Exact solution of some friendly directed walker problems

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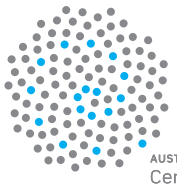
Workshop on Random Polymers, EURANDOM



AUSTRALIAN RESEARCH COUNCIL
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DIRECTED WALKS

- Exact solutions of single and multiple directed walk models
- Recurrence and functional equation
- Rational, algebraic, Differentially-finite and non D-finite solutions
- Multiple walks: Bethe Ansatz & Lindström-Gessel-Viennot
- LGV Lemma: multiple walks = determinant of single walks
- LGV problems result in generating functions that are D-finite

SOLVING FUNCTIONAL EQUATIONS

- Functional equation for an expanded generating function
- Uses an extra catalytic variable
- Answer is a 'boundary' value
- Fix catalytic variable $\rightarrow$ 'bulk' term disappears (Kernel method)
- Obstinate kernel method: multiple values of catalytic variable
- See Bousquet-Mélou *Math. and Comp. Sci 2* (2002)), Bousquet-Mélou, Mishna *Contemp. Math.* **520** (2010)
- Solutions are not always D-finite

Polymer Adsorption

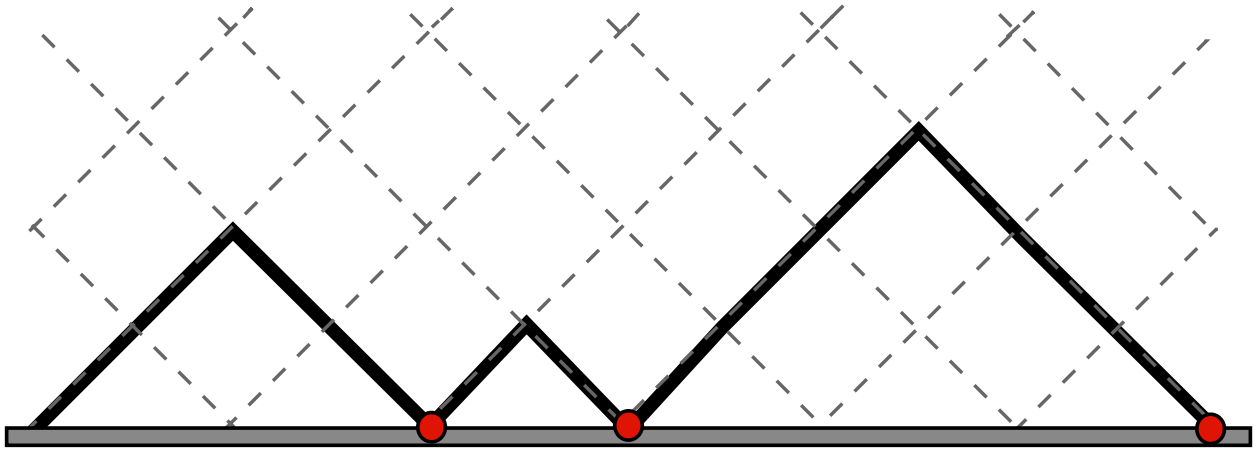
The physical motivation is the adsorption phase transition

- 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 in a half space
- Energy $-\varepsilon_a$ for each time (number m_a) it visits the surface
- Boltzmann weight $a = e^{\varepsilon_a / k_B T}$



ADSORPTION: ONE DIRECTED WALK

A complete solution exists and the generating function is algebraic

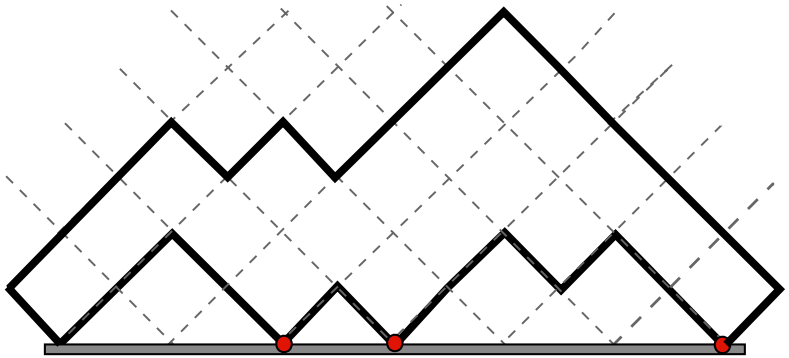
Consider the density of visits

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

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



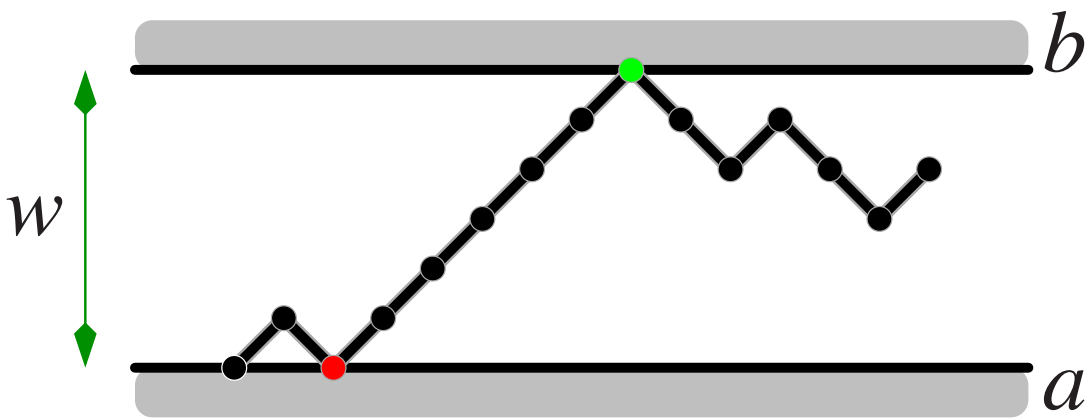
- Exact solution of two directed walks joined making a simple "vesicle" (Brak, Essam, Owczarek , *J. Stat. Phys.* **93**, 155 (1998))
- Vesicles with interactions for visits of the *bottom* walk to height 0 and height 1 (Lonsdale, Brak, Essam, Owczarek, Rechnitzer, *J. Phys. A.: Math. and Theor.* **42**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

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

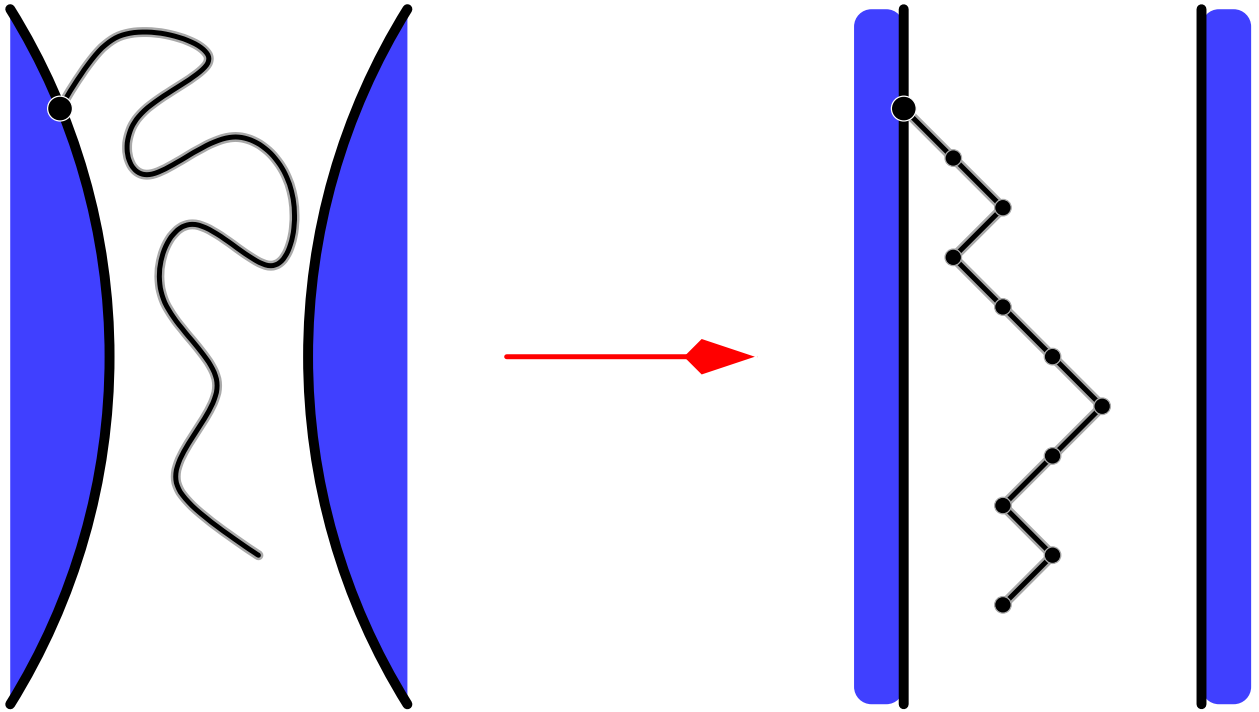
More motivation: polymers in a slit

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

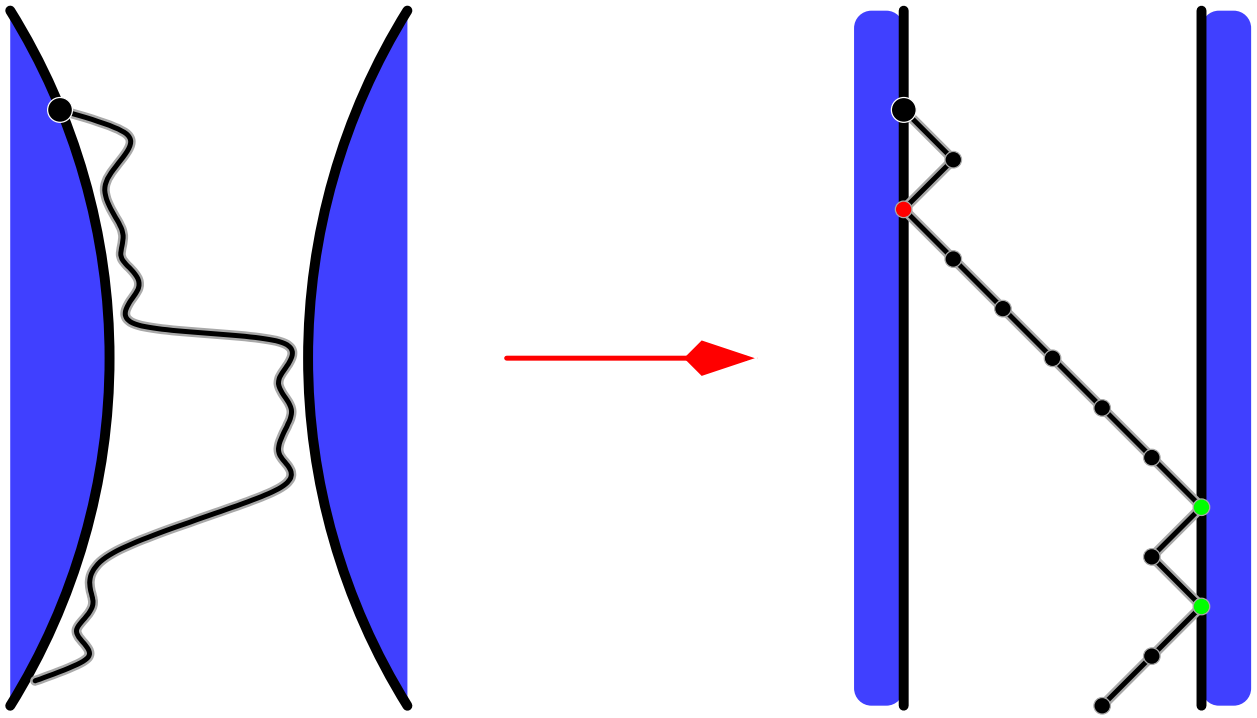


WHAT IS STERIC STABILISATION?



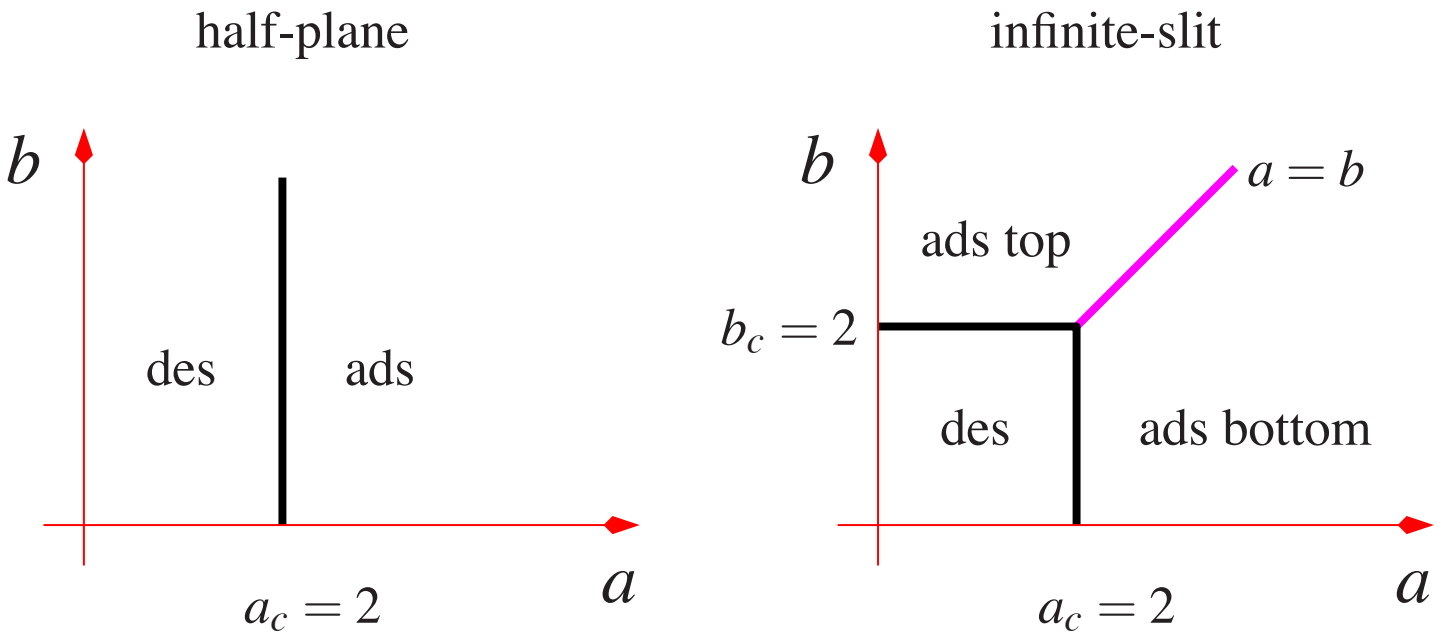
- Entropic repulsion between the colloidal particles.

WHAT IS SENSITISED FLOCCULATION?



- Polymer adsorbs and pulls the particles together.

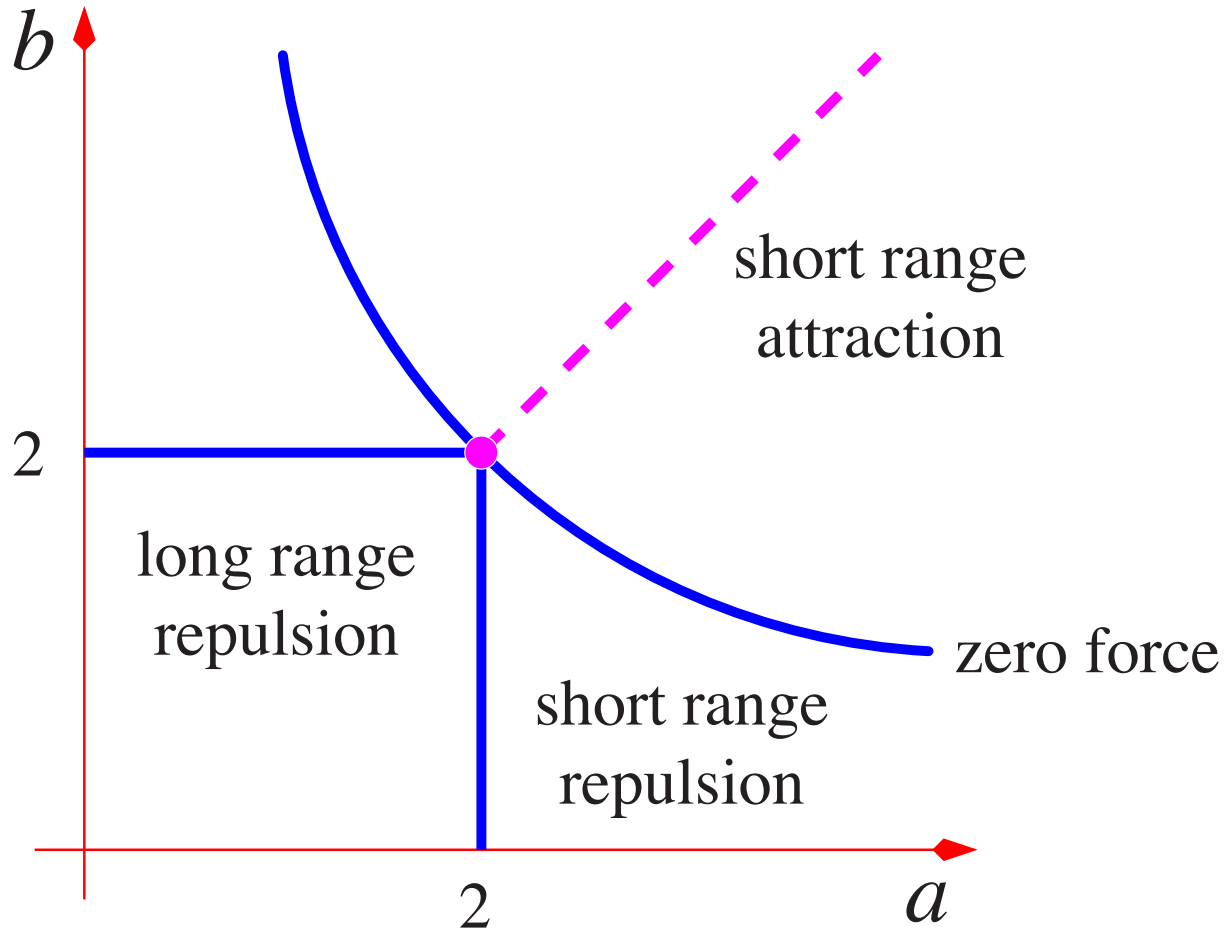
THE PHASE DIAGRAM POLYMERS IN A SLIT



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

Model

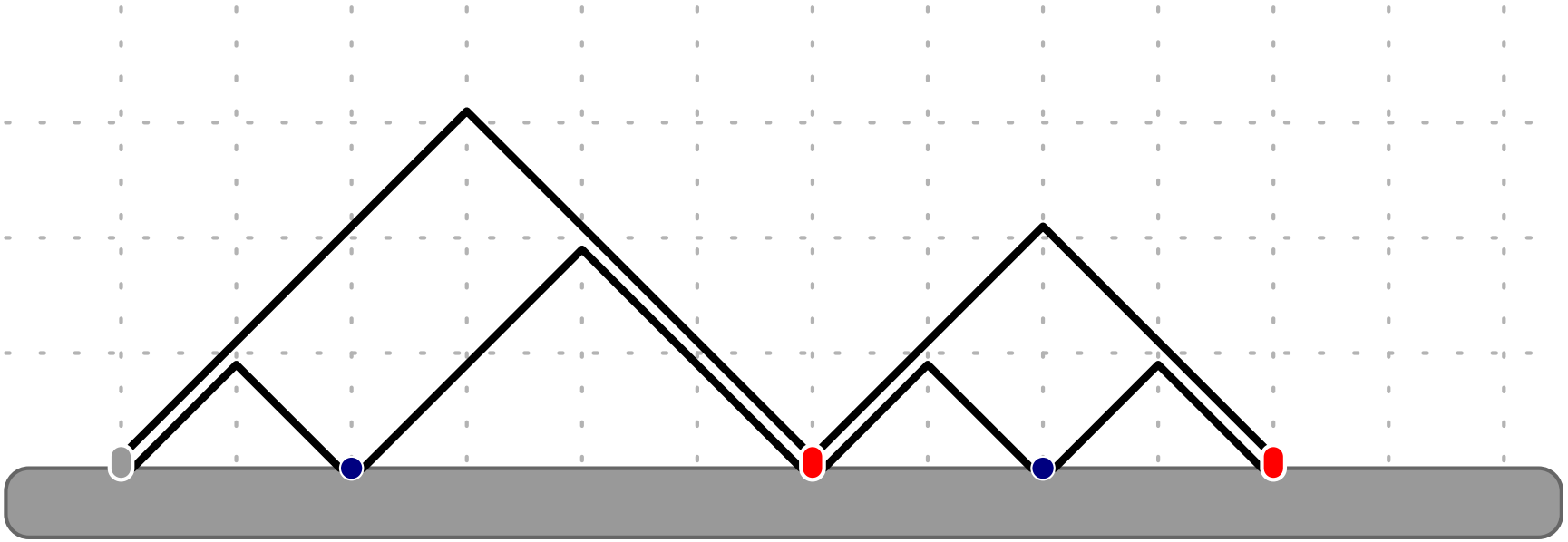


Figure: Two directed walks with single and "double" visits to the the surface.

- *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

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

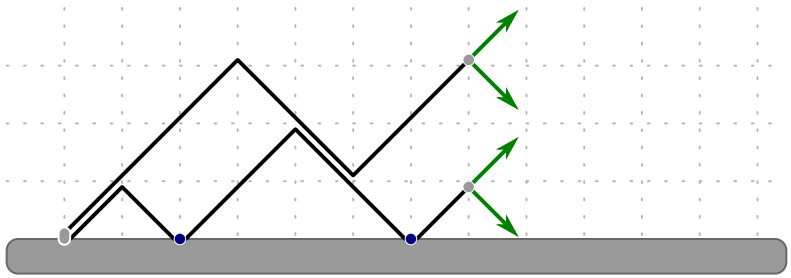


Figure: Adding steps to the walks when the walks are away from the wall.

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

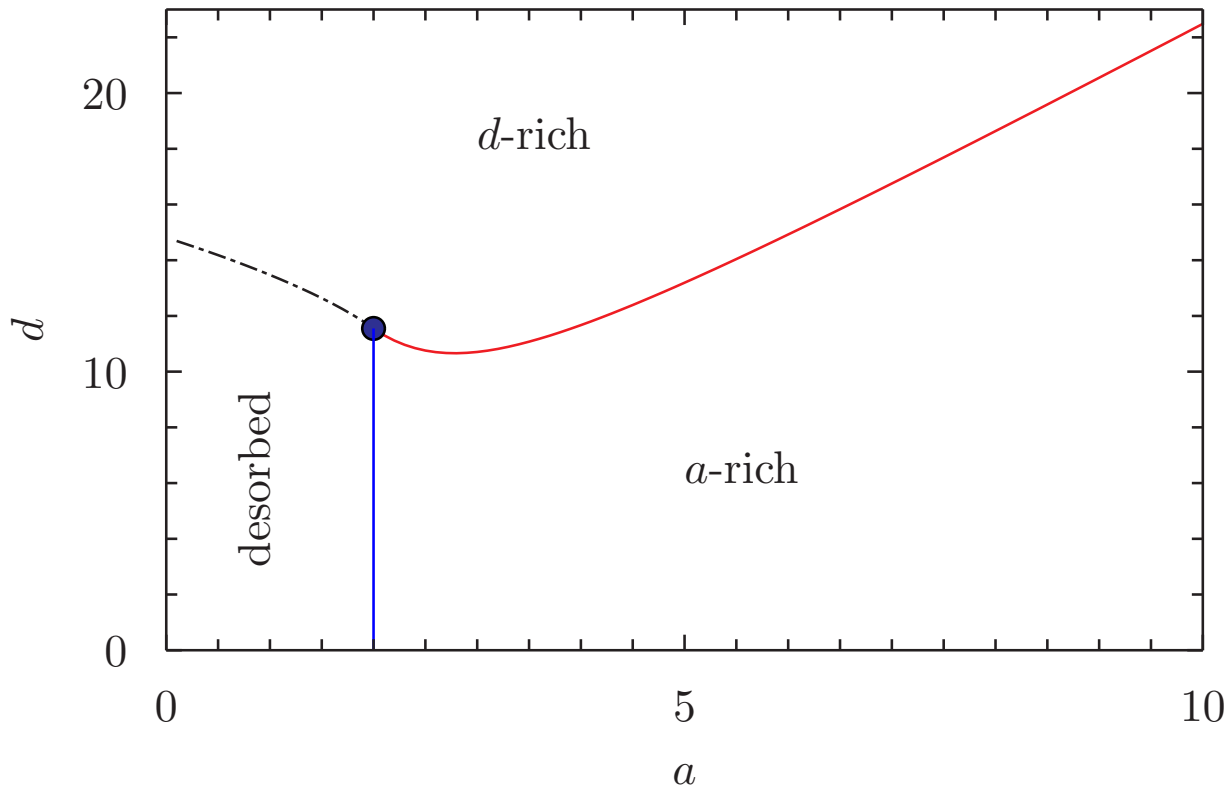
There are two singularities of $G(a,a;z)$ giving rise to two phases:

- 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*

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

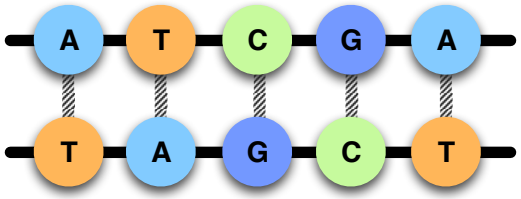
- $r = 2$ model has *two* phase transitions as temperature changed .
- At very low temperatures the model is in a d-rich phase
- while at high temperatures the model is in the desorbed state.
- At intermediate temperatures the system is in an a-rich phase.
- Both transitions are second-order with jumps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

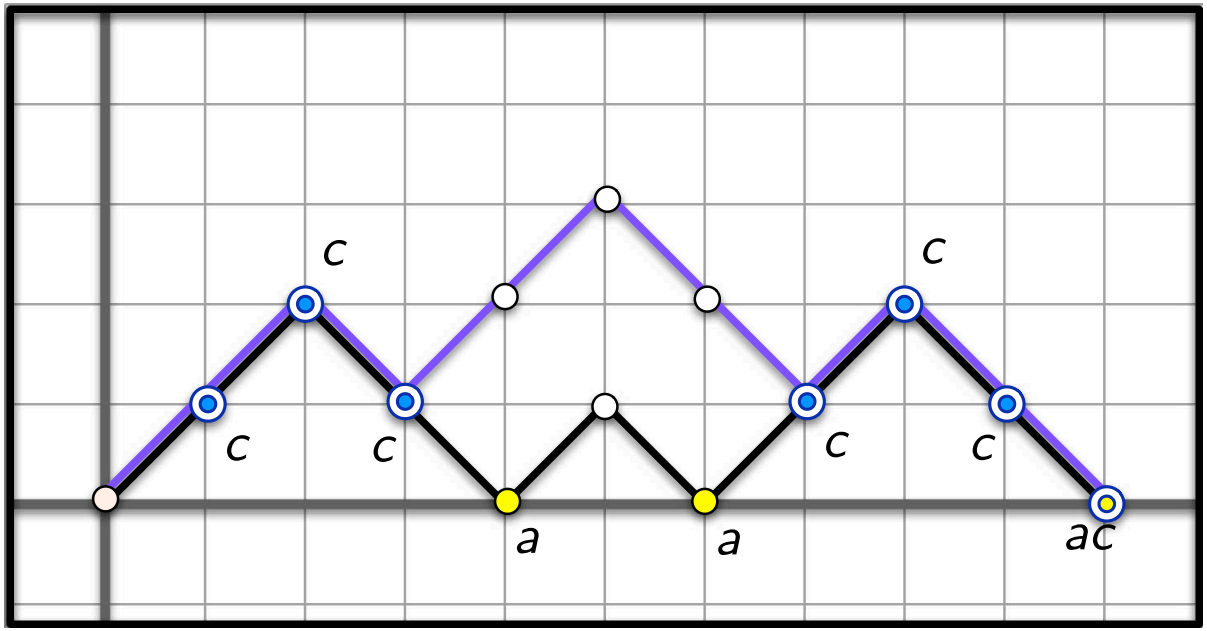
(Our model — Adsorption and Unzipping)

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

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:

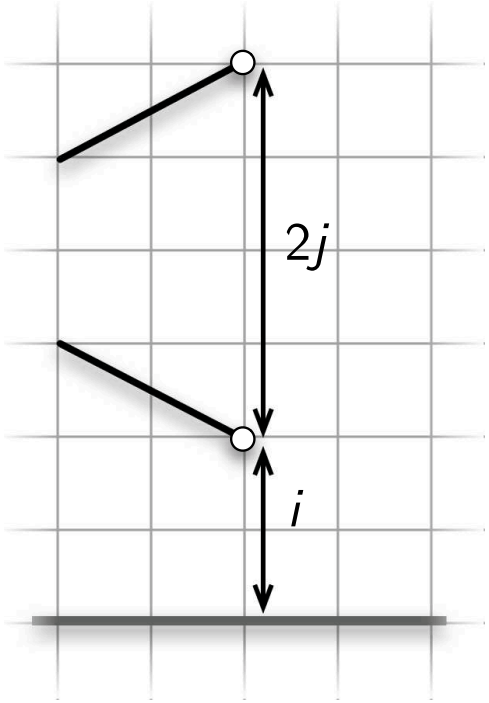
$$\mathcal{A}(a,c) = \lim_{n\to\infty} \frac{\langle m_a \rangle}{n} \qquad \text{and} \qquad \mathcal{C}(a,c) = \lim_{n\to\infty} \frac{\langle m_c \rangle}{n},$$

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:

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



FUNCTIONAL EQUATION

As before:

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

where

$$A(a) = \frac{a-1}{a}, \quad C(c) = \frac{c-1}{c}$$

and the same kernel $K(r,s)$ is

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

Magic decomposition of $G(a,c)$

We can re-write $G(a,c)$ in terms of $G(a,1)$ and $G(1,c)$:

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

SOLUTION FOR $G(a,1)$

Exact solution for $G(a,1)$ is known from first part of talk!

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 have: $G(1, c) = [r^1]\text{mess}(r, a, c; z) \equiv [r^1]H(r; z)$
- Traditionally, get series rep. for H. Sometimes an art — see first part of this talk!
- Alternative — find differential equation satisfied by generating function
- Difficult to solve, but DE just as useful for analysis!
- Use Zeilberger-Gosper algorithm: Maple: DETools package, Zeilberger hyperexp. implementation
- Result: DE for $G(1, c)$ is order 6 with poly. coeff of $\deg_z = 12$

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:

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

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

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

ORDER PARAMETERS AND PHASES

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

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

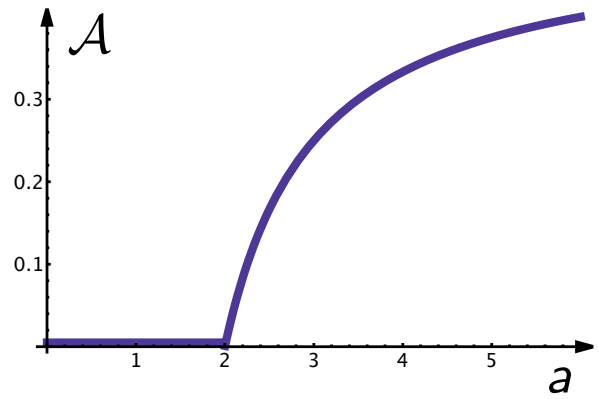
Four Phases:

- 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) $\mathcal{A} > 0, \mathcal{C} > 0$

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

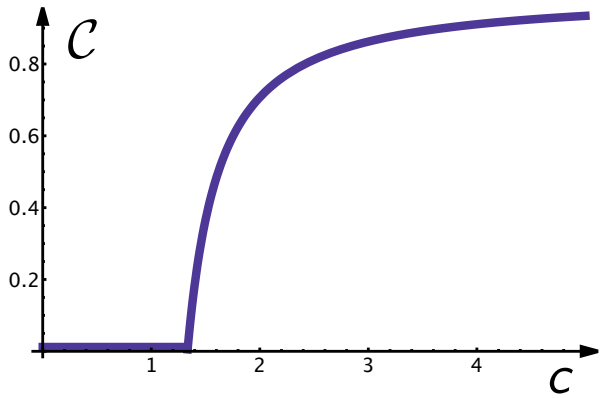
- For $G(a,1)$:

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



- For $G(1,c)$:

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



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

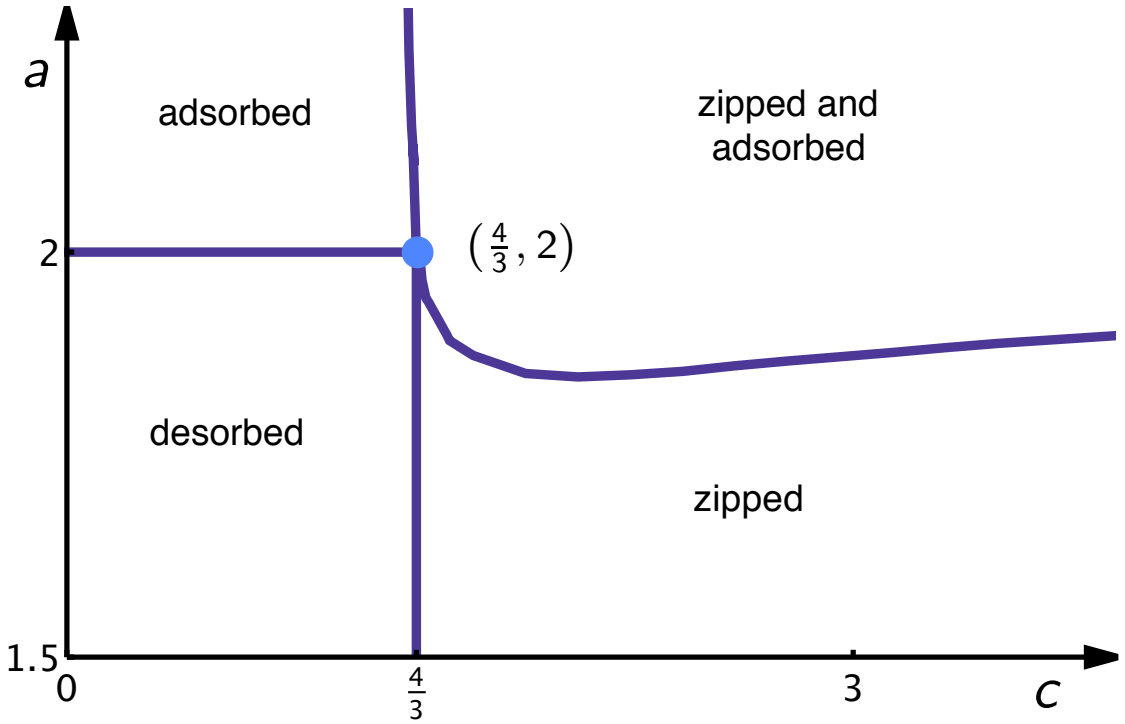
Analysing $G(a, c)$

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.
- Can find location of pole precisely

PHASE DIAGRAM



Low-temp argument

- $c \to \infty$, crit. $a = 2$
- $a \to \infty$, crit. $c = \sqrt{5} - 1$

Conclusion

- Simple model of DNA as two friendly walks near a boundary
- Used obstinate kernel method to produce two sets refined fn. eqns
- Combined these eqn to relate $G(a, c)$ to both $G(a, 1)$ and $G(1, c)$
- Used Zeilberger-Gosper algorithm to find lin. DE for $G(1, c)$
- Started analysis of phase diagram

FUTURE WORKS

- Finish analysis of (a, c)- model
- Combine single, double surface and unzipping interactions
- Also in progress is work in a slit
- Extend these to various interactions