Three Interacting Friendly Directed Walks; A Simple Model of Polymer Gelation

[†]Aleks Owczarek, [‡]Andrew Rechnitzer, and [†]Rami Tabbara

[†]MASCOS and School of Mathematics and Statistics, The University of Melbourne

[‡]Department of Mathematics and Statistics, University of British Columbia

June, 2015

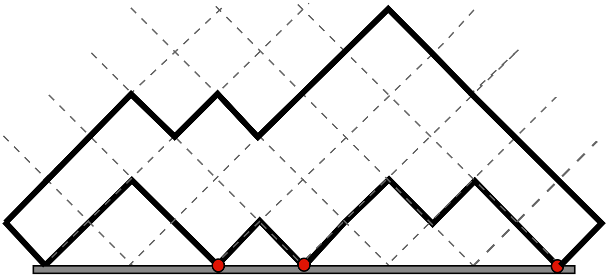
CANADAM 2015

AUSTRALIAN RESEARCH COUNCIL
Centre of Excellence for Mathematics and Statistics of Complex Systems

THE UNIVERSITY OF MELBOURNE

Directed walks lattice models

- Simple lattice models of polymers in solution
- Interface of combinatrorics, probability theory and statistical physics
- There are many exact solutions of single and multiple directed walk models



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
- Multiple walks: Bethe Ansatz & Lindström-Gessel-Viennot (LGV) Lemma
- LGV Lemma: multiple walks = determinant of single walks (partition functions)
- Interactions have been added to a single walk of various types
- Multiple walks where interaction confined to a single walk
- Recently we have considered some problems where there are interactions between walks
- These can give non-D-finite solutions

Some known exact solutions: geometries

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

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)

SOME KNOWN EXACT SOLUTIONS: INTERACTIONS

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)

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)

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

SO HOW DO WE FIND A SOLUTION: KERNEL METHOD

- Consider generating function
- Combinatorial decompose a 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″ where bulk term is product of kernel and bulk generating function
- Answer needed is one of the boundary generating functions so try to remove bulk by setting the value of a catalytic variable to a value that makes the kernel vanish
- Standard kernel method due to *Knuth* (1968): use values of ″catalytic variable’ to ″kill″ kernel
- From ≈ 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 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)

Double Interaction Adsorption Model

Two walks above a surface — both walks can interact with wall

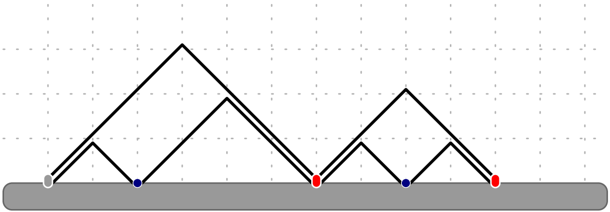


Figure : Two directed walks with single and “double” visits to the wall the surface.

- 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 denoted m_a,
- number of *double visits* denoted m_d.

The partition function is

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

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

- *a is associated with (weights or counts) each single visit to the wall*
- *d is associated with (weights or counts) each double visit to the wall*

The generating function is

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

Double Interaction Adsorption Model

- Used combinatorial decomposition to obtain linear functional equation
- Exact solution of generating function can be found
- Obstinate kernel method with a generalisation for inclusion of interactions
- "Group of walk" has eight elements
- $D(a, d)$ can be written in terms of $D(a, a)$ via "primitive piece" argument or using obstinate kernel method
- $D(a, a)$ can be found via obstinate kernel method or other methods
- Solution is not D-finite — LGV lemma does not apply directly
- Interesting discrete maths
- Phase diagram with second and first order transitions
- Interesting physics
- Scaling of partition function calculated
- Owczarek, Rechnitzer, and Wong, *J. Phys. A: Math. Theor.*, **45** 425002, (2012)

UNZIPPING ADSORPTION MODEL

Simple model of DNA as two friendly walks near a boundary

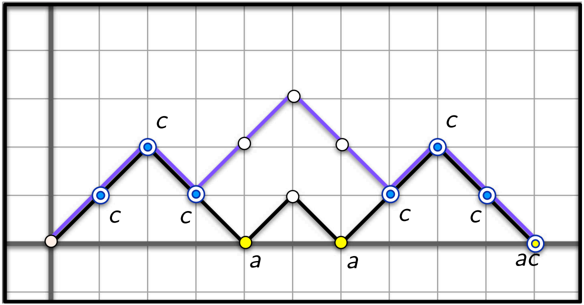


Figure : An allowed configuration of length 10. The overall weight is a^3c^7

- 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*)

MODEL

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

The partition function is

$$Z_n^{(u)}(a,c) = \sum_{\hat{\varphi} \ni |\hat{\varphi}|=n} e^{(m_a(\hat{\varphi})\cdot\varepsilon_a + m_d(\hat{\varphi})\cdot\varepsilon_c)/k_B T}$$

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

- *a is associated with (weights or counts) each single visit to the wall*
- *c is associated with (weights or counts) each joint visit of the two walks to site*

The generating function is

$$U(a,c;z) = \sum_{n=0}^{\infty} Z_n^{(u)}(a,c) z^n.$$

Summary for Unzipping-adsorption model

- Exact solution of generating function can be found
- Used combinatorial decomposition to obtain linear functional equation
- Obstinate kernel method with a generalisation for inclusion of interactions
- "Group of walk" has eight elements
- $U(a,c)$ can be written in terms of $U(a,1)$ and $U(1,c)$ using observed functional equation relationship after applying obstinate kernel method
- No obvious combinatorial explanation (e.g. primitive pieces)
- $U(a,1) = D(a,a)$ already known
- $U(1,c)$ can be found via obstinate kernel method
- Explicit series solutions for $U(a,1)$ and $U(1,c)$
- Also used Zeilberger-Gosper algorithm to find linear DE for $U(1,c)$
- Phase diagram with four phases and second order transitions
- Scaling of partition function calculated
- 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 — gelation

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

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

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

- Energy $-\varepsilon_c$ for visits of any two walks to a single lattice site
- An extra energy $-\varepsilon_d$ when all three walks visit a single site
- That is, a total energy $(-2\varepsilon_c - \varepsilon_d)$ when all three walks visit a single site

WEIGHTS

- double visits weight: $c \equiv e^{\varepsilon_c / k_B T}$
- triple visits extra weight factor: $d \equiv e^{\varepsilon_d / k_B T}$
- total weight for triple visits: $t = c^2 d$
- trivial walk consisting of zero steps has weight 1.

- number of *shared contact sites* between the top-to-middle and the middle-to-bottom walks is denoted m_c
- number of *triple shared contact sites* where all three walks coincide is denoted m_d

THE MODEL

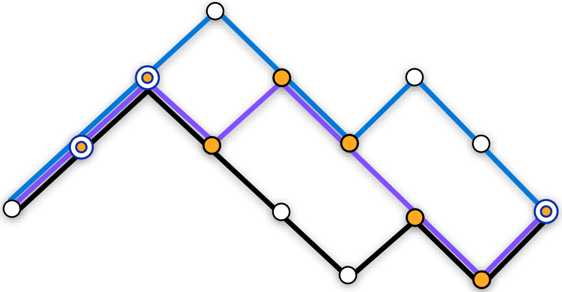


Figure : An example of an allowed configuration of length 8. Here, we have $m_c = 11$ double shared contact steps and $m_d = 3$ triple shared contact steps. Thus, the overall Boltzmann weight for this configuration is $c^{11}d^3 = c^5t^3$

Generating function

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

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

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

PRIMITIVE PIECES

- Let $\widehat{\Omega}_P$ be the subclass where *all* three walks share a common site only at the very beginning and end of the configuration.
- Then the *primitive* generating function $P(c;z)$

$$P(c;z) = \sum_{\varphi \in \widehat{\Omega}_P} z^{|\varphi|} c^{m_c(\varphi)} \tag{1}$$

- Importantly any $\varphi \in \widehat{\Omega}$ can be uniquely decomposed into a sequence of primitive walks. Hence

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

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

Hence solve for our full model it suffices to solve for the model that ignores triple shared contact effects with corresponding generating function $G(c,1;z)$

Generalised generating function

We consider walks φ in the larger set, where each walk can end at any possible position and not necessarily together.

- Let $\Omega(i,j)$ be the class of triple walks that consists of configurations with final top to middle walk distance i and middle to bottom distance j, that still obey friendly constraints
- To find $G(c,1)$, consider larger class of configurations $\widehat{\Omega} \equiv \bigcup_{i\geq 0, j\geq 0} \Omega(i,j)$
- Generalised generating function:

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

- $G(c,1) = F(0,0)$

where z is conjugate to the length $|\varphi|$ of a configuration $\varphi \in \widehat{\Omega}$, r and s are conjugate to *half* the distance $h(\varphi)$ and $f(\varphi)$ between the final vertices of the top to middle and middle to bottom walks respectively.

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

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

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 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')

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

- *We make use these 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):

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

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

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 partially-gelated phase is observed when

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

and finally we have a fully-gelated phase when

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

ANALYSING $G(a, c)$

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

$$z_s(c,d) = \begin{cases} z_b \equiv 1/8, & c \le 4/3, d < 9/8 \\ z_b, & c \le \alpha(d), d \ge 9/8 \\ z_p(c,d), & c > \alpha(d), d \ge 9/8 \\ z_c(c) \equiv \frac{1-c+\sqrt{c^2-c}}{2c}, & c > 4/3, d < \beta(c), \\ z_p(c,d), & c > 4/3, d \ge \beta(c), \end{cases}$$

- $\alpha(d)$ is boundary between free and fully-gelated phases
- $\beta(c)$ is the boundary between partially-gelated and fully-gelated phases

where each of the different singularities are associated with different phases:

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

Phase diagram

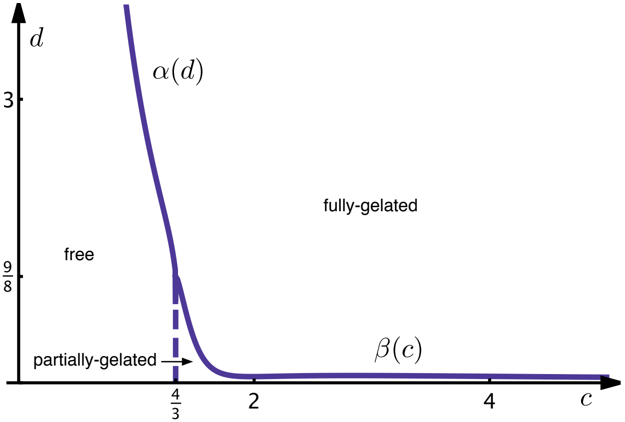


Figure : The phase diagram of our full model. First and second order phase transitions are observed when crossing solid and dashed lined boundaries respectively. All phase boundaries coincide at $c = 4/3$ and $d = 9/8$.

TRANSITIONS

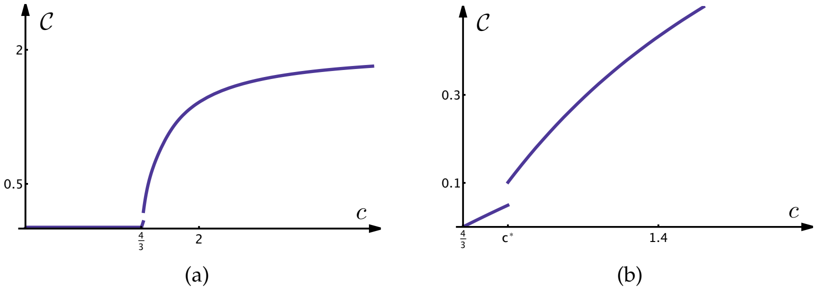


Figure : The limiting average number of shared contacts $\mathcal{C}$ when $d = 1$. There is a second and first order phase transition at $c = 4/3$ and $c = c^\star \approx 1.34865$ respectively. Figure (b) is a rescaling of the plot (a) to highlight the finite-jump discontinuity at $c = c^\star$.

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	$8^n n^{-3}$
free to partial-gelation boundary	$8^n n^{-2}$
free to full-gelation boundary	$8^n n^{-1/2}$
$c = 4/3, d = 9/8$	$8^n n^{-1/2}$
partial-gelation	$z_c(c)^{-n} n^{-3/2}$
partial to full-gelation boundary	$z_c(c)^{-n} n^{-1/2}$
full-gelation	$z_p(c, d)^{-n} n^0$

Phase diagram in different variables

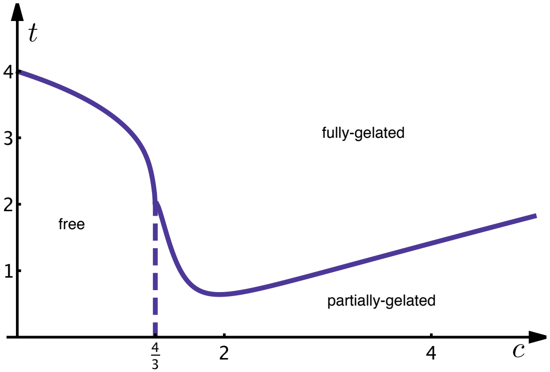


Figure : The phase diagram of our full model when setting $d = t/c^2$. First and second order phase transitions are observed when crossing sold and dashed lined boundaries respectively. All phase boundaries coincide at $c = 4/3$ and $t = 2$.

Conclusion

- Simple model of 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 in preparation