Exact Solutions of Interacting Friendly Directed Walkers

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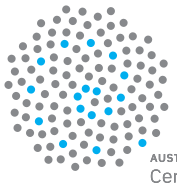

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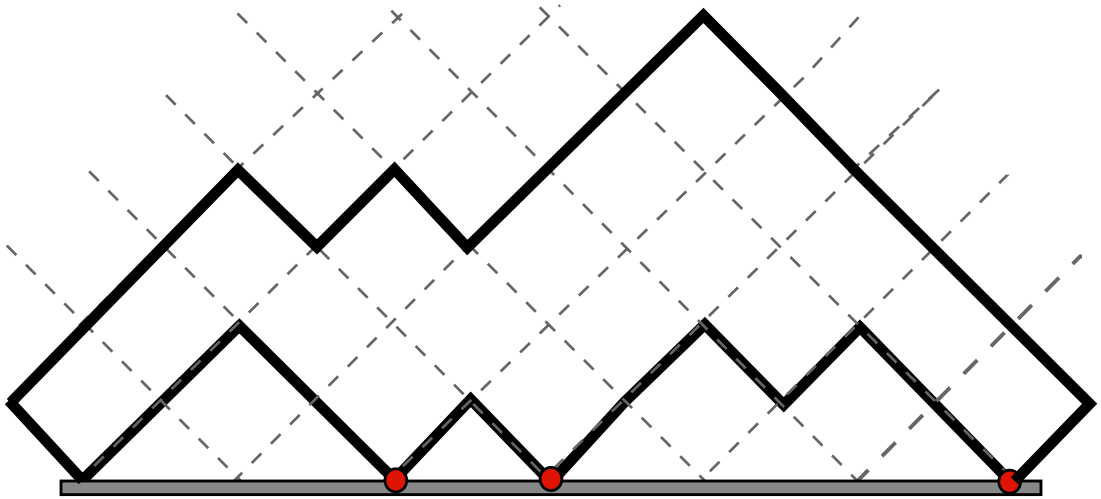
DIRECTED WALKS LATTICE MODELS

- 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
- Interest is in adding multiple interactions



EXACT SOLUTION OF DIRECTED LATTICE WALKS LATTICE

- Recurrence and functional equation for partition or generating function
- Rational, algebraic, Differentially-finite (D-finite)
- and non D-finite solutions (e.g. q-series) for generating functions
- Vicious walks are related to free fermions
- 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 thm.* ('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 (submitted)

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

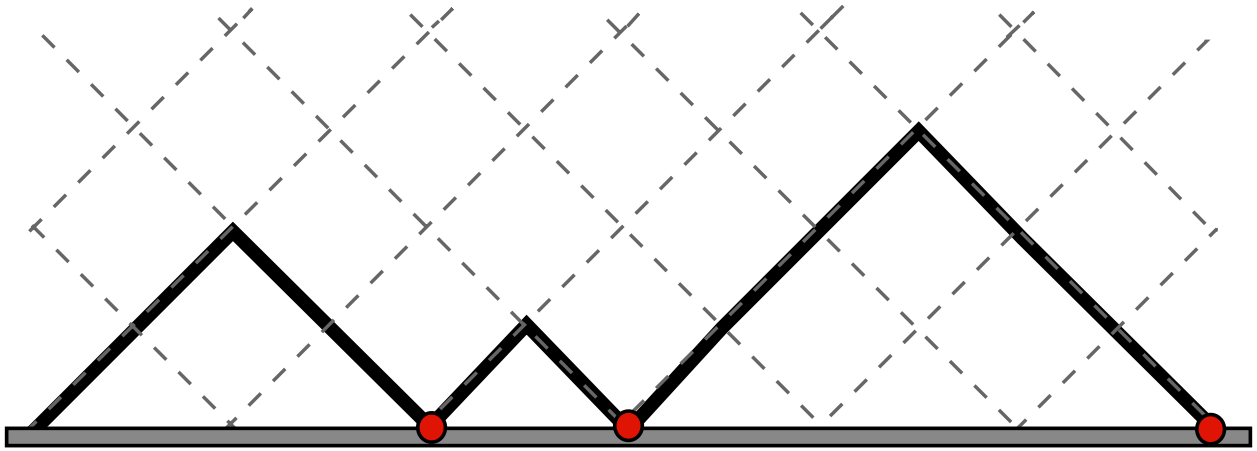
- Our problems have several catalytic variables
- Need multiple values of catalytic variables: obstinate kernel method
- Earliest combinatorial application due to *Bousquet-Mélou* ('02).
- Bousquet-Mélou *Math. and Comp. Sci 2* (2002)
- Bousquet-Mélou, Mishna *Contemp. Math.* **520** (2010)
- Solutions 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 $a = e^{\varepsilon_a / k_B T}$
- 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

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

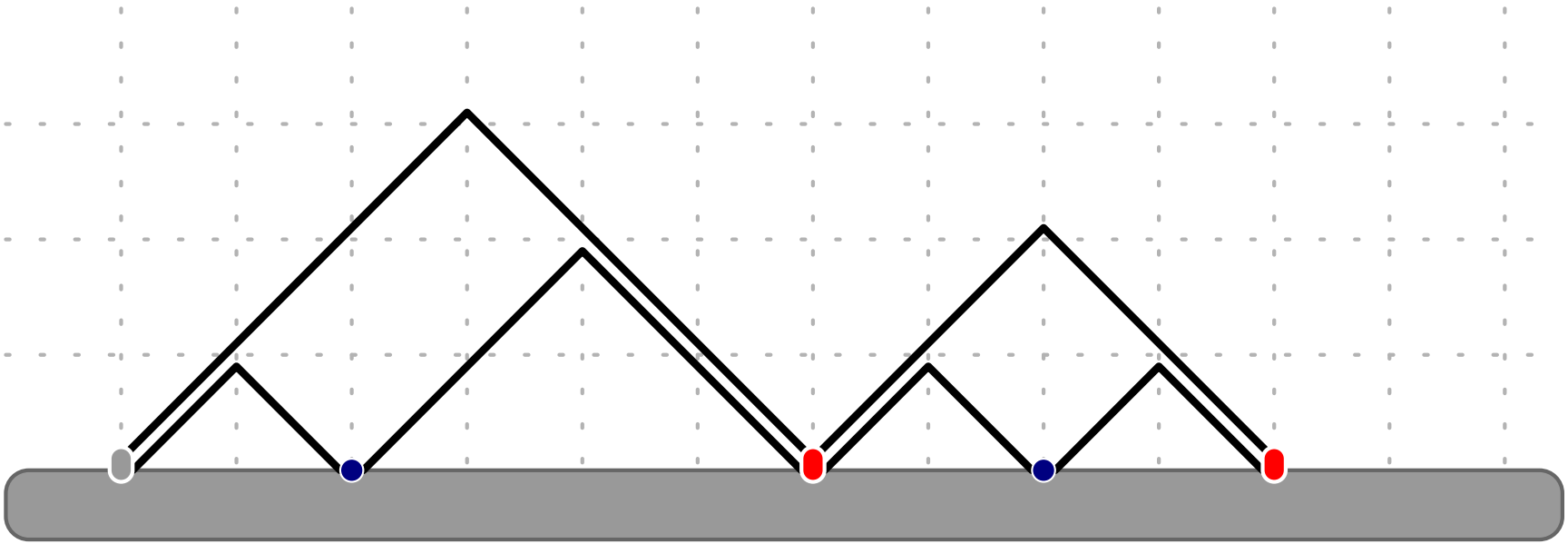


Figure : Two directed walks with single and "double" visits to the the surface.

- *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:

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

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

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

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

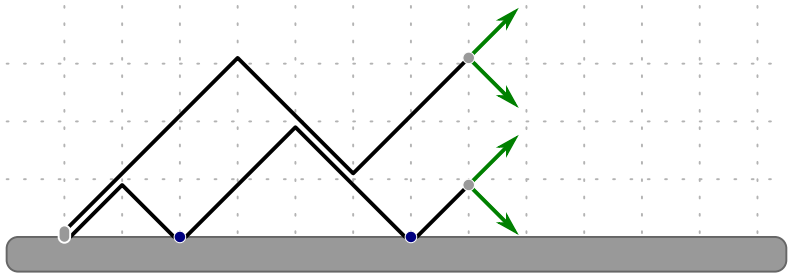


Figure : Adding steps to the walks when the walks are away from the wall.

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.

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

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

where

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

EXTRACTING THE SOLUTION $a = 1$

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

- 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 $1-dP(a;z)=0$.*

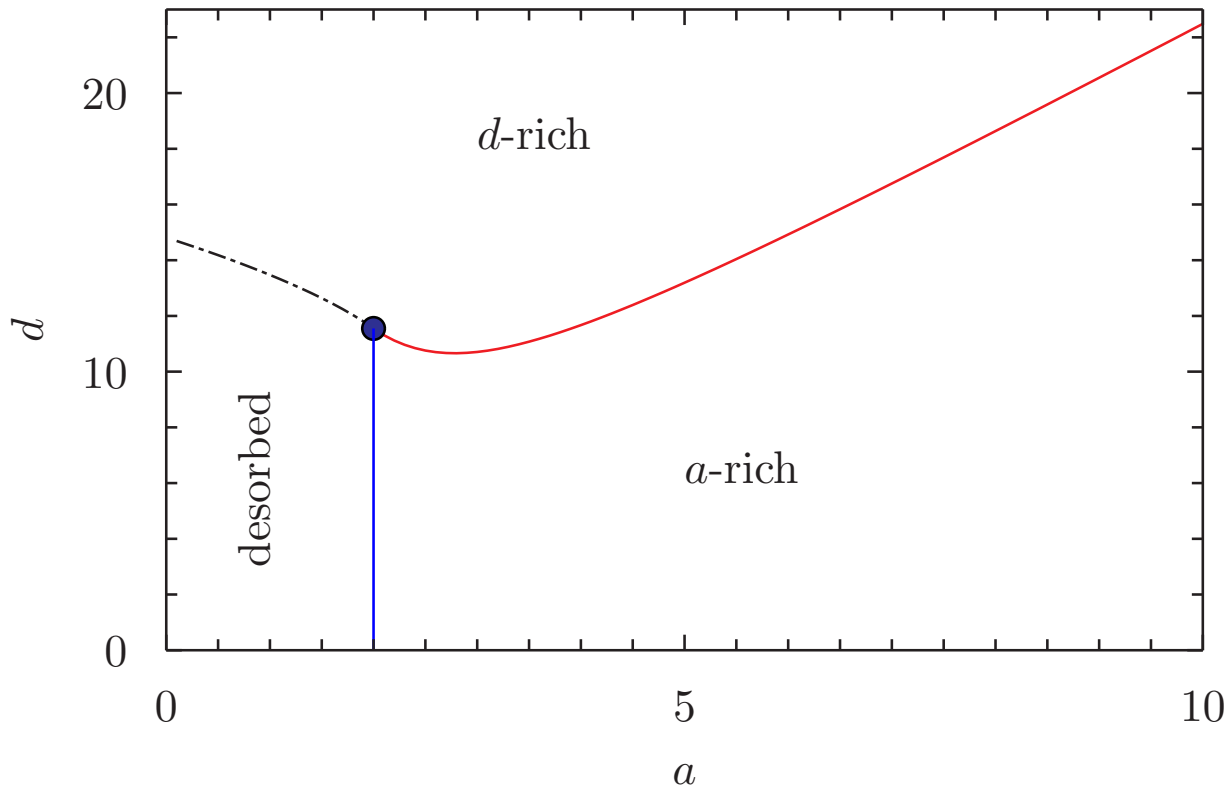
There are two singularities of $G(a,a;z)$ giving rise to two phases:

- 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 $(a, d) = (a^*, d^*) = (2, 11.55\ldots)$.

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.*

FIXED ENERGY RATIO MODEL FAMILY

Family of models parameterised by $-\infty < r < \infty$ *where*

$$\varepsilon_d = r\varepsilon_a \qquad \text{and so} \qquad d = a^r$$

- $r = 2$ model has *two* phase transitions as temperature changed .
- At very low temperatures the model is in a d-rich phase
- while at high temperatures the model is in the desorbed state.
- At intermediate temperatures the system is in an a-rich phase.
- Both transitions are second-order with jumps in specific heat.

Conclusions for Double Interaction model

- 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

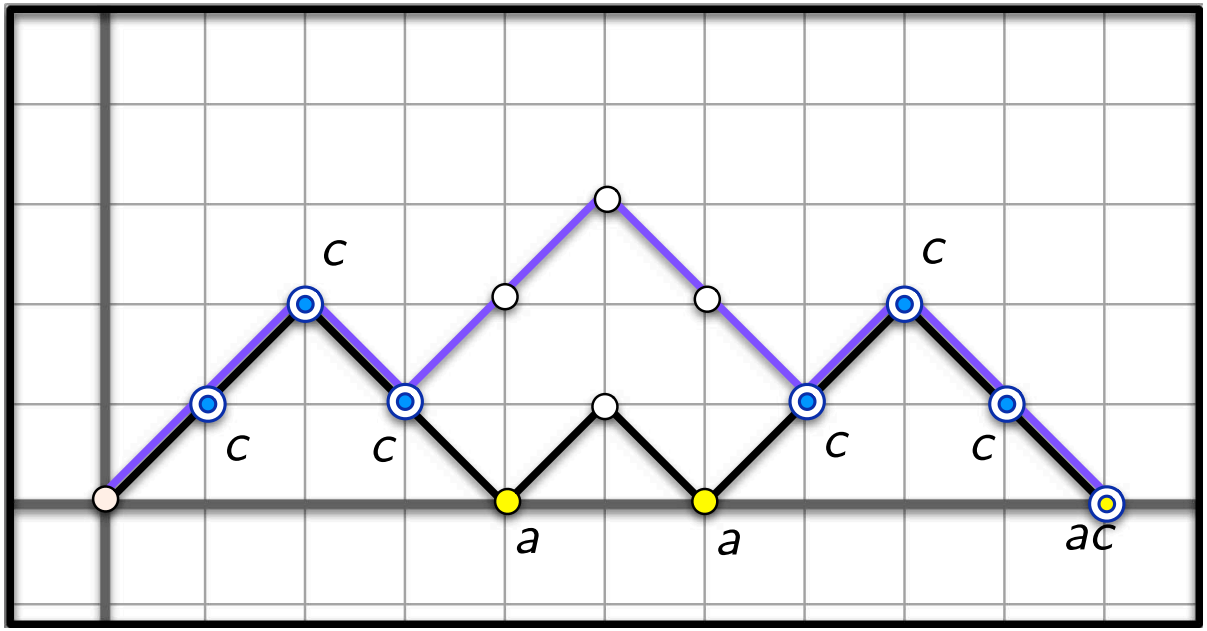


Figure : An allowed configuration of length 10. The overall weight is a^3c^7

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

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

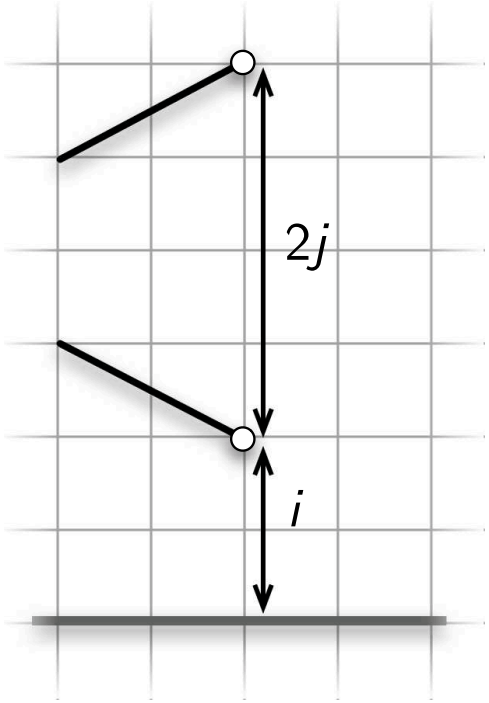
Generalised generating function

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')

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

- *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

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

- 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

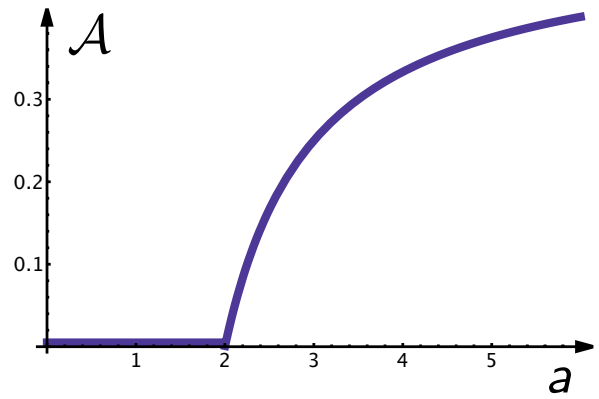
Recall lim. avg. surface and shared site contacts resp.

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

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

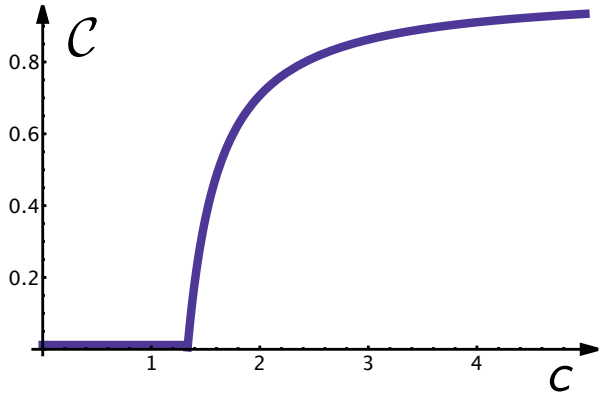
- For $G(a,1)$: the order parameter associated with the phase transition is the surface coverage

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



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

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



- 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

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

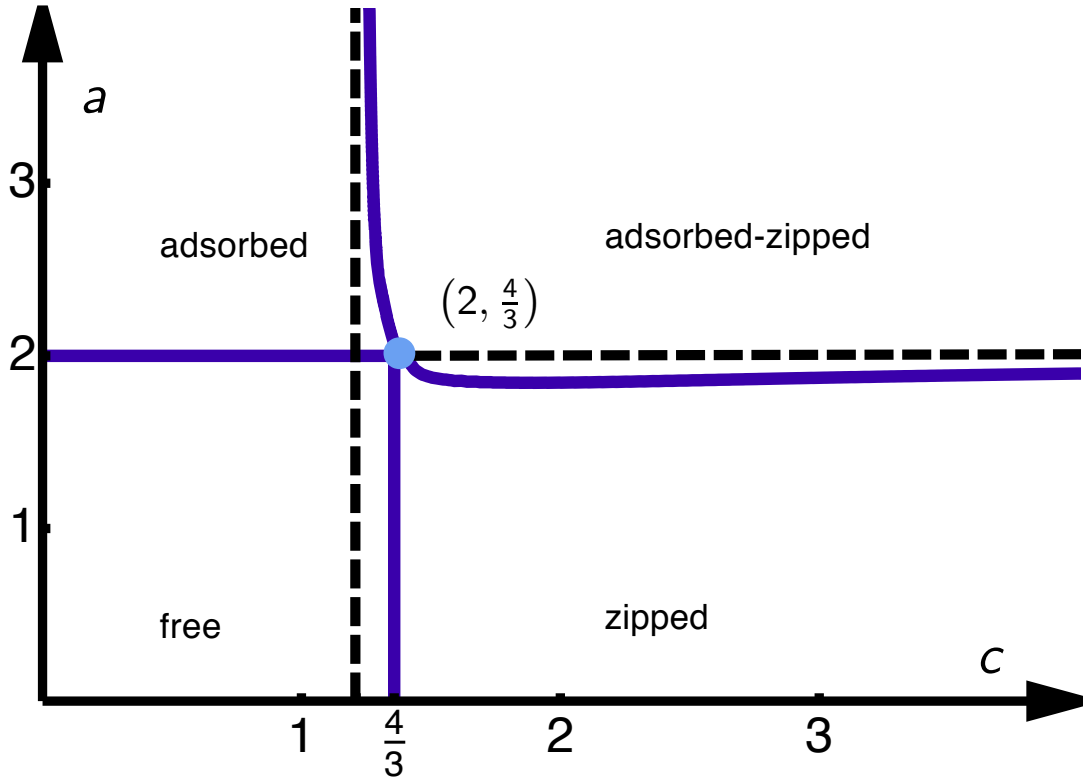
- $\Rightarrow$ Singularities: Look at $G(a,1)$, $G(1,c)$ and root of above denom.
- root of denominator is associated with the zipped-adsorbed phase

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	$z_{ac}(a,c)^{-n} n^{-1}$

Conclusion

- 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

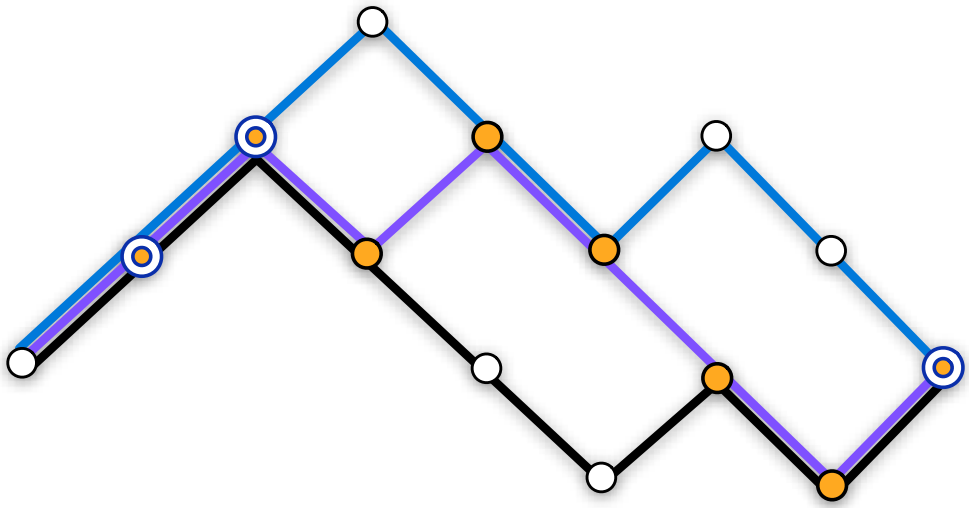


Figure : An example of an allowed configuration of length 8. Here, we have $m_c = 11$ double shared contact steps and $m_d = 3$ triple shared contact steps. Thus, the overall Boltzmann weight for this configuration is $c^{11}d^3 = c^5t^3$

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:

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

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

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:

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

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

- *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.

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

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

and

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

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 $\deg_z = 26$

ORDER PARAMETERS FOR THE FULL MODEL

Two order parameters:

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

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 $G(c, d; z)$

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

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

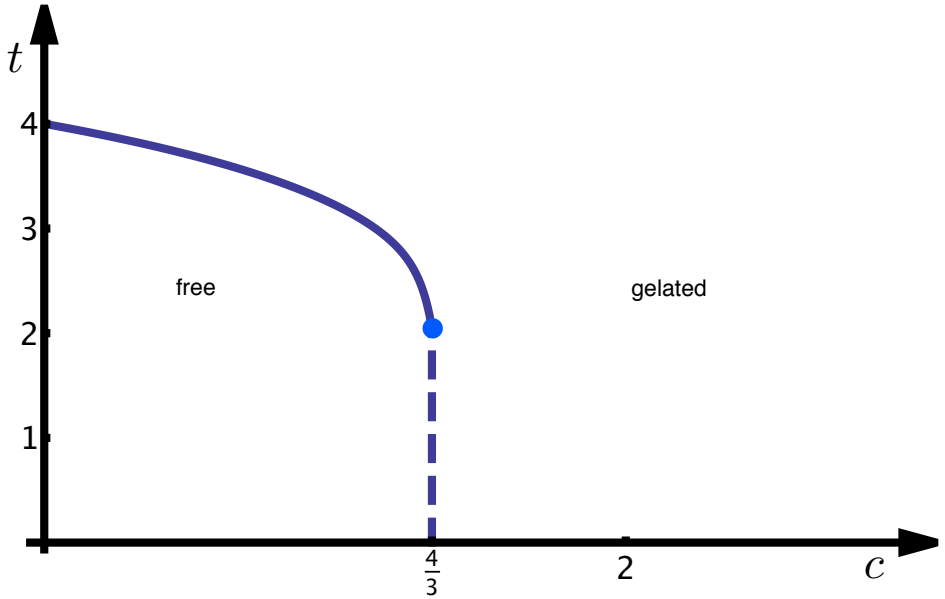


Figure 10. The phase diagram of our full model when setting $d = t/c^2$. First and second-order transitions are indicated by solid and dashed lines respectively. All phase boundaries coincide at $c = 4/3$ and $t = 2$.

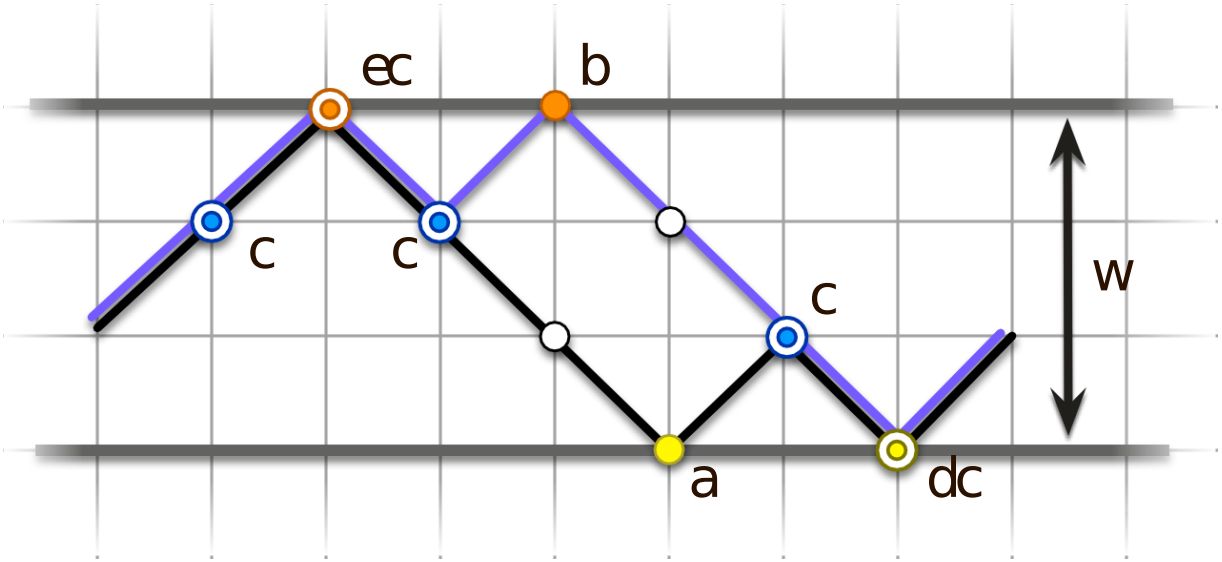
Conclusion

- 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
- Used obstinate kernel method 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
- Again interesting physics and mathematics
- Manuscript submitted to *J. Phys. A: Math. Theor.*

FUTURE WORKS

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

- Combine single, double surface and unzipping interactions
- Consider three walks with multiple unzipping interactions
- Three walks and a wall
- Four walks
- Working in a slit



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}
\tag{A.1}
$$