n-k)}$$

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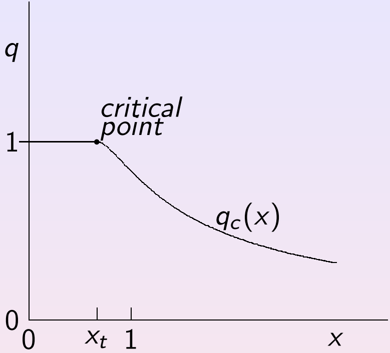
Understanding $Q_n^{as}(q)$:

- Counting rectangles: $\sum_{k=1}^{n-1} q^{k(n-k)}$
- Corners are Ferrer diagrams:
$$(q;q)_\infty^{-1} = (1-q)^{-1}(1-q^2)^{-1}(1-q^3)^{-1}\cdots$$

Phase Diagram



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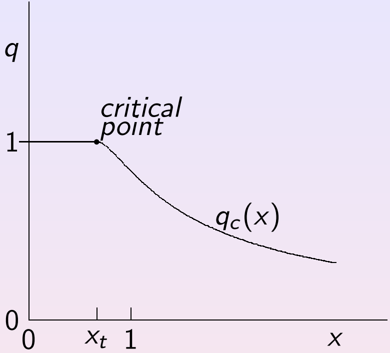

Physicist's folklore: upon approaching the critical point

- scaling function f with crossover exponent ϕ:

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

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

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  - Langevin equation for BE (Kearney and Majumdar)

Partially Directed Vesicles

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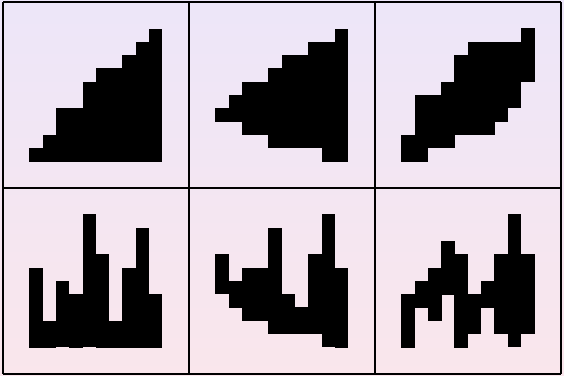
Partial directedness leads to solvability:



Methods

Solution via e.g.

- recurrence relations (Temperley '52, Brak '90)
- q-extension of an algebraic language (Delest '84)
- functional equations (Bousquet-Melou '93)

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Structure of generating function:

- single-variable: algebraic or rational
- two-variable: (quotient of) q-series

Method of Inflation

Distinguish horizontal (x) and vertical (y) steps:

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

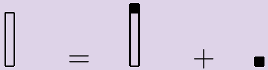
Inflated a (directed) polygon by increasing the height of each column by one:

$$G(x, y, q) \to G(qx, y, q)y$$

Partition the set of all polygons using this inflation process

Example: Columns

$\{\text{columns}\} = \{\text{columns with height} \geq 2\} \,\dot{\cup}\, \{\text{single square}\}$



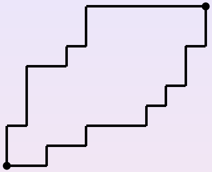
$$C(x, y, q) = C(qx, y, q)y + qxy$$

can be solved

$$C(x, y, q) = \frac{qxy}{1 - qy}$$

Non-linear Functional Equations

Staircase polygons lead to a non-linear equation



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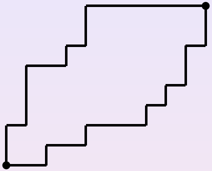

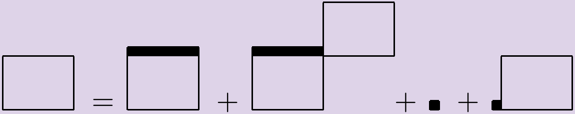

$$G(x) = G(qx)y + G(qx)G(x) + qxy + qxG(x)$$

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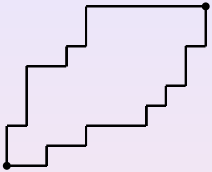

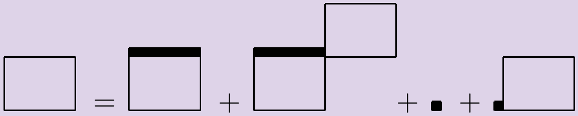

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Deeper analysis via bijection to heaps of pieces (Viennot)

Solving the Functional Equation

$$G(x,y,q) = \left[G(qx,y,q) + qx\right]\left[y + G(x,y,q)\right]$$

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$$G(x, y, q) = [G(qx, y, q) + qx]\,[y + G(x, y, q)]$$

- Consider the transformation

$$G(x, y, q) = y\frac{H(qx, y, q)}{H(x, y, q)} - 1$$

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$$0 = yH(q^2x,y,q) + (qx - 1 - y)H(qx,y,q) + H(x,y,q)$$

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

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Structure of GF is explainable combinatorially (Viennot)

Solving the Functional Equation

To summarise,

$$G(x,y,q) = [G(qx,y,q) + qx]\,[y + G(x,y,q)]$$

is solved by

$$G(x,y,q) = y\left(\frac{\sum_{n=0}^{\infty} \frac{(-q^2x)^n q^{\binom{n}{2}}}{(q;q)_n (qy;q)_n}}{\sum_{n=0}^{\infty} \frac{(-qx)^n q^{\binom{n}{2}}}{(q;q)_n (qy;q)_n}} - 1\right)$$

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Statistical Physicist: So what? Can you please tell me $q_c(x, y)$?

A Puzzle

The full generating function is a quotient of q-series

$$G(x,y,q) = y\left(\frac{H(q^2x,qy,q)}{H(qx,qy,q)} - 1\right)$$

where

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

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However, the perimeter-generating function is algebraic

$$G(x,y,1) = [G(x,y,1)+x]\,[y+G(x,y,1)]$$

gives

$$G(x,y,1) = \frac{1-x-y}{2} - \sqrt{\left(\frac{1-x-y}{2}\right)^2 - xy}$$

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

Answer

We obtain

$$G(x, y, q) = \frac{1 - x - y}{2} + G^{sing}(x, y, q)$$

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

as $q \to 1$ with $x_t = 1/4$, $\gamma_t = -1/3$, and $\phi = 2/3$.

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as $q \to 1$ with $x_t = 1/4$, $\gamma_t = -1/3$, and $\phi = 2/3$. The scaling function $f(z)$ is obtained explicitly

$$f(z) = -4^{-2/3}\frac{\mathrm{Ai}'(4^{4/3}z)}{\mathrm{Ai}(4^{4/3}z)}$$

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$$f(z)=-4^{-2/3}\frac{\mathrm{Ai}'(4^{4/3}z)}{\mathrm{Ai}(4^{4/3}z)}$$

The limit $q\to 1$ is *uniform* near $x=x_t$

$$G(x,y,1)=\frac{1-x-y}{2}-\sqrt{\left(\frac{1-x-y}{2}\right)^2-xy}$$

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

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$$f(z) = -4^{-2/3}\frac{\mathrm{Ai}'(4^{4/3}z)}{\mathrm{Ai}(4^{4/3}z)}$$

The limit $q \to 1$ is *uniform* near $x = x_t$

$$G(x,y,1) = \frac{1-x-y}{2} - \sqrt{\left(\frac{1-x-y}{2}\right)^2 - xy}$$

Stronger than scaling limit

Sketch of Proof

We need to evaluate

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

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Standard Trick: write an alternating series as a contour integral

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

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Find suitable q-version for this trick

Contour Integral Representation

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

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Lemma

For complex x with $|\arg(x)| < \pi$, complex y with $y \neq q^{-n}$ for non-negative integer n, and $0 < q < 1$ we have for $0 < \rho < 1$

$$H(x,y,q) = \frac{1}{2\pi i} \frac{(q;q)_\infty}{(y;q)_\infty} \int_{\rho - i\infty}^{\rho + i\infty} \frac{(y/z;q)_\infty}{(z;q)_\infty} z^{-\frac{\log x}{\log q}} dz$$

Integral Asymptotics

Restrict to $0 < x, y, q < 1$ and write $\varepsilon = -\log q$. A careful approximation gives

Lemma

For $y < \rho < 1$,

$$H(x,y,q) = \frac{1}{2\pi i}\int_{\rho-i\infty}^{\rho+i\infty} e^{\frac{1}{\varepsilon}[\log(z)\log(x)+\mathrm{Li}_2(z)-\mathrm{Li}_2(y/z)]}\sqrt{\frac{1-y/z}{1-z}}dz \times e^{\frac{1}{\varepsilon}\left[\mathrm{Li}_2(y)-\frac{\pi^2}{6}\right]}\sqrt{\frac{2\pi}{\varepsilon(1-y)}}\,[1+O(\varepsilon)]$$

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This is a genuine Laplace-type integral

$$\int_{\mathcal{C}} e^{\frac{1}{\varepsilon}g(z)}f(z)dz$$

Saddle Point Analysis

The asymptotics of

$$\int_{\mathcal{C}} e^{\frac{1}{\varepsilon}g(z)} f(z) dz$$

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As d changes sign, the saddles coalesce

Coalescing Saddle Points

Reparametrize locally by a cubic $\Rightarrow$ normal form.

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Write

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$g(z_i) = u_i$ determines α and β:

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The transformation is one-to-one and analytic in a neighbourhood of $d = 0$.

Finally: Ai(x)

We substitute $z = z(u)$ into

$$I(\epsilon) = \int_{\mathcal{C}} e^{\frac{1}{\varepsilon}g(z)} f(z)dz = \int_{\mathcal{C}'} e^{\frac{1}{\varepsilon}g(z(u))} f(z(u))\frac{dz}{du}du$$

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The Main Lemma

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Lemma

Let $0 < x, y < 1$ *and* $q = e^{-\varepsilon}$ *for* $\varepsilon > 0$. *Then*

$$H(x,y,q) = \left[p_0 \varepsilon^{1/3} \mathrm{Ai}(\alpha \varepsilon^{-2/3}) + q_0 \varepsilon^{2/3} \mathrm{Ai}'(\alpha \varepsilon^{-2/3})\right]$$

$$\times e^{\frac{1}{\varepsilon}\left[\mathrm{Li}_2(y) - \frac{\pi^2}{6} + \log(x)\log(y)/2\right]} \sqrt{\frac{2\pi}{\varepsilon(1-y)}}\,[1 + O(\varepsilon)]$$

where

$$\frac{4}{3}\alpha^{3/2} = \log(x) \log \frac{z_1}{z_2} + 2\mathrm{Li}_2(z_1) - 2\mathrm{Li}_2(z_2)$$

and

$$p_0 = \left(\frac{\alpha}{d}\right)^{1/4} (1 - x - y)\,, \qquad q_0 = \left(\frac{d}{\alpha}\right)^{1/4} .$$

Asymptotics for Staircase Polygons

Theorem (TP)

Let $0 < x, y < 1$ *and* $q = e^{-\varepsilon}$ *for* $\varepsilon > 0$. *Then*

$$G(x,y,q) = \frac{1-x-y}{2} + \sqrt{\frac{(1-x-y)^2}{4} - xy}\,\frac{\mathrm{Ai}'(\alpha\varepsilon^{-2/3})}{\alpha^{1/2}\varepsilon^{-1/3}\mathrm{Ai}(\alpha\varepsilon^{-2/3})} \times [1 + O(\varepsilon)]$$

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$$\frac{4}{3}\alpha^{3/2} = \log(x)\log\frac{z_m - \sqrt{d}}{z_m + \sqrt{d}} + 2\mathrm{Li}_2(z_m - \sqrt{d}) - 2\mathrm{Li}_2(z_m + \sqrt{d})$$

and

$$z_{1,2} = z_m \pm \sqrt{d}\ , \quad z_m = \frac{1+y-x}{2} \quad \textit{and} \quad d = z_m^2 - y\ .$$

Brownian Motion

Langevin Equation for BM

- One-dimensional Brownian Motion with drift

$$\frac{dy(t)}{dt} = -u_d + \xi(t)$$

$\xi(t)$ zero mean white noise with $\langle \xi(t)\xi(t') \rangle = \delta(t - t')$

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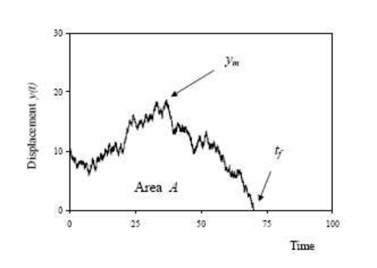
Area

$$A = \int_0^{t_f} y(\tau) d\tau$$



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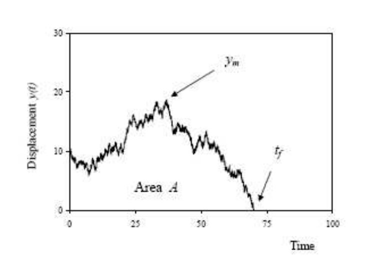

Compute probability distribution $P(A, y_0)$

Fokker-Planck approach

The Laplace transform $\tilde{P}(s, y_0) = \int_0^\infty P(A, y_0) e^{-sA} dA$ satisfies

$$\frac{1}{2} \frac{\partial^2 \tilde{P}(s, y_0)}{\partial y_0^2} - u_d \frac{\partial \tilde{P}(s, y_0)}{\partial y_0} - s y_0 \tilde{P}(s, y_0) = 0$$

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- Solution

$$\tilde{P}(s, y_0) = e^{u_d y_0} \frac{\mathrm{Ai}(2^{1/3} s^{1/3} y_0 + u_d^2 / [2^{2/3} s^{2/3}])}{\mathrm{Ai}(u_d^2 / [2^{2/3} s^{2/3}])}$$

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- Keep $z = u_d^2/[2^{2/3} s^{2/3}]$ fixed, let $u_d, s \to 0$ and expand in $u_d y_0$

$$\tilde{P}(s, y_0) = 1 + u_d y_0 - u_d y_0 z^{-1/2} F(z) + O[(u_d y_0)^2]$$

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$$F(z) = -\frac{\mathrm{Ai}'(z)}{\mathrm{Ai}(z)}$$

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- q-series solution
- contour integral
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Continuum models

- Brownian motion is well understood
- Connection with lattice models?

The End