Exact solution of some friendly directed walker problems on two-dimensional lattices

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DIRECTED WALKS ON TWO-DIMENSIONAL LATTICES

- Integrable models in lattice statistical mechanics (usually two-dimensional) have been a mathematical goldmine for 70 years
- Simple lattice models of polymers have been studied from near the beginning of this era
- There are many exact solutions of single and multiple directed walk models
- Different though related techniques to Ising type models
- Strong connection to combinatorics
- Techniques interplay with probability theory
- Some three-dimensional solutions

EXACT SOLUTION OF DIRECTED WALKS LATTICE MODELS

- Recurrence and functional equation
- Rational, algebraic, Differentially-finite (D-finite) and non D-finite solutions (e.g. q-series)
- Multiple walks: Bethe Ansatz & Lindström-Gessel-Viennot (LGV) Lemma
- LGV Lemma: multiple walks = determinant of single walks
- LGV problems result in generating functions that are D-finite

TYPES OF MULTIPLE WALK SYSTEMS

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

Some exact solutions of directed walk systems

No wall/interaction:

- Vicious directed walks: *Fisher* ('84), *Lindström-Gessel-Viennot thm.* ('85), *Essam & Guttmann* ('95), *Guttmann, Owczarek & Viennot* ('98)
- Friendly walks & Osculating walks: *Brak* ('97), *Guttmann & Vöge* ('02), *Bousquet-Mélou* ('06)

With wall (but no interaction)

- Vicious: *Krattenhaler, Guttmann & Viennot* ('00)

With wall (interaction)

- Vicious: *Brak, Essam & Owczarek* ('98, '01)
- Friendly: *Owczarek, Rechnitzer & Wong* ('12)

DIRECTED WALKS AND FUNCTIONAL EQUATIONS

- Focus on generating function
- Combinatorially decompose the walks
- Find a functional equation for an expanded generating function
- Uses an extra catalytic variable
- Answer is a 'boundary' value
- Equation is written as "bulk = boundary terms" where bulk term is product of a kernel function and the bulk generating function
- Answer needed is one of the boundary generating functions
- Fix catalytic variable $\rightarrow$ 'bulk' term disappears (Kernel method)
- Standard kernel method due to *Knuth* (1968): use values of "catalytic variable' to "kill" kernel

SOLVING FUNCTIONAL EQUATIONS: KERNEL METHODS

- Fix catalytic variable $\rightarrow$ 'bulk' term disappears (Kernel method)
- Standard kernel method due to *Knuth* (1968): use values of "catalytic variable' to "kill" kernel
- From $\approx$ early '00's applied to a number of dir. walk problems
- Obstinate kernel method: multiple values of catalytic variable are needed
- Earliest combinatorial application of the obstinate kernel method due to *Bousquet-Mélou* ('02).
- See Bousquet-Mélou *Math. and Comp. Sci 2* (2002)), Bousquet-Mélou, Mishna *Contemp. Math.* **520** (2010)
- Solutions are not always D-finite

Polymer Adsorption

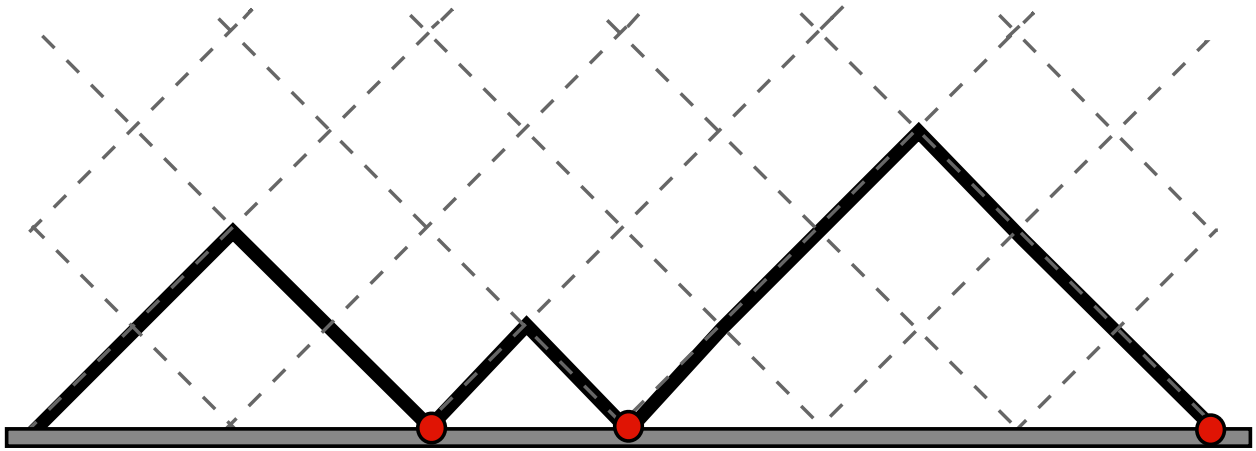
The physical motivation is the adsorption phase transition

- Second order phase transition with jump in specific heat
- Crossover exponent $\phi = 1/2$ for directed walks and SAW
- Order parameter is density of visits to surface by the polymer

ADSORPTION: ONE DIRECTED WALK

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

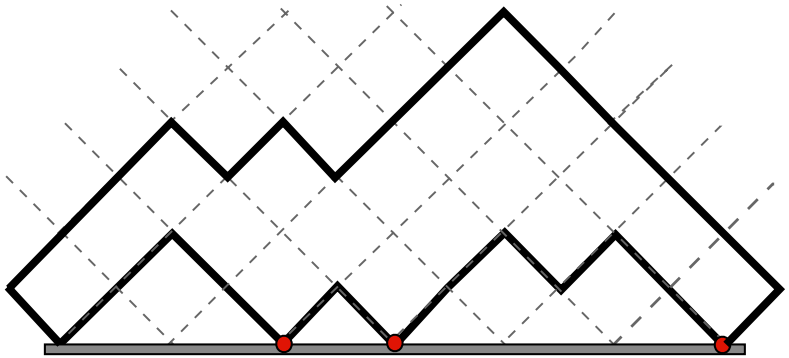
Consider the density of visits

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

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

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

VESICLE ADSORPTION



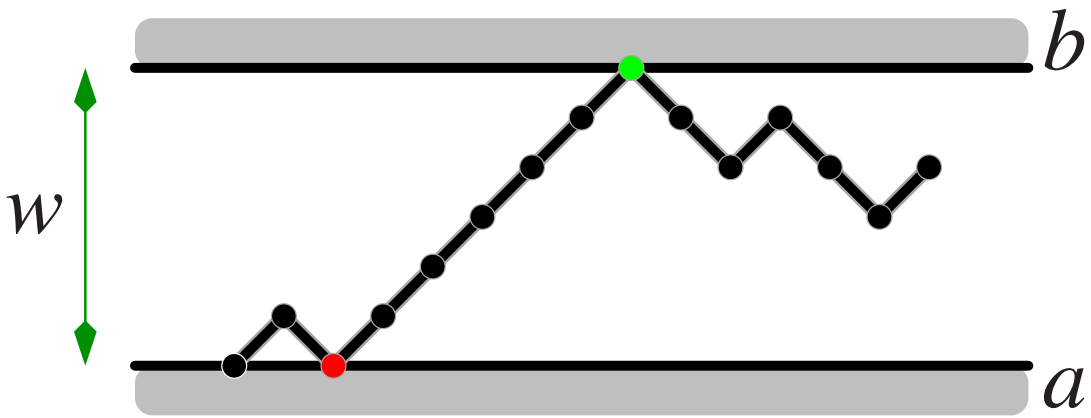
- Exact solution of two directed walks joined making a simple "vesicle" (Brak, Essam, Owczarek , *J. Stat. Phys.* **93**, 155 (1998))
- Vesicles with interactions for visits of the *bottom* walk to height 0 and height 1 (Lonsdale, Brak, Essam, Owczarek, Rechnitzer, *J. Phys. A.: Math. and Theor.* **42** 1, (2009).)

Single second order transition — similar to the single walk adsorption transition

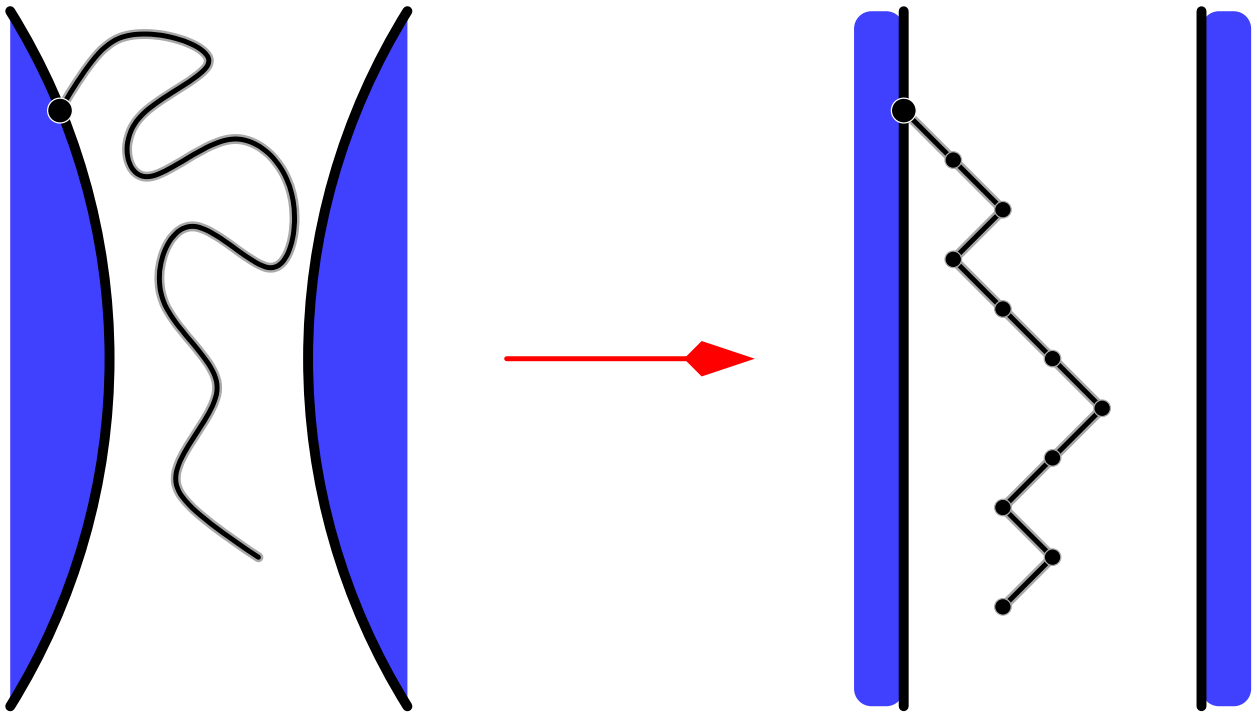
POLYMERS IN A SLIT

Paths in a slit

- A directed path of length n in a slit of width w.
- Boltzmann weights a and b for interactions with lines (walls).
- Brak, Owczarek, Rechnitzer and Whittington *J. Phys. A*, **38** (2005) 4309–4325
- Subsequent works on undirected SAW

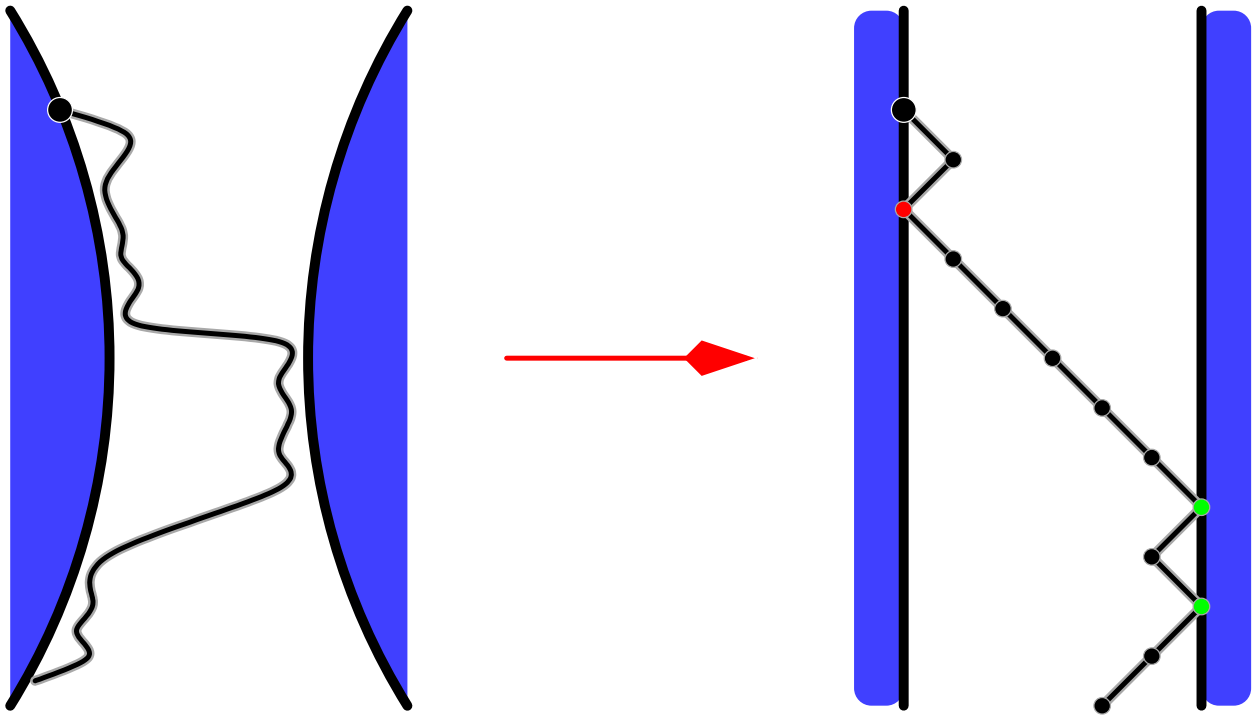


WHAT IS STERIC STABILISATION?



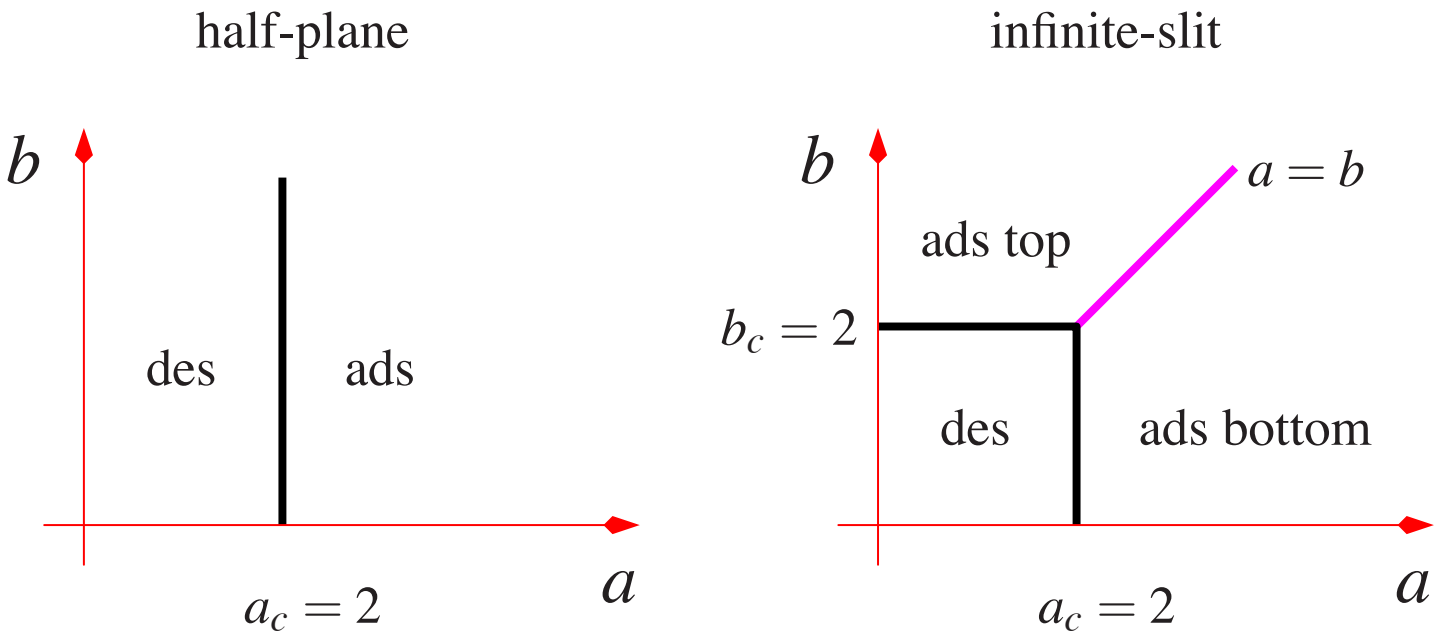
- Entropic repulsion between the colloidal particles.

WHAT IS SENSITISED FLOCCULATION?



- Polymer adsorbs and pulls the particles together.

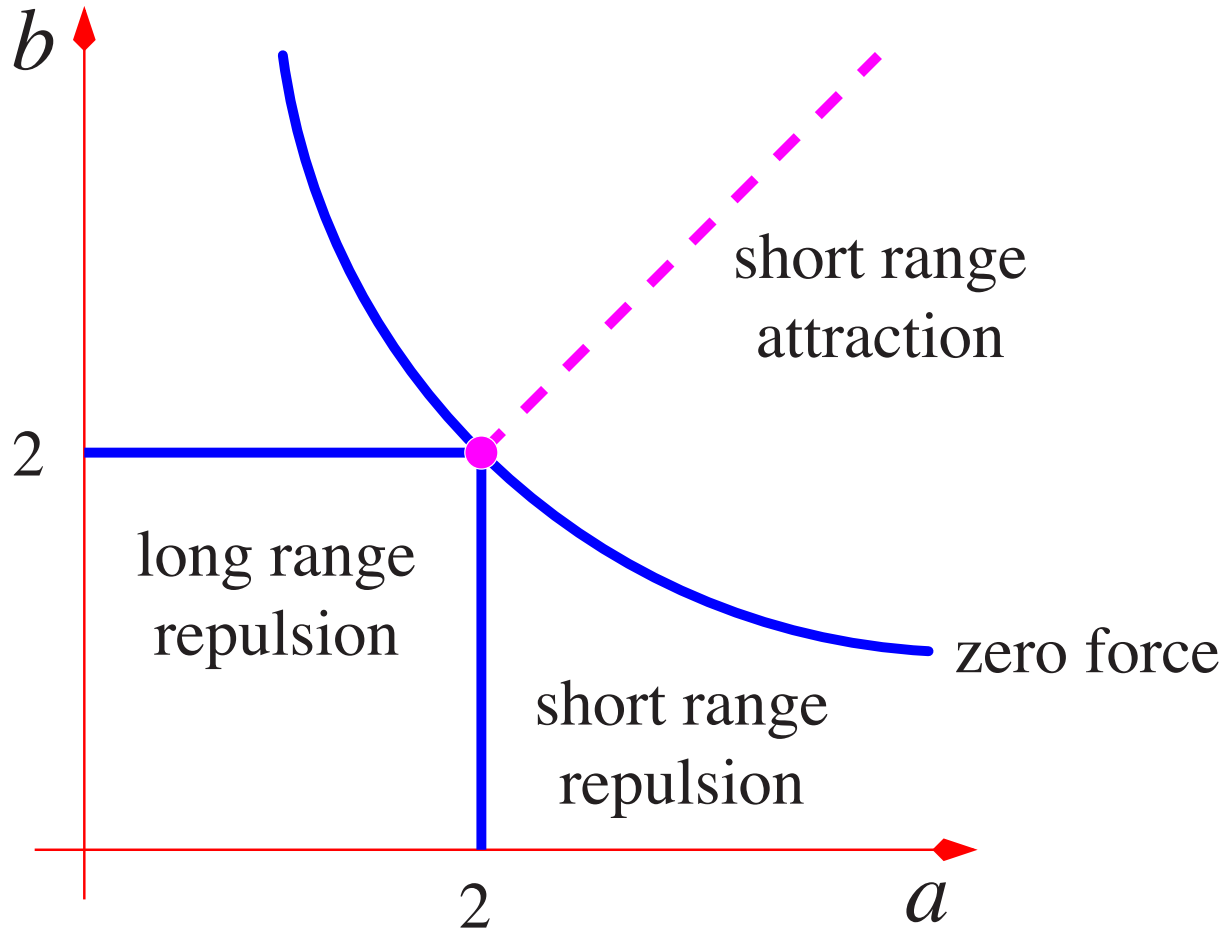
THE PHASE DIAGRAM POLYMERS IN A SLIT



Phase diagram depends on order of limits

- Black = 2^{nd} order and pink = 1^{st} order.
- Left-hand diagram: $w \to \infty$ and then $n \to \infty$.
- Right-hand diagram: $n \to \infty$ and then $w \to \infty$.
- The order of n and w limits really does matter!

More motivation: polymers in a slit



RING POLYMERS IN A SLIT

- Our motivation is a recent Monte Carlo study of ring polymers in a slit
- Here both sides of the polygon interact with the surfaces of the slit Alvarez, Janse van Rensburg, Soteros and Whittington *J. Phys. A.: Math. and Theor.* **41**, 185004 (2008)
- Novel zero force curve

(Our Model)

Directed vesicle where both walks can interact with a single surface

Work with Thomas Wong

Model

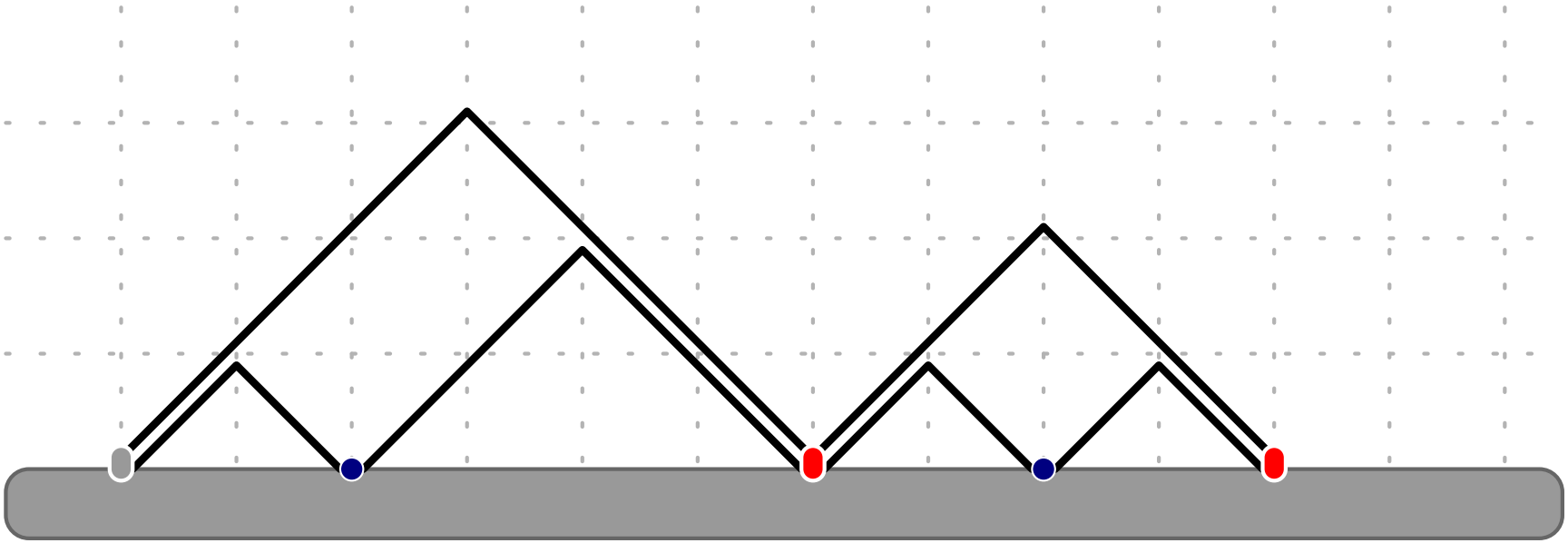


Figure : Two directed walks with single and "double" visits to the the surface.

- *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

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

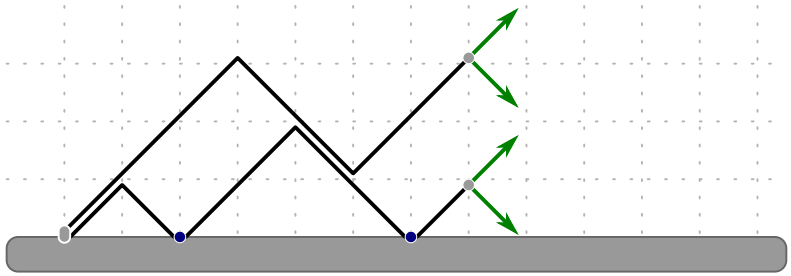


Figure : Adding steps to the walks when the walks are away from the wall.

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

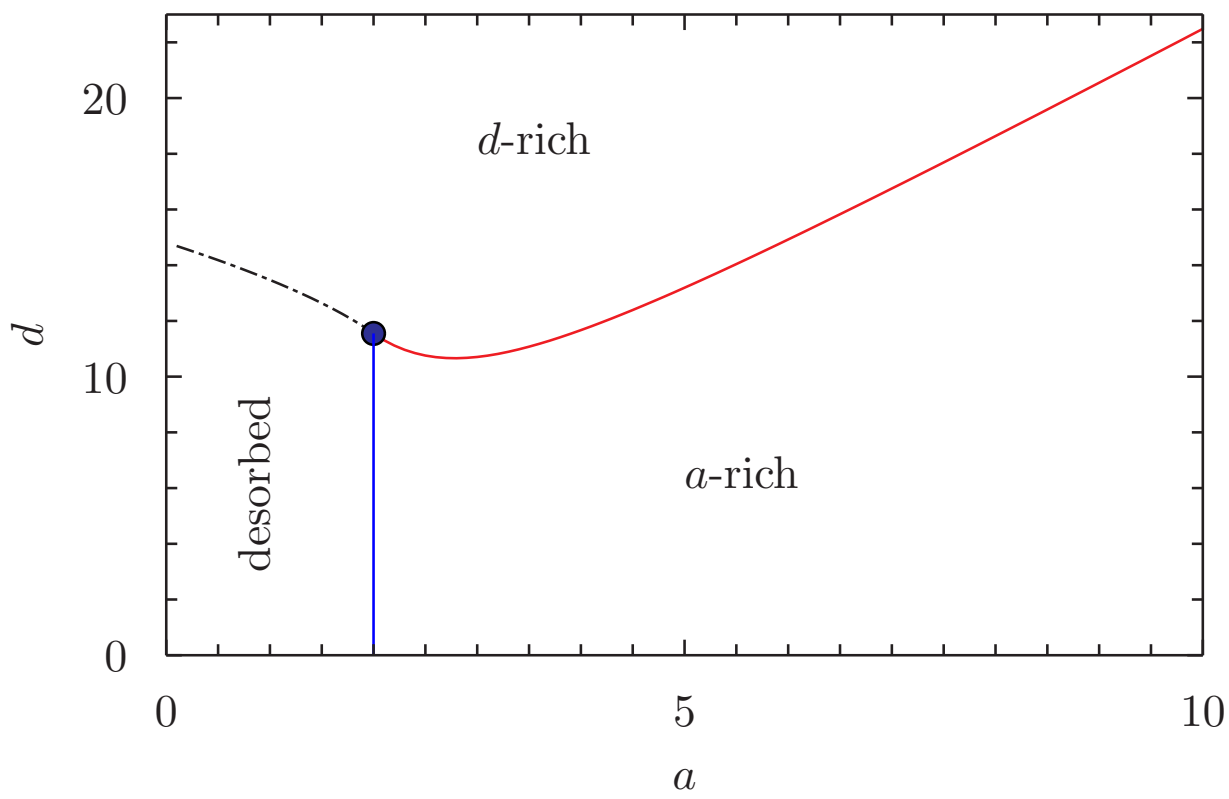
There are two singularities of $G(a,a;z)$ giving rise to two phases:

- 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*

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

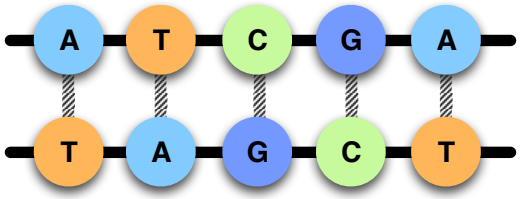
- $r = 2$ model has *two* phase transitions as temperature changed .
- At very low temperatures the model is in a d-rich phase
- while at high temperatures the model is in the desorbed state.
- At intermediate temperatures the system is in an a-rich phase.
- Both transitions are second-order with jumps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

DNA

- DNA is a polymer consisting of four repeating nucleic bases A,C,G,T.
- Two strands entwined with a helix structure
- Denaturation: At high T, strands pulled apart



Work with Rami Tabbara

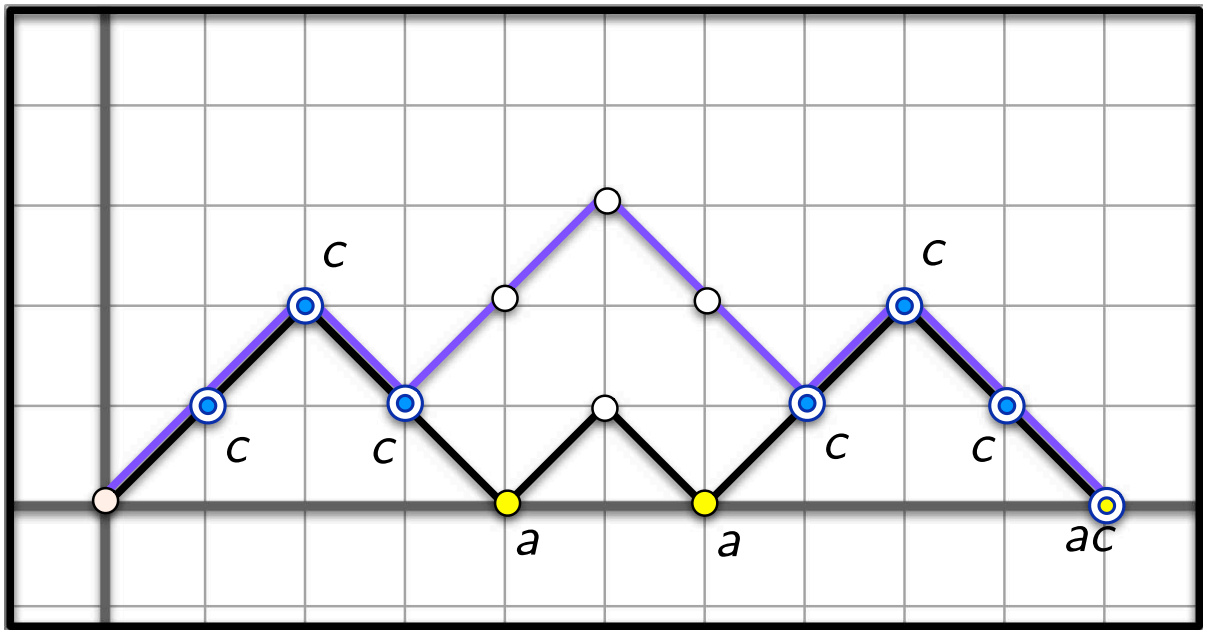
(Our model — Adsorption and Unzipping)

- *double DNA strand in a solvent*
- *near attractive surface*
- *assume aligned base sequence*
- *Use* (∞) *- friendly directed walks again*

ALLOWED WALKS

Consider two directed walks along the square lattice.
Let our model contain the class of allowed configs. with n steps as described:

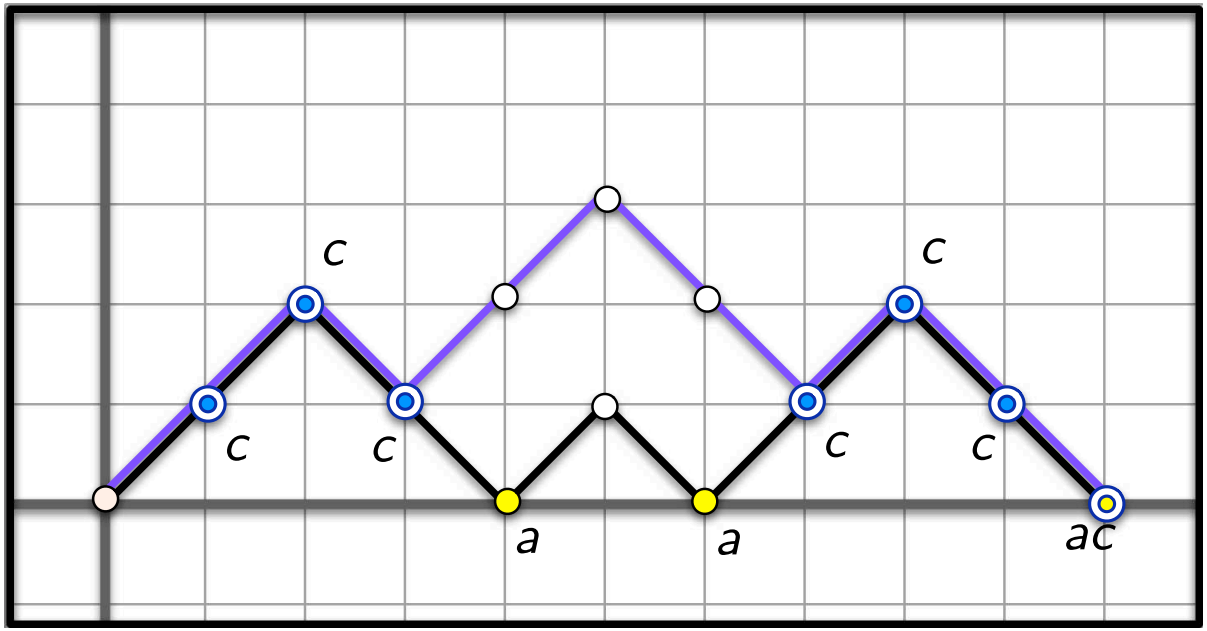
- both walks begin at $(0,0)$, end at $(2n,0)$.
- directed: can only take steps in the $(\pm 1, 0)$ directions.
- (∞) - friendly: walks can share sites, but cannot cross



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: $c \equiv e^{\varepsilon_c / k_B T}$
- trivial walk consisting of zero steps has weight 1.



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

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:

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

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

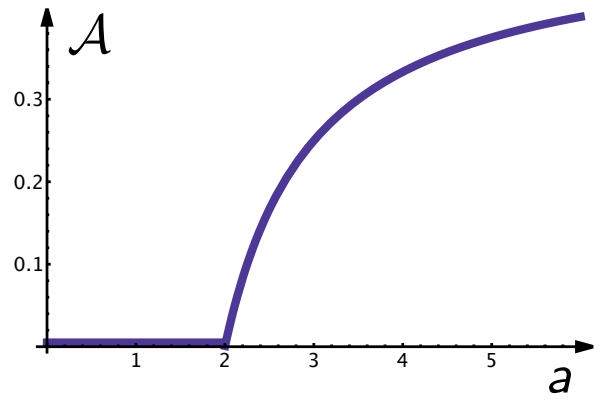
Recall lim. avg. surface and shared site contacts resp.

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

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

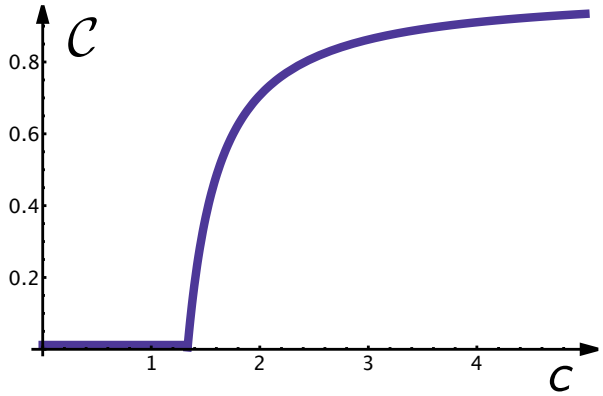
- For $G(a,1)$: the order parameter associated with the phase transition is the surface coverage

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



- 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

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

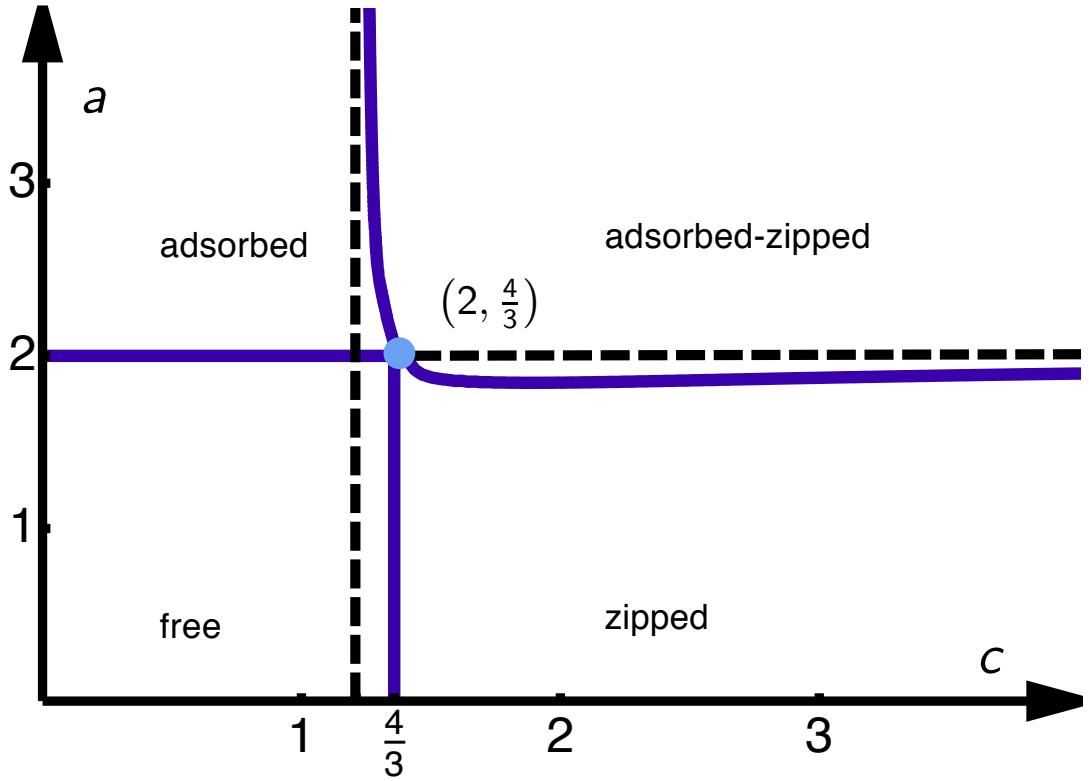
- $\Rightarrow$ Singularities: Look at $G(a,1)$, $G(1,c)$ and root of above denom.
- root of denominator is associated with the zipped-adsorbed phase

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

FUTURE WORKS

- Combine single, double surface and unzipping interactions: work in progress
- Consider three walks with multiple unzipping interactions: work in progress
- Also in progress is work in a slit
- Extend these to various interactions