Counting shared sites of three friendly directed lattice paths and related problems

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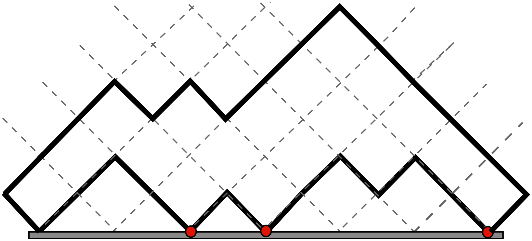
BIRS

DIRECTED WALKS LATTICE MODELS

- Simple lattice models of polymers in solution
- Interface of combinatorics, probability theory and statistical physics
- There are many exact solutions of single and multiple directed walkers
- Focus on the exact *generating function* for fixed number of walks
- Interactions are features of the configurations such as vertices of the walks shared with a wall or between two walks
- Interest is in adding multiple interactions for multiple walks: how many different properties can we count at the same time
- Counting different properties related to different statistical physics



EXACT SOLUTION OF DIRECTED LATTICE WALKS LATTICE

- Recurrence and functional equation for partition or generating function
- Rational, Algebraic, D-finite, D-algebraic generating functions
- non D-finite solutions (e.g. q-series) for generating functions
- Vicious walks are related to free fermions (lattice model)
- Six vertex model can be mapped to walks that touch (osculating)
- Bethe Ansatz & Lindström-Gessel-Viennot (LGV) Lemma
- LGV: multiple walks = determinant of single walks (partition functions)
- LGV problems result in generating functions that are D-finite

INTERACTING MODELS

- Previously, interactions applied to single walk of various types
- Multiple walks where interaction confined to a single walk
- Recently interactions between walks
- and/or multiple interactions have been considered
- These can give non-D-finite solutions

Vicious	No intersection
Osculating	Shared sites but not lattice bonds (touch or kiss)
Friendly	Shared sites and bonds

Some known exact solutions: geometries

No wall or interaction

- Many vicious directed walks: *Fisher* ('84), *Lindström-Gessel-Viennot Lemma* ('85), *Essam & Guttmann* ('95), *Guttmann*, *Owczarek & Viennot* ('98)
- Many friendly walks & Osculating walks: *Brak* ('97), *Guttmann & Vöge* ('02), *Bousquet-Mélou* ('06)

With wall but no interaction (LGV)

- Many vicious walks: *Krattenhaler, Guttmann & Viennot* ('00)

Single walk involved in interactions (recurrence, Bethe Ansatz, LGV):

- Two Vicious walks: with wall interactions *Brak, Essam & Owczarek* ('98)
- Many Vicious walks: with wall interactions *Brak, Essam & Owczarek* ('01)

Exact solutions: multiple walks and interactions

How can we extend the numbers of walks with complex and different types of interactions that can be solved exactly?

Inter-walk interactions using (obstinate) kernel method:

- Two Friendly walks: with both walks interacting with the wall *Owczarek, Rechnitzer & Wong* ('12)
- Two Friendly walks: with both wall and inter-walk interactions *Tabbara, Owczarek, Rechnitzer* ('14)
- Three Friendly walks: with two types of inter-walk interactions *Tabbara, Owczarek, Rechnitzer* ('16)

SO HOW DO WE FIND A SOLUTION: KERNEL METHOD

- Combinatorial decomposition of the set of walks
- Find a functional equation for an expanded generating function
- This leads to the use of extra catalytic variables
- Answer is a 'boundary' value
- Equation is written as "bulk = boundary terms"
- Bulk term is product of a rational kernel and bulk generating function
- Set the value of a catalytic variable to make the kernel vanish
- Origin of kernel method due to *Knuth* (1968)
- From $\approx$ early '00's applied to a number of dir. walk problems

Obstinate kernel method

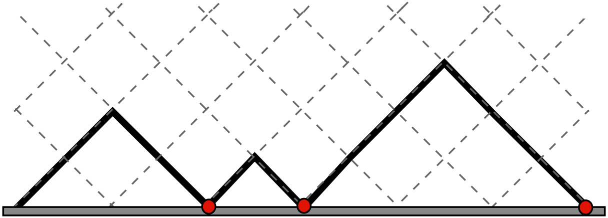
- Our problems have several catalytic variables
- Need multiple values of catalytic variables: obstinate kernel method
- Earliest combinatorial application due to *Bousquet-Mélou* ('02).
- Bousquet-Mélou *Math. and Comp. Sci 2* (2002)
- Bousquet-Mélou, Mishna *Contemp. Math.* **520** (2010)
- Solutions are not always D-finite
- Quarter plane random walk problems
- Diagonals of multi-variate rational functions

Polymer Adsorption: one directed walk

The physical motivation is the adsorption phase transition

Exact solution and analysis of single and multiple directed walk models exist

- Single Dyck path, $\widehat{\varphi}$, in a half space
- Energy $-\varepsilon_a$ for each time (number m_a) it visits the surface
- Boltzmann weight (counting variable) $a = e^{\varepsilon_a / k_B T}$
- Partition function $Z_n(a) = \sum_{|\widehat{\varphi}|=n} a^{m_a(\widehat{\varphi})}$
- Generating function: $G(a; z) = \sum_{n=0}^{\infty} Z_n(a)\, z^n$



ADSORPTION: ONE DIRECTED WALK

A complete solution exists and the generating function is algebraic

The thermodynamic reduced free energy:

$$\kappa(a) = \lim_{n\to\infty} n^{-1} \log\left(Z_n(a)\right).$$

is known exactly from location of closest singularity to the origin of generating function:

$$\kappa(a) = \log(z_c(a)^{-1}).$$

It has a single non-analytic point —- that is, a phase transition.

Adsorption transition charactisation

Consider the density of visits (derivative of the free energy)

$$\mathcal{A}(a) = \lim_{n\to\infty} \frac{\langle m_a \rangle}{n}$$

There exists a phase transition at a temperature T_a given by $a = 2$:

- For $T > T_a$ ($a < 2$) the walk moves away entropically and $\mathcal{A}(a) = 0$
- For $T < T_a$ ($a > 2$) the walk is adsorbed onto the surface and $\mathcal{A}(a) > 0$

- *Second order phase transition with jump in second derivative of the free energy*
- *Order parameter is density of visits to surface by the polymer*

Double Interaction Adsorption Model

Motivation arising from Monte Carlo studies of ring polymers in slits in two dimensions

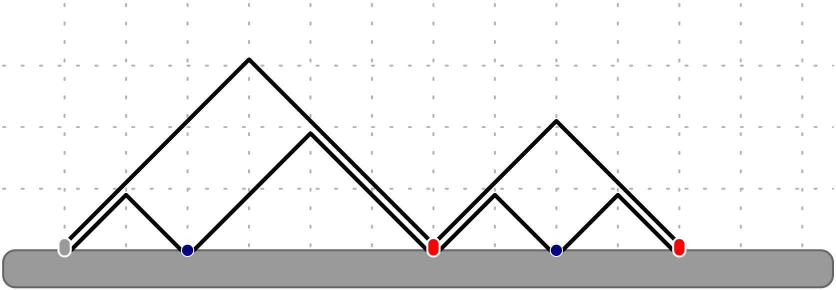


Figure: Two directed walks with single and "double" visits to the the surface.

- *energy $-\varepsilon_a$ for visits of the bottom walk only (single visits) to the wall,*
- *energy $-\varepsilon_d$ when both walks visit a site on the wall (double visits)*

MODEL

- number of *single visits* to the wall will be denoted m_a,
- number of *double visits* will be denoted m_d.

The partition function:

$$Z_n(a, d) = \sum_{\widehat{\varphi} \ni |\widehat{\varphi}|=n} e^{(m_a(\widehat{\varphi})\cdot\varepsilon_a + m_d(\widehat{\varphi})\cdot\varepsilon_d)/k_B T}$$

where $a = e^{\varepsilon_a/k_B T}$ and $d = e^{\varepsilon_d/k_B T}$.

The thermodynamic reduced free energy:

$$\kappa(a, d) = \lim_{n\to\infty} n^{-1} \log\left(Z_n(a, d)\right).$$

Generating Function

To find the free energy we will instead solve for the generating function

$$G(a,d;z) = \sum_{n=0}^{\infty} Z_n(a,d) z^n.$$

The radius of convergence of the generating function $z_c(a,d)$ is directly related to the free energy via

$$\kappa(a,d) = \log(z_c(a,d)^{-1}).$$

Two order parameters:

$$\mathcal{A}(a,d) = \lim_{n\to\infty} \frac{\langle m_a \rangle}{n} \qquad \text{and} \qquad \mathcal{D}(a,d) = \lim_{n\to\infty} \frac{\langle m_d \rangle}{n},$$

FUNCTIONAL EQUATION

We consider walks φ in the larger set, where each walk can end at any possible height.

The expanded generating function

$$F(r,s;z) \equiv F(r,s) = \sum_{\varphi\in\Omega} z^{|\varphi|} r^{\lfloor\varphi\rfloor} s^{\lceil\varphi\rceil/2} a^{m_a(\varphi)} d^{m_d(\varphi)},$$

where

- z is conjugate to the length $|\varphi|$ of the walk,
- r is conjugate to the distance $\lfloor\varphi\rfloor$ of the bottom walk from the wall and
- s is conjugate to *half* the distance $\lceil\varphi\rceil$ between the final vertices of the two walks.

and we recover $G(a,d;z) = F(0,0)$.

Functional equation

Consider adding steps onto the ends of the two walks

This gives the following functional equation

$$\begin{aligned} F(r,s) =& 1 + z\left(r + \frac{1}{r} + \frac{s}{r} + \frac{r}{s}\right) \cdot F(r,s) \\ & - z\left(\frac{1}{r} + \frac{s}{r}\right) \cdot [r^0]F(r,s) - z\frac{r}{s} \cdot [s^0]F(r,s) \\ & + z(a-1)(1+s) \cdot [r^1]F(r,s) + z(d-a) \cdot [r^1 s^0]F(r,s). \end{aligned}$$

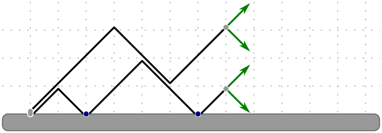


Figure: Adding steps to the walks when the walks are away from the wall.

THE KERNEL

Rewrite equation as "Bulk = Boundary"

$$K(r,s)\cdot F(r,s)=\frac{1}{d}+\left(1-\frac{1}{a}-\frac{zs}{r}-\frac{z}{r}\right)\cdot F(0,s)-\frac{zr}{s}\cdot F(r,0)+\left(\frac{1}{a}-\frac{1}{d}\right)\cdot F(0,0)$$

where the *kernel* K is

$$K(r,s)=\left[1-z\left(r+\frac{1}{r}+\frac{s}{r}+\frac{r}{s}\right)\right].$$

Recall, we want $F(0,0)$ so we try to find values that kill the kernel

Symmetries of the Kernel

The kernel is symmetric under the following two transformations:

$$(r,s) \mapsto \left(r, \frac{r^2}{s}\right), \qquad (r,s) \mapsto \left(\frac{s}{r}, s\right)$$

Transformations generate a family of 8 symmetries ('group of the walk')

$$(r,s), \left(r, \frac{r^2}{s}\right), \left(\frac{s}{r}, \frac{s}{r^2}\right), \left(\frac{r}{s}, \frac{1}{s}\right), \left(\frac{1}{r}, \frac{1}{s}\right), \left(\frac{1}{r}, \frac{s}{r^2}\right), \left(\frac{r}{s}, \frac{r^2}{s}\right), \text{ and } \left(\frac{s}{r}, s\right)$$

We make use of 4 of these which only involve positive powers of r.

This gives us four equations - this is the "half-orbit" sum methodology.

Magic combination

Following Bousquet-Mélou when $a = 1$ we form the simple alternating sum

$$Eqn1 - Eqn\ 2 + Eqn\ 3 - Eqn\ 4.$$

- When $a \neq 1$ one needs to generalise that approach
- Multiply by rational functions,

The form of the Left-hand side of the final equation being

$$a^2 rK(r,s)\left(sF(r,s) - \frac{r^2}{s}F\left(r,\frac{r^2}{s}\right) + \frac{Lr^2}{s^2}F\left(\frac{r}{s},\frac{r^2}{s}\right) - \frac{L}{s^2}F\left(\frac{r}{s},\frac{1}{s}\right)\right)$$

where

$$L = \frac{zas - ars + rs + zar^2}{zas - ar + r + zar^2}.$$

EXTRACTING THE SOLUTION $a = 1$

$$K(r,s) \cdot (\text{linear combination of } F) = \frac{r(s-1)(s^2+s+1-r^2)}{s^2}\,(1+(d-1)F(0,0)) - zd(1+s)sF(0,s) + \frac{zd(1+s)}{s^2}F\left(0,\frac{1}{s}\right).$$

- The kernel has two roots
- choose the one which gives a positive term power series expansion in z
- with Laurent polynomial coefficients in s:

$$\hat{r}(s;z) \equiv \hat{r} = \frac{s\left(1-\sqrt{1-4\frac{(1+s)^2z^2}{s}}\right)}{2(1+s)z} = \sum_{n\geq 0} C_n \frac{(1+s)^{2n+1}z^{2n+1}}{s^n},$$

where $C_n = \frac{1}{n+1}\binom{2n}{n}$ is a Catalan number.

EXTRACTING THE SOLUTION $a = 1$

- *Make the substitution* $r \mapsto \hat{r}$
- *rewrite to remove* z*:* $z = (\hat{r} + 1/\hat{r} + \hat{r}/s + s/\hat{r})^{-1}$.

Setting $r \mapsto \hat{r}$ gives

$$0 = ds^4 F(0,s) - dsF\left(0, \frac{1}{s}\right) - (s-1)(s^2+s+1-\hat{r}^2)(s+\hat{r}^2)\left(1+(d-1)F(0,0)\right)$$

Note coefficients of $F(0,s)$ and $F(0,1/s)$ are independent of $\hat{r}$.

If we divide by equation by s *— then* $F(0,0)$ *is the constant term in* s*.*

SOLUTION FOR $a = 1$

Now extract the coefficient of s^1:

$$0 = -\left(1 + \sum_{n=0}^{\infty} \frac{12(2n+1)}{(n+2)^2(n+3)} C_n^2 z^{2n+2}\right) \cdot (1 + (d-1)F(0,0)) - d \cdot F(0,0).$$

Solving the above when $d = 1$ gives

$$G(1,1;z) = 1 + \sum_{n=0}^{\infty} \frac{12(2n+1)}{(n+2)^2(n+3)} C_n^2 z^{2n+2},$$

and hence for general d we have

$$F(0,0) = G(1,d;z) = \frac{G(1,1;z)}{d + (1-d)G(1,1;z)}.$$

$a = d$

Need to extract coefficients term by term in a to give

$$[a^k z^{2n}]F(0,0) = \sum_{k'=0}^{k} \frac{k'(k'+1)(2+4n-k'n-2k')}{(k'-1-n)(n+1)^2(-2n+k')(n+2)} \binom{2n-k'}{n}\binom{2n}{n}$$
$$= \frac{k(k+1)(k+2)}{(2n-k)(n+1)^2(n+2)} \binom{2n-k}{n}\binom{2n}{n}$$

which gives us

$$G(a,a) = \sum_{n\geq 0} z^{2n} \sum_{k=0}^{n} a^k \frac{k(k+1)(k+2)}{(n+1)^2(n+2)(2n-k)} \binom{2n}{n}\binom{2n-k}{n}.$$

Agrees with Brak *et al.* (1998) that used LGV

One can now consider $d \neq a$:

$$G(a,d;z) = \frac{aG(a,a;z)}{d+(a-d)G(a,a;z)}.$$

Combinatorial structure

- Combinatorial structure in the underlying the functional equation.
- Breaking up our configurations into pieces between double visits gives

$$G(a,d;z) = \frac{1}{1 - dP(a;z)}$$

where $P(a;z)$ is the generating function of so-called primitive factors or pieces.

- Rearranging this expression gives

$$P(a;z) = \frac{G(a,d;z) - 1}{dG(a,d;z)} = \frac{G(a,a;z) - 1}{aG(a,a;z)}.$$

- This allows us to calculate $P(a;z)$ from a known expression for $G(a,a;z)$

PHASES

The phases determined by dominant singularity of the generating function

The singularities of $G(a, d; z)$ are

- *those of $P(a; z)$ which are related to those of $G(a, a; z)$ and*
- *the simple pole at $1 - dP(a; z) = 0$.*

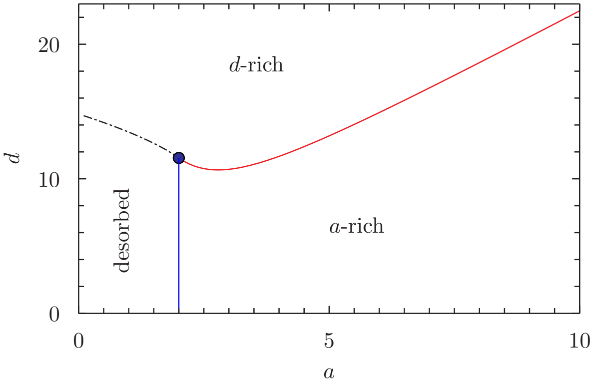
There are two singularities of $G(a, a; z)$ giving rise to two phases:

- A desorbed phase: $\mathcal{A} = \mathcal{D} = 0$
- The bottom walk is adsorbed (an a-rich phase): $\mathcal{A} > 0$ with $\mathcal{D} = 0$

The simple pole in $1 - dP(a; z) = 0$ gives rise to the third phase

- Both walks are adsorbed and this is a d-rich phase: $\mathcal{D} > 0$, and $\mathcal{A} > 0$

PHASE DIAGRAM



The first-order transition is marked with a dashed line, while the two second-order transitions are marked with solid lines. The three boundaries meet at the point $(a, d) = (a^*, d^*) = (2, 11.55\dots)$.

Phase transitions

- The Desorbed to a-rich transition is
  - the standard second order adsorption transition
  - on the line $a = 2$ for $d < d^*$
- On the other hand the Desorbed to d-rich transition is first order
- While the a-rich to d-rich transition is also second order.

The other two phase boundaries are solutions to equations involving $G(a, a)$

The point where the three phase boundaries meet can be computed as

$$(a^*, d^*) = \left(2, \frac{16(8 - 3\pi)}{64 - 21\pi}\right)$$

Note that d^* is not algebraic.

NATURE OF THE SOLUTION

Desorbed to d-rich transition occurs at a value of $d_c(a)$ for $a < 2$.
We found

$$d_c(1) = \frac{8(512 - 165\pi)}{4096 - 1305\pi}$$

which is not algebraic.

- *If generating function were D-finite then $d_c(1)$ must be algebraic*
- *Hence generating function is not D-finite*
- *though it is calculated in terms of one.*

DOUBLE INTERACTION MODEL SUMMARY

- Vesicle above a surface — both sides of the vesicle can interact
- Exact solution of generating function
- Obstinate kernel method with a minor generalisation
- Solution is not D-finite — LGV lemma does not apply directly
- There are two low temperature phases
- Line of first order transition and usual second order adsorption.
- Owczarek, Rechnitzer, and Wong, *J. Phys. A*, 45 425002, (2012)

UNZIPPING ADSORPTION MODEL OF DNA DENATURATION

Simple model of DNA as two friendly walks near a boundary

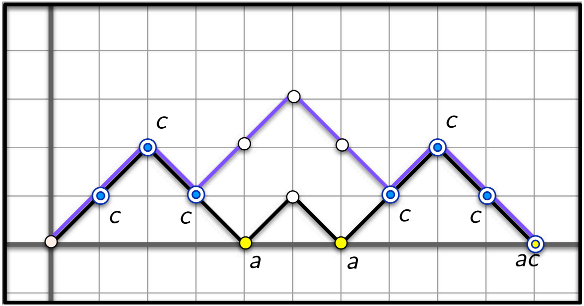


Figure: An allowed configuration of length 10. The overall weight is a^3c^7

- *a is a fugacity for each single visit to the wall*
- *c is a fugacity for each contact of the two walks to site*

Unzipping Adsorption Model

Let T be the system temperature, k_B the Boltzmann constant.

- surface visit step: $a \equiv e^{\varepsilon_a/k_B T}$
- shared site contact: $c \equiv e^{\varepsilon_c/k_B T}$

- *Energy $-\varepsilon_a$ for visits of the bottom walk only (single visits) to the wall*
- *Energy $-\varepsilon_c$ when both walks visit the same site (contacts)*

The partition function is

$$Z_n(a,c) = \sum_{\widehat{\varphi} \ni |\widehat{\varphi}|=n} a^{m_a(\widehat{\varphi})} c^{m_c(\widehat{\varphi})}$$

- *number of visits to the wall denoted m_a,*
- *number of joint contacts denoted m_c.*

Generating function

- Partition function: $Z_n(a,c) = \sum_{\hat{\varphi} \ni |\hat{\varphi}|=n} a^{m_a(\hat{\varphi})} c^{m_c(\hat{\varphi})}$
- Generating function: $G(a,c) \equiv G(a,c;z) = \sum_{n\geq 1} Z_n(a,c) z^n$
- Reduced free energy:

$$\kappa(a,c) = \lim_{n\to\infty} n^{-1} \log Z_n(a,c) = \log z_s(a,c)$$

where $z_s(a,c)$ is dominant singularity of G w.r.t. z

Two order parameters:

$$\mathcal{A}(a,c) = \lim_{n\to\infty} \frac{\langle m_a \rangle}{n} \qquad \text{and} \qquad \mathcal{C}(a,c) = \lim_{n\to\infty} \frac{\langle m_c \rangle}{n},$$

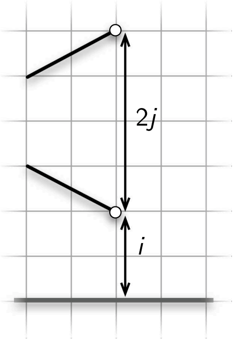
GENERALISED GENERATING FUNCTION

We consider walks φ in the larger set, where each walk can end at any possible height.

- To find $G(a, c)$, consider larger class of configs.
- Generalised generating function:

$$F(r, s) \equiv F(r, s, a, c; z) = \sum_{\varphi \in \Omega} a^{m_a(\varphi)} c^{m_c(\varphi)} r^i s^j z^n$$

- $G(a, c) = F(0, 0)$



Establishing a functional equation

- By considering the addition of a single column onto a configuration, and the types of walks obtained, we can find a decomposition of all configurations
- Translating back to generating functions we end up with

$$K(r,s)F(r,s) = \frac{1}{ac} + \left(\frac{c-1}{c} - \frac{zr}{s}\right) F(r,0) + \left[\frac{a-1}{a} - \frac{z}{r}(s+1)\right] F(0,s) - \frac{(a-1)}{a}\frac{(c-1)}{c} F(0,0)$$

where the kernel $K(r,s)$ is

$$K(r,s) \equiv K(r,s;z) = \left(1 - z\left[r + \frac{s}{r} + \frac{r}{s} + \frac{1}{r}\right]\right).$$

Symmetries of the Kernel

The kernel is symmetric under the following two transformations, which are involutions:

$$(r, s) \mapsto \left(r, \frac{r^2}{s}\right), \qquad (r, s) \mapsto \left(\frac{s}{r}, s\right)$$

Transformations generate a family of 8 symmetries ('group of the walk')

$$(r, s), \left(r, \frac{r^2}{s}\right), \left(\frac{s}{r}, \frac{s}{r^2}\right), \left(\frac{r}{s}, \frac{1}{s}\right), \left(\frac{1}{r}, \frac{1}{s}\right), \left(\frac{1}{r}, \frac{s}{r^2}\right), \left(\frac{r}{s}, \frac{r^2}{s}\right), \text{ and } \left(\frac{s}{r}, s\right)$$

- *Use "half-orbit" sum methodology*
- *We make use of four of these which only involve positive powers of r.*
- *This gives us four equations.*
- *One can eliminate many of the unknown generating functions by a clever choice of adding these equations*

Roots of the Kernel

- The kernel has two roots as function of either r or s
- choose the one which gives a positive term power series expansion in z
- with Laurent polynomial coefficients in s (r):

$$\hat{r}(s;z) \equiv \hat{r} = \frac{s\left(1-\sqrt{1-4\frac{(1+s)^2z^2}{s}}\right)}{2(1+s)z} = \sum_{n\geq 0} C_n \frac{(1+s)^{2n+1}z^{2n+1}}{s^n},$$

where $C_n = \frac{1}{n+1}\binom{2n}{n}$ is a Catalan number.

- *Make the substitution* $r \mapsto \hat{r}$

Finding the solution

Key idea

- Treat K as fn. of r or s to get roots $\hat{r}$ and $\hat{s}$
- Then use subset of $\mathcal{F}$ to get system of eqns. E.g. Using $\hat{r}$:

$(\hat{r}, s)$	$F(\hat{r}, 0)$	$F(0, s)$	$F(0, 0)$
$(\hat{r}, \hat{r}^2/s)$	$F(\hat{r}, 0)$	$F(0, \hat{r}^2/s)$	$F(0, 0)$
$(\hat{r}/s, \hat{r}^2/s)$	$F(\hat{r}/s, 0)$	$F(0, \hat{r}^2/s)$	$F(0, 0)$
$(\hat{r}/s, 1/s)$	$F(\hat{r}/s, 0)$	$F(0, 1/s)$	$F(0, 0)$

- Combine these eqns. to get new fn. eqn

$$N_1^\star(s;z)F(0,1/s)+N_2^\star(s;z)F(0,s) = \left[M^\star(s) - c^2H^\star(s;z)\right]\left(\frac{1}{ac} - ACF(0,0)\right),$$

- Can do the same using $\hat{s}$!
- Nice things happen when $a = 1$ or $c = 1$ to $N_1^\star(s;z)$ etc

Solution for $G(a, 1)$

Exact solution for $G(a, 1)$ is known and can be found using the kernel method
In fact, the exact solution for $G(a, 1)$ is known from first part of talk!

- Brak, Essam & Owczarek (1998, 2001): Partition fn. using Lindström-Gessel-Viennot Thm.
- Owczarek, Rechnitzer & Wong (2012): Gen. fn calculated by employing same kernel method techniques.

Specifically:

$$G(a,1) = \sum_{n\geq 0} z^{2n} \sum_{k=0}^{n} a^k \frac{k(k+1)(k+2)}{(2n-k)(n+1)^2(n+2)} \binom{2n-k}{n} \binom{2n}{n}.$$

Solution for $G(1,c)$

- No known previous solution for $G(1,c)$

We can write functional equation as

$$G(1,c) = [r^1]\frac{\hat{s}\left(r^2-1\right)\left[r-cr+cz\left(1+r^2-\hat{s}\right)\right]}{(c-1)\left(\hat{s}-c\hat{s}+crz\right)},$$

where $\hat{s}(r)$ is the appropriate root of the kernel, expanding RHS as power series in c and so obtain, after some work:

$$G(1,c;z) = 1 + c^2z^2 + c^3\left(1+2z\right)z^4$$
$$+\sum_{i=3}^{\infty} z^{2i}\sum_{m=3}^{2i} c^m \sum_{k=3}^{m}(-1)^{k+1}\frac{k(k-1)(k-2)(2i-k+1)(i-k+2)}{i^2(i-1)^2(i+1)(i-2)}\binom{m}{k}\binom{2i-k}{i-2}\binom{2i-k-1}{i-3}.$$

SOLUTION FOR $G(1, c)$

- While we have an explicit solution for $G(1, c)$ it is advantageous for analysis to directly read off the singularities
- Alternative — find differential equation satisfied by generating function
- Use Zeilberger-Gosper algorithm: Maple: DETools package, Zeilberger hyperexp. implementation
- Result: DE for $G(1, c)$ is order 6 with poly. coeff of $\deg_z = 12$

Fortunate decomposition of $G(a, c)$

Using various combinatorial relationships between the generating functions we can re-write $G(a, c)$ in terms of $G(a, 1)$ and $G(1, c)$:

$$G(a,c) = \frac{1}{(a-1)(c-1)} + \frac{p_1(a,c,z)}{p_2(a,c,z) + p_3(a,c,z)G(a,1) + p_4(a,c,z)G(1,c)}$$

where p_i are polynomials in a, c and z: quadratics in z^2.

Key point: With solutions to $G(a, 1)$ and $G(1, c)$ we additionally have solved for $G(a, c)$.

SINGULARITIES OF $G(a,1)$ & $G(1,c)$

- Recall, free energy $\kappa(a,c) = \log z_s(a,c)$
- For $G(a,1)$, prev. known:

$$z_s(a,1) = \begin{cases} z_b \equiv 1/4, & a \leq 2 \\ z_a \equiv \frac{\sqrt{a-1}}{2a}, & a > 2 \end{cases}$$

- For $G(1,c)$, we use the DE (roots of leading poly. coeff.):

$$z_s(1,c) = \begin{cases} z_b \equiv 1/4, & c \leq 4/3 \\ z_c \equiv \frac{1-c+\sqrt{c^2-c}}{c}, & c > 4/3 \end{cases}$$

Recall Order parameters

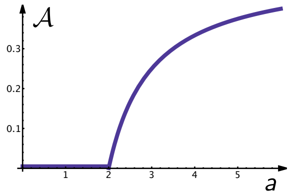
Recall lim. avg. surface and shared site contacts resp.

$$\mathcal{A}(a,c) = \lim_{n\to\infty} \frac{\langle m_a \rangle}{n} = a\frac{\partial \kappa}{\partial a}, \qquad \mathcal{C}(a,c) = \lim_{n\to\infty} \frac{\langle m_c \rangle}{n} = c\frac{\partial \kappa}{\partial c}$$

Transitions of $G(a,1)$ & $G(1,c)$

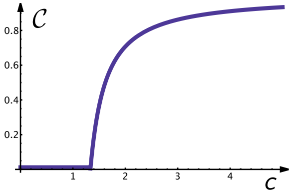
- For $G(a,1)$: the order parameter associated with the phase transition is the surface coverage

$$\mathcal{A}(a,1) = \begin{cases} 0, & a \le 2 \\ \frac{a-2}{2(a-1)}, & a > 2 \end{cases}$$



- For $G(1,c)$: the order parameter associated with the phase transition is the shared site density

$$\mathcal{C}(1,c) = \begin{cases} 0, & c \le 4/3 \\ \frac{c-2+\sqrt{c(c-1)}}{2(c-1)}, & c > 4/3 \end{cases}$$



- Second-order adsorption and zipping phase trans. resp.

SINGULARITIES AND PHASES

This leads us to associate the singularities of $G(a,1)$ and $G(1,c)$ with the phases as

- $z_b = 1/4$ with a desorbed phase where $\mathcal{A} = 0$ and $\mathcal{C} = 0$
- $z_a = \frac{\sqrt{a-1}}{2a}$ with an adsorbed phase where $\mathcal{A} > 0$
- $z_c = \frac{1-c+\sqrt{c^2-c}}{c}$ with a zipped phase where $\mathcal{C} > 0$

ORDER PARAMETERS FOR THE FULL MODEL

Four possible phases:

- Desorbed: $\mathcal{A} = \mathcal{C} = 0$
- Adsorbed: (a-rich) $\mathcal{A} > 0, \mathcal{C} = 0$
- Zipped: (c-rich) $\mathcal{A} = 0, \mathcal{C} > 0$
- Zipped & Adsorbed: (ac-rich) $\mathcal{A} > 0, \mathcal{C} > 0$

Analysing $G(a, c)$

Recall

$$G(a,c) \sim \frac{p_1(a,c,z)}{p_2(a,c,z) + p_3(a,c,z)G(a,1) + p_4(a,c,z)G(1,c)}$$

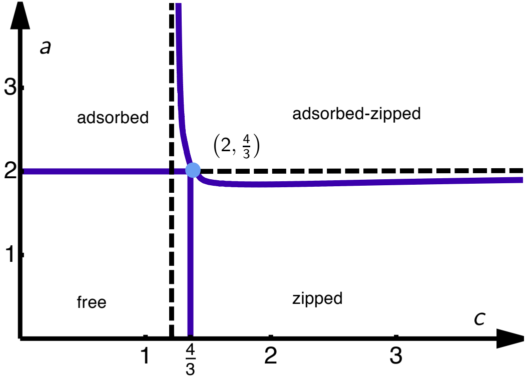
- $\Rightarrow$ Singularities: Look at $G(a,1)$, $G(1,c)$ and root of above denom.
- root of denominator is associated with the zipped-adsorbed phase

The dominant singularity $z_s(a,c)$ of the generating function $G(a,c;z)$ is one of four types associated with the four phases

$$z_s(a,c) = \begin{cases} z_b \equiv 1/4, & a \le 2, c \le 4/3 \\ z_a(a) \equiv \frac{\sqrt{a-1}}{2a}, & a > 2, c \le \alpha(a) \\ z_c(c) \equiv \frac{1-c+\sqrt{c^2-c}}{c}, & a \le \gamma(c), c > 4/3 \\ z_{ac}(a,c), & a > \gamma(c), c > \alpha(a) \end{cases}$$

- $\alpha(a)$ is boundary between adsorbed and zipped-adsorbed phases
- $\gamma(c)$ is the boundary between zipped and zipped-adsorbed phases

PHASE DIAGRAM



All transitions found to be second order

Low-temp argument gives

- $c \to \infty, \gamma(c) \to 2$
- $a \to \infty, \alpha(a) \to \sqrt{5} - 1$

ASYMPTOTICS

Table: The growth rates of the coefficients $Z_n(a,c)$ modulo the amplitudes of the full generating function $G(a,c;z)$ over the entire phase space.

phase region	$Z_n(a,c) \sim$
free	$4^n n^{-5}$
free to adsorbed boundary	$4^n n^{-3}$
free to zipped boundary	$4^n n^{-3}$
$a = 2, c = 4/3$	$4^n n^{-3}$
adsorbed	$z_a(a)^{-n} n^{-3/2}$
zipped	$z_c(c)^{-n} n^{-3/2}$
adsorbed to adsorbed-zipped boundary ($\alpha(a)$)	$z_a(c)^{-n} n^{-1/2}$
zipped to adsorbed-zipped boundary ($\gamma(c)$)	$z_c(c)^{-n} n^{-1/2}$
adsorbed-zipped	$z_{ac}(a,c)^{-n}$

UNZIPPING SUMMARY

- Simple model of DNA as two friendly walks near a boundary
- Used combinatorial decomposition to obtain linear functional equation
- Used obstinate kernel method to solve functional equations (using symmetries to provide sufficient information)
- Explicit series solutions for $G(a, 1)$ and $G(1, c)$
- Combined these equations to relate $G(a, c)$ to both $G(a, 1)$ and $G(1, c)$
- Also used Zeilberger-Gosper algorithm to find linear DE for $G(1, c)$
- Full analysis of asymptotics and phase diagram
- R. Tabbara, A. L. Owczarek and A. Rechnitzer, *J. Phys. A.: Math. Theor*, **47**, 015202 (34pp), 2014

Three walks and gelation interactions: two types

Model set of polymers in solution that can attract each other — finite gelation

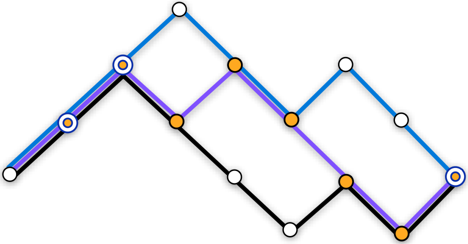


Figure: An example of an allowed configuration of length $n = 8$. Here, we have $m_c = 11$ double shared sites and $m_d = 3$ triple shared sites. Thus, the overall Boltzmann weight for this configuration is $c^{11}d^3 = c^5t^3$

THREE WALKS AND GELATION INTERACTIONS: TWO TYPES

Model set of polymers in solution that can attract each other — finite gelation

- **Start with three walks in the "bulk" (no walls) with interactions**

- double visits fugacity: c and triple visits fugacity: d
- total weight for triple visits: $t = c^2 d$
- Walks start and end together

- *m_c is the number of double contacts between pairs of walks*
- *m_d is the number of triple contacts between all three walks*

- Partition function: $Z_n(c,d) = \sum_{\varphi \in \widehat{\Omega}, |\varphi|=n} c^{m_c(\varphi)} d^{m_d(\varphi)}$
- Generating function: $G(c,d) \equiv G(c,d;z) = \sum_{n \geq 1} Z_n(c,d) z^n$

Primitive pieces

- Primitive walks [$P(c; z)$] only have triple visits at either end
- Any walk can be uniquely decomposed into a sequence of primitive pieces:

$$G(c, d; z) = \frac{1}{1 - dP(c; z)}$$

$$G(c, d; z) = \frac{G(c, 1; z)}{d\left[1 - G(c, 1; z)\right] + G(c, 1; z)}.$$

Hence it suffices to solve for $G(c, 1; z)$

GENERALISED GENERATING FUNCTION

We consider walks in a larger set, where they do not necessarily end together.

- Generalised generating function:

$$F(r,s) \equiv F(r,s,c;z) = \sum_{\varphi \in \widehat{\Omega}} r^{h(\varphi)/2} s^{f(\varphi)/2} c^{m_c(\varphi)} z^{|\varphi|}$$

- $G(c,1) = F(0,0)$
- where $h(\varphi)$ and $f(\varphi)$ are *half* the distance between the final vertices of the top to middle and middle to bottom walks respectively.

Establishing a functional equation

The decomposition of the set of walks gives

$$K(r,s)F(r,s) = \frac{1}{c^2} - \frac{(r - cr + cz + csz)}{cr}F(0,s) - \frac{(s - cs + cz + crz)}{cs}F(r,0) - \frac{(c-1)^2}{c^2}F(0,0)$$

where the kernel $K(r,s)$ is

$$K(r,s) \equiv K(r,s;z) = 1 - \frac{z(r+1)(s+1)(r+s)}{rs}.$$

SYMMETRIES OF THE KERNEL

The kernel $K(r, s)$ is

$$K(r,s) \equiv K(r,s;z) = 1 - \frac{z(r+1)(s+1)(r+s)}{rs}.$$

The kernel is symmetric under the following two transformations, which are involutions:

$$(r,s) \mapsto (s,r)\,, \qquad\qquad (r,s) \mapsto \left(r, \frac{r}{s}\right)$$

Transformations generate a family of 12 symmetries ('group of the walk')

$$(r,s), (s,r), \left(r,\frac{r}{s}\right), \left(s,\frac{s}{r}\right), \left(\frac{r}{s},r\right), \left(\frac{s}{r},s\right), \left(\frac{r}{s},\frac{1}{s}\right), \left(\frac{s}{r},\frac{1}{r}\right),$$
$$\left(\frac{1}{s},\frac{r}{s}\right), \left(\frac{1}{r},\frac{s}{r}\right), \left(\frac{1}{r},\frac{1}{s}\right), \left(\frac{1}{s},\frac{1}{r}\right).$$

- *Proceed in a similar way to previously*

USING THE SYMMETRIES

- *Again use half-orbit summary methodology*
- *We make use of the symmetries of the kernel to produce multiple equations making sure we have either only positive powers of r or s.*
- *Re-combine to leave only say $F(0,0)$, $F(1/s,0)$ and $F(0,s)$*

$$N_1(s;z)F\left(1/s,0\right)+N_2(s;z)F(0,s)+N_3(s;z)\left[(c-1)^2F(0,0)-1\right]=0$$

where N_j can be considered simple polynomials of $\hat{r}$, s and z.

- *Note also that $F(s,0)=F(0,s)$ because of vertical symmetry.*
- *N_1/N_2 is actually a rational function of s and z*

Roots of the Kernel

- *Substitute root of the kernel*
- *Use Lagrange inversion to find answer term-by-term*

- The kernel has two roots as function of either r or s
- choose the one which gives a positive term power series expansion in z
- with Laurent polynomial coefficients in s (r):

$$\hat{r}_{\pm}(s;z) = \frac{s - z\left(s^2+2s+1\right) \pm \sqrt{s^2 - 2zs(1+s)^2 + z^2\left(s^2-1\right)^2}}{2z(s+1)}$$

Lagrange Inversion gives us

$$\hat{r}(s;z)^k = \sum_{n\geq k} \frac{k}{n} z^n (1+s)^n \sum_{j=k}^{n} \binom{n}{j}\binom{n}{j-k} s^{j-n}$$

SOLUTION FOR $G(c,1)$

$$G(c,1;z) = \frac{1}{(c-1)^2}\left(1 + \frac{c\left(c^2z + c^2 - 3c\right)\sqrt{1-4cz}}{G_b(c,1;z)}\right)$$

where

$$\begin{aligned} G_b(c,1;z) &= -1 - c^2z - c^3z + c(2z+1) \\ &\quad + \sqrt{1-4cz}\left[-cz + c^2z - c^3z + \left(-2c^2z + 2c^3z\right) J(c;z)\right]. \end{aligned}$$

and

$$\begin{aligned} J(c;z) = \sum_{i\geq 3} z^i \sum_{m=1}^{i-1} c^m \sum_{k=1}^{i-m-1} \binom{m}{k} \sum_{j=k}^{i-m-1} &\left\{ \frac{k}{i-m-1}\binom{i-m-1}{j}\binom{i-m-1}{j-k} \right. \\ &\left[\binom{m+i-k}{i-j} + \binom{m+i-k}{i-j-2}\right] \\ &\left. - \frac{k}{i-m}\binom{i-m}{j}\binom{i-m}{j-k}\binom{m+i-k-1}{i-j-1} \right\} \\ &- \sum_{i\geq 2} z^i \sum_{m=1}^{i-1} c^m \sum_{k=1}^{i-m} \binom{m}{k} \frac{k}{i-m}\binom{i-m}{i-k-m}\binom{m+i-k-1}{m-1} \end{aligned}$$

DE FOR $G(c, 1)$

- While we have an explicit solution for $G(c, 1)$ it is advantageous for analysis to directly read off the singularities
- Alternative — find differential equation satisfied by generating function
- Use Zeilberger-Gosper algorithm: Maple: DETools package, Zeilberger hyperexp. implementation
- Result: DE for $G(c, 1)$ is order 7 with poly. coeff of $\deg_z = 26$

COEFFICIENT

Appendix A. $J(c,z)$: Leading coefficient of the differential equation

The following is the leading polynomial coefficient of the linear homogeneous differential equation (55) satisfied by the generating function $J(c;z)$.

$$
\begin{aligned}
&-2(-1+c)^{15}\left(2-10c+5c^2\right)z^3-(-1+c)^{13}\left(-39+161c+5c^2-222c^3+100c^4+10c^5\right)z^4\\
&+(-1+c)^{12}\left(37+868c-4988c^2+6268c^3-2741c^4+1048c^5-894c^6+276c^7\right)z^5\\
&-(-1+c)^{11}\left(144-2972c+5580c^2+25430c^3-54470c^4+30904c^5-6709c^6+5072c^7-2974c^8+340c^9\right)z^6\\
&+(-1+c)^{10}\left(64-4392c+50474c^2-199461c^3+206342c^4-40697c^5+80412c^6-165265c^7+79458c^8-4196c^9-2640c^{10}+144c^{11}\right)z^7\\
&+(-1+c)^9c\left(32+1124c+196538c^2-1302168c^3+2311239c^4-1877980c^5+1680410c^6-1880689c^7+1132844c^8\right.\\
&\left.-267138c^9+11452c^{10}+1008c^{11}\right)z^8\\
&-(-1+c)^8c\left(-768+35664c-760080c^2+2816159c^3-2310559c^4-765330c^5-299959c^6+349759c^7+4145937c^8\right.\\
&\left.-4922524c^9+1924892c^{10}-255032c^{11}+5616c^{12}\right)z^9\\
&-2(-1+c)^7c^2\left(2272+323820c-4500222c^2+19063995c^3-37596741c^4+48558131c^5-56624432c^6+52032149c^7-25304076c^8\right.\\
&\left.+2280008c^9+2360242c^{10}-676758c^{11}+49032c^{12}\right)z^{10}\\
&-(-1+c)^6c^2\left(44544-230784c+3551112c^2-38087632c^3+180802288c^4-453709471c^5+757037039c^6\right.\\
&\left.-984837233c^7+964461909c^8-610442720c^9+210975064c^{10}-28939008c^{11}-1107832c^{12}+435024c^{13}\right)z^{11}\\
&+(-1+c)^5c^2\left(70656-986624c+3821136c^2-835488c^3+18490772c^4-384953050c^5+1637076179c^6\right.\\
&\left.-3696376911c^7+5534602531c^8-5744764453c^9+3949902310c^{10}-1648705682c^{11}+364273136c^{12}-32000516c^{13}+400464c^{14}\right)z^{12}\\
&+2(-1+c)^4c^2\left(-12288+486912c-7890144c^2+47462076c^3-120173060c^4+146708495c^5-604330390c^6+2911050330c^7-7397407941c^8\right.\\
&\left.+11555022726c^9-12066613597c^{10}+8462237673c^{11}-3794267461c^{12}+989457534c^{13}-128435640c^{14}+6705720c^{15}\right)z^{13}\\
&+(-1+c)^4c^3\left(270336-17143296c+205053760c^2-1034863488c^3+2602602184c^4-3573368080c^5+5348902942c^6-13198755668c^7\right.\\
&\left.+25758949628c^8-33181320397c^9+28810239411c^{10}-16430320530c^{11}+5648981962c^{12}-1011435820c^{13}+72248976c^{14}\right)z^{14}\\
&+(-1+c)^3c^4\left(8306688-167047680c+1173463616c^2-4823571904c^3+11089729840c^4-12279891800c^5+3293103356c^6+4133511414c^7\right.\\
&\left.+2455498351c^8-18471969408c^9+28896185625c^{10}-24138273334c^{11}+11229185308c^{12}-2621954160c^{13}+223736688c^{14}\right)z^{15}
\end{aligned}
\qquad (A.1)
$$

Primitive pieces

Consider the primitive pieces generated by

$$P(c;z) = \frac{[G(c,1;z) - 1]}{G(c,1;z)}$$

Now, put $c = 1$

In 2017 Jensen showed that $P(1,z)$ is D-algebraic with non-linear DE given by

$$\begin{aligned} &z^2(1+z)(1-8z)P''P - 2z^2(1-z^2)(1-8z)P'' - 2z^2(1+z)(1-8z)(P')^2 \\ &+ 2z(4-21z-16z^2)P'P - 4z(4-23z-9z^2)P' - 12P^3 \\ &+ (60-32z+16z^2)P^2 - (96-96z+132z^2)P + (48-64z+176z^2-48z^3) = 0. \end{aligned}$$

Order parameters for the full model

Two order parameters:

$$\mathcal{C}(c,d) = \lim_{n\to\infty} \frac{\langle m_c \rangle}{n} \quad \text{and} \quad \mathcal{D}(c,d) = \lim_{n\to\infty} \frac{\langle m_d \rangle}{n},$$

The system is in a free phase when

$$\mathcal{C} = \mathcal{D} = 0,$$

while a gelated phase is observed when

$$\mathcal{C} > 0, \mathcal{D} > 0$$

and finally we do not observe a phase where

$$\mathcal{C} > 0, \mathcal{D} = 0.$$

ANALYSING $G(a, c)$

The dominant singularity $z_s(c, d)$ of the generating function $G(c, d; z)$

$$z_s(c,d) = \begin{cases} z_b \equiv 1/8, & c \leq 4/3, d < 9/8 \\ z_b, & c \leq \alpha(d), d \geq 9/8 \\ z_p(c,d), & c > 4/3, d < 9/8 \\ z_p(c,d), & c > \alpha(d), d \geq 9/8 \end{cases} \quad (1)$$

where the boundary $\alpha(d)$ corresponds to when the singularities $z_p(c, d) = z_b$ coincide respectively.
where each of the different singularities are associated with different phases:

- z_b with the free phase
- $z_p(c, d)$ with the gelated phase

There is another singularity $z_c(c)$ of the generating function but one can show that $z_p < z_c$ for all c, d where z_c exists.

Phase diagram

Figure 9. The phase diagram of our full model. First and second-order transitions are indicated by solid and dashed lines respectively. All phase boundaries coincide at $c = 4/3$ and $d = 9/8$.

ASYMPTOTICS

Table: The growth rates of the coefficients $Z_n(c,d)$ modulo the amplitudes of the full generating function $G(c,d;z)$ over the entire phase space.

phase region	$Z_n(c,d) \sim$
free	$8^n n^{-4}$
gelated	$z_p(c,d)^{-n} n^0$
free to gelated boundary, $d < 9/8$	$8^n n^{-1} \log n$
free to gelated boundary, $d > 9/8$	$8^n n^0$
$c = 4/3, d = 9/8$	$8^n n^{-1}$

PHASE DIAGRAM IN DIFFERENT VARIABLES

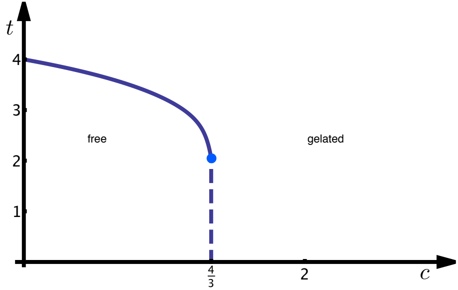


Figure 10. The phase diagram of our full model when setting $d = t/c^2$. First and second-order transitions are indicated by solid and dashed lines respectively. All phase boundaries coincide at $c = 4/3$ and $t = 2$.

THREE WALKS WITH ASYMMETRIC INTERACTIONS

Differentiating types of shared sites between upper two and lower two walks

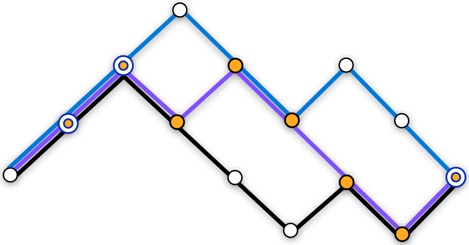


Figure: An example of an allowed configuration of length 8. Here, we have $m_a = 5$ shared sites between the upper two walks and $m_b = 6$ shared sites between the lower two walks. Thus, the overall Boltzmann weight for this configuration is $a^5 b^6$

THREE WALKS WITH ASYMMETRIC INTERACTIONS BUT NO EXPLICIT TRIPLE INTERATIONS

- shared sites between upper two walks fugacity: a
- shared sites between lower two walks fugacity: b
- previous symmetric model: $c = a = b$
- Walks start and end together

- *m_a is the number of shared sites between the upper pair of walks*
- *m_b is the number of shared sites between the lower pair of walks*

- Generating function: $G(a,b) \equiv G(a,b;z) = \sum_{n\geq 1} \sum_{\varphi\in\widehat{\Omega},|\varphi|=n} a^{m_a} b^{m_b} z^n$

GENERALISED GENERATING FUNCTION

Again, we consider walks in a larger set, where they do not necessarily end together.

- Generalised generating function:

$$F(r,s) \equiv F(r,s,a,b;z) = \sum_{\varphi \in \widehat{\Omega}} r^{h(\varphi)/2} s^{f(\varphi)/2} a^{m_a(\varphi)} b^{m_b(\varphi)} z^{|\varphi|}$$

- $G(a,b) = F(0,0)$
- where $h(\varphi)$ and $f(\varphi)$ are *half* the distance between the final vertices of the top to middle and middle to bottom walks respectively.

Find initial functional equation as above with same kernel as there is no fugacity dependence in the kernel $K(r,s)$

$$K(r,s) \equiv K(r,s;z) = 1 - \frac{z(r+1)(s+1)(r+s)}{rs}.$$

USING THE HALF-ORBIT METHODOLOGY

$$\color{red}{K(r,s)}F(r,s) = \frac{1}{ab} - \frac{(r - ar + az + asz)}{ar}F(0,s) - \frac{(s - bs + bz + brz)}{bs}F(r,0) - \frac{(a-1)}{a}\frac{(b-1)}{b}F(0,0)$$

- *We make use of the same symmetries of the kernel to produce multiple equations making sure we have either only positive powers of r or s.*
- *Re-combine to leave only say $F(0,0)$, $F(1/s,0)$ and $F(0,s)$*

$$N_1(s;z)F\left(1/s,0\right) + N_2(s;z)F(0,s) + N_3(s;z)\left[(c-1)^2F(0,0) - 1\right] = 0$$

- *The function $F(s,0;a,b) \neq F(0,s;a,b)$ so the symmetry is broken (as expected)*
- *N_j are now algebraic functions of s which cannot be made rational*

What about full-orbit methodology?

This results in an equation of the form

$$K(r,s) \cdot (\text{linear combination of } F)$$
$$= (a-1)(b-1)M_1(r,s;a,b)F(0,0) + (a-b)M_2(r,s;a,b)F(s,0) + M_3(r,s;a,b)$$

If $a = b$ this removes one of our unknown functions and allows us to find $F(0,0)$

Even if $b = 1$ with $a \neq 1$ the generating function seems to be D-finite but explicit solution eludes us

Is there a way to write $G(a,b)$ in terms of $G(a,a)$, $G(b,b)$ and/or $G(a,1)$ and $G(1,b)$?

CONCLUSION

- Simple model of finite gelation with three friendly walks in the bulk
- Used combinatorial decomposition to obtain linear functional equation
- $G(c,d)$ can be written in terms of $G(c,1)$ via "primitive piece" argument
- Even with $c=1$ primitive pieces are D-algebraic and not D-finite
- Used obstinate kernel method (half-orbit sum) to solve functional equations
- Explicit series solutions for $G(c,1)$
- Also used Zeilberger-Gosper algorithm to find linear DE for $G(c,1)$
- Full analysis of asymptotics and phase diagram
- R. Tabbara, A. L. Owczarek and A. Rechnitzer, *J. Phys. A: Math. Theor.* **49** (2016) 154004 (27pp)
- Asymmetric model seems intractable! — not enough information in kernel functional equations?

FUTURE WORKS

How far can we extend this? — where does integrability end?

- Four walks with double interactions (Xu, O and R)
- Combine single, double surface and unzipping interactions
- Is there another way for the asymmetric three walks model?
- Three walks and a wall
- Working in a slit — currently two walks: asymptotic solutions (O and R, 2017)
- Kreweras walks and counting boundary sites of the quarter plane (O and R, last week)