Exact Solutions of Interacting Friendly Directed Walkers

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

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

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

July, 2015

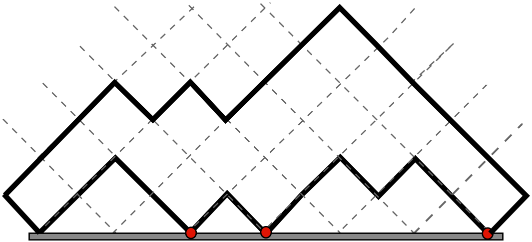
AUSTRALIAN RESEARCH COUNCIL
Centre of Excellence for Mathematics and Statistics of Complex Systems

Baxter 2015

THE UNIVERSITY OF MELBOURNE

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
  in progress/almost complete ('15)

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 ≈ 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

UNZIPPING ADSORPTION MODEL

Simple model of DNA as two friendly walks near a boundary

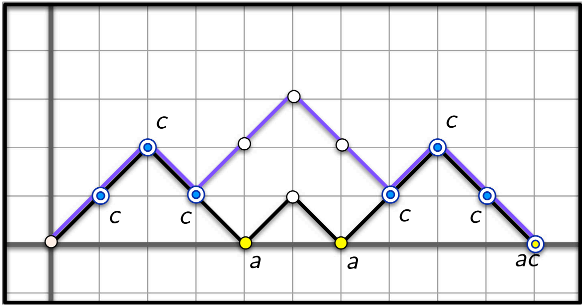


Figure : An allowed configuration of length 10. The overall weight is a^3c^7

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

MODEL

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

The partition function is

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

The generating function is

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

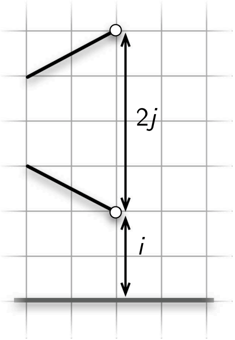
GENERALISED GENERATING FUNCTION

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

- Generalised generating function:

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

$$G^{(u)}(a,c) = F(0,0)$$



ESTABLISHING A FUNCTIONAL EQUATION

- Adding a single column onto a configuration leads to a decomposition
- Translating back to generating functions we end up with

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

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

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

Symmetries of the Kernel

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

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

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

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

- *Use of four of these which only involve positive powers of r.*
- *Then eliminate some of the unknown generating functions*

Combining the equations

Key idea

- Treat K as function 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 $\hat{r}$:

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

- *These combinations generalise the alternating sum of the orbit sum in previous applications of the obstinate kernel method*
- *Factors that look like Bethe amplitudes*

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 $r \mapsto \hat{r}$ or $s \mapsto \hat{s}$*
- *Use Lagrange Inversion to find $\hat{r}^k$ as a series*

SOLUTION FOR $G^{(u)}(1, c)$

Exact solution for $G^{(u)}(a, 1)$ was already known though it can be found using the method described

- No known previous solution for $G^{(u)}(1, c)$

We can write functional equation as

$$G^{(u)}(1, c) = F(0, 0, 1, c; z) = [r^1] \frac{\hat{s}\,(r^2 - 1)\,[r - cr + cz\,(1 + r^2 - \hat{s})]}{(c - 1)\,(\hat{s} - c\hat{s} + crz)},$$

expanding RHS as power series in c and so obtain, after some work:

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

SOLUTION FOR $G^{(u)}(1, c)$

- While we have an explicit solution for $G^{(u)}(1, c)$ 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 $G^{(u)}(1, c)$ is order 6 with poly. coeff of $\deg_z = 12$

FORTUNATE DECOMPOSITION OF $G^{(u)}(a, c)$

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

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

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

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

ANALYSING $G(a,c)$

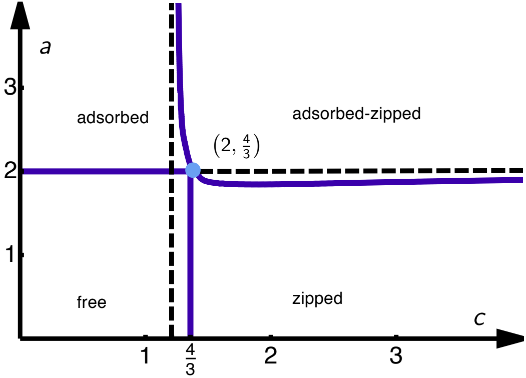
- Singularities: Look at $G^{(u)}(a,1)$, $G^{(u)}(1,c)$ and root of above denom.
- Four Phases: Free, zipped, adsorbed and zipped-adsorbed

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

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

- $\alpha(a)$ 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 $G^{(u)}(a, c; z)$ 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	$z_{ac}(a, c)^{-n} n^{-1}$

Double Interaction Adsorption Model

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

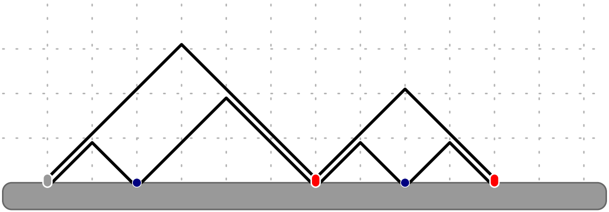


Figure : Two directed walks with single and "double" visits to the wall the surface. This walk has weight $a^2 d^2$.

- *a is a fugacity for each single visit to the wall*
- *d is a fugacity for each double visit to the wall*

MODEL

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

The partition function is

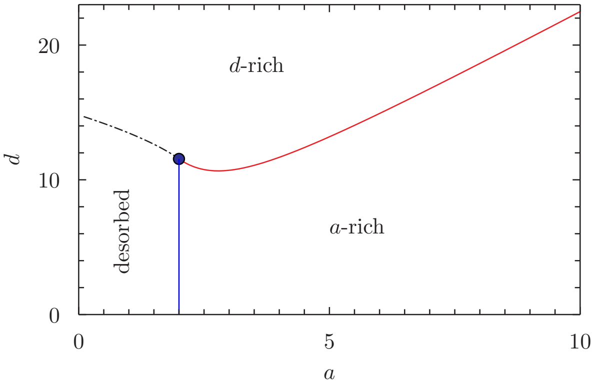
$$Z_n^{(d)}(a,d) = \sum_{\widehat{\varphi} \ni |\widehat{\varphi}|=n} a^{m_a(\widehat{\varphi})} d^{m_d(\widehat{\varphi})}$$

The generating function

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

can be found by the obstinate kernel method.

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 $(a, d) = (a^*, d^*) = \left(2, \frac{16(8-3\pi)}{64-21\pi}\right)$. Note that d^* is not algebraic.

Double Interaction Adsorption Model

- Exact solution of generating function can be found in the same way
- Exactly the same kernel (two walks above a wall)
- Key idea here: one can prove that the solution is not D-finite
- LGV lemma does not apply directly
- Phase diagram with second and first order transitions
- Scaling of partition function calculated

THREE WALKS AND GELATION INTERACTIONS: TWO TYPES

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

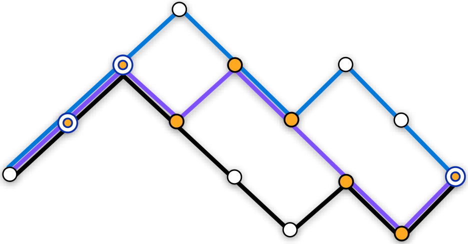


Figure : An example of an allowed configuration of length 8. Here, we have $m_c = 11$ double shared contact steps and $m_d = 3$ triple shared contact steps. Thus, the overall Boltzmann weight for this configuration is $c^{11}d^3 = c^5t^3$

THREE WALKS AND GELATION INTERACTIONS: TWO TYPES

Model set of polymers in solution that can attract each other — 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: $Z_n^{(t)}(c,d) = \sum_{\varphi \in \widehat{\Omega}, |\varphi|=n} c^{m_c(\varphi)} d^{m_d(\varphi)}$

- Generating function: $G(c,d) \equiv G(c,d;z) = \sum_{n \geq 1} Z_n^{(t)}(c,d) z^n$

Primitive pieces

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

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

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

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

Generalised generating function

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

- Generalised generating function:

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

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

The decomposition of the set of walks gives

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

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*

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

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

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 have used Zeilberger-Gosper algorithm to find linear DE for denominator of $G(c,1)$
- Full analysis of asymptotics and phase diagram almost complete
- All transitions seem to be first order

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