Exact Solution of Asymmetric Gelation between Three Walks on the Square Lattice

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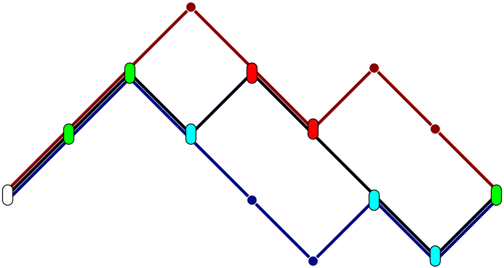
DIRECTED WALKS LATTICE MODELS

- 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

- Interactions have been applied to single walk problems of various types
- Also, multiple walks have been considered where interactions are confined to a single walk
- Later 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

Extending the problems that can be solved exactly by increase in the numbers of walks and adding different types of interactions

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 symmetric inter-walk interactions
  Tabbara, Owczarek, Rechnitzer, J. Phys. A: Math. Theor. 49 154004 (27pp) (2016)

ONE WAY TO 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 and Mishna* Contemp. Math. **520** (2010)
- Solutions are not always D-finite
- Quarter plane random walk problems
- Diagonals of multi-variate rational functions

THREE WALK WATERMELONS WITH GELATION INTERACTIONS

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

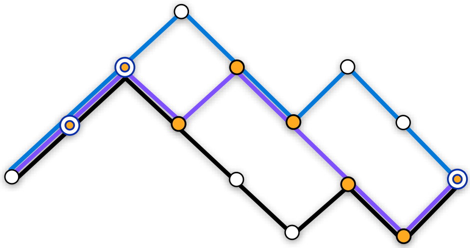


Figure: A watermelon configuration, that starts and ends together, of length 8. There are $m_c = 11$ double shared contact sites (a triple contact counts two double contacts). The Boltzmann weight for this configuration is c^{11}.

Three walks and gelation interactions

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
- total weight for triple visits: $t = c^2$
- Walks start and end together: Watermelons
- m_c is the number of *double contacts* between pairs of walks
- Partition function: $Z_n^{(t)}(c) = \sum_{\varphi \in \widehat{\Omega}, |\varphi| = n} c^{m_c(\varphi)}$
- Generating function: $G_f(c) \equiv G_f(c; z) = \sum_{n \geq 1} Z_n^{(t)}(c) z^n$

Generalised generating function

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

- Generalised generating function:

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

- $G_f(c) = F(0,0)$: $r = s = 0$ gives watermelon configurations

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

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

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')

Friendly Watermelon Generating Function

$$G_f(c;z) = \frac{1}{(c-1)^2}\left(1 + \frac{c\left(c^2 z + c^2 - 3c\right)\sqrt{1-4cz}}{D(c;z)}\right)$$

where

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

and

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

GENERALISING

Can we solve a model where the interaction between the top two walks is different to the interaction between the bottom two walks?

- We tried!
- However, the breaking of the symmetry meant we didn't have enough equations arising in the obstinate kernel method to solve the problem.
- The complication of the symmetric solution: D-Finite but of high order DE meant "guessing" was difficult
- So let's try a different walk problem: back to osculating!
- Stars vs Watermelons

Osculating Stars

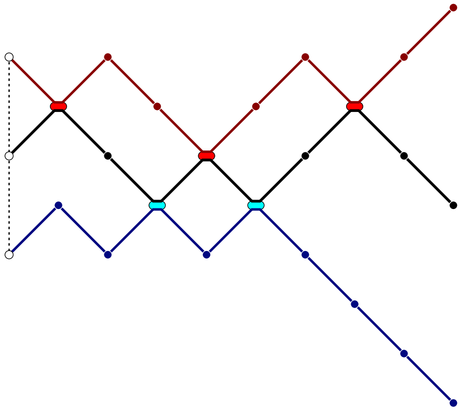


Figure: Three osculating walks in a star configuration of length $n = 9$. We have $m_a = 3$ shared sites between the upper two walks and $m_b = 2$ shared sites between the lower two walks. The Boltzmann weight is $a^3 b^2$.

THREE WALK OSCULATING STARS

For any configuration $\varphi \in \Omega_3$, we assign a weight a to the $m_a(\varphi)$ *shared contact sites* and a weight b to the $m_b(\varphi)$ *shared contact sites* between the top-to-middle and the middle-to-bottom walks respectively. Note, all three walks cannot share the same site. The partition function for our model consisting of n triple steps is

$$Z_n(a,b) = \sum_{\varphi \in \Omega_3, |\varphi|=n} a^{m_a(\varphi)} b^{m_b(\varphi)},$$

where $|\varphi|$ denotes the length of the configuration φ.

$$G_3(a,b;z) = \sum_{n=0}^{\infty} Z_n(a,b) z^n$$

Free energy, growth constant and order parameters

The free energy κ is

$$\kappa(a, b) = \log z_s(a, b),$$

where $z_s(a, b)$ is the real and positive singularity of the generating function that is closest to the origin. Moreover, it is expected that for any fixed a and b the partition function scales with growth constant μ as

$$Z_n(a, b) \sim A(a, b)\ \mu(a, b)^n\ n^{\gamma-1},$$

$$\mu(a, b) = z_s(a, b)^{-1} = e^{-\kappa(a,b)}.$$

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

and

$$\mathcal{B}(a, b) = \lim_{n\to\infty} \frac{\langle m_b \rangle}{n} = b\frac{\partial \kappa}{\partial b}.$$

Phases

We can then characterise the possible phases in the following way. We say that the system is in a *free* phase when

$$\mathcal{A} = \mathcal{B} = 0.$$

A *top zipped* phase with the top two walks only bound together is indicated by the situation when

$$\mathcal{A} > 0 \text{ with } \mathcal{B} = 0,$$

whilst a *bottom zipped* phase with the bottom two walks only bound together is indicated by the situation when

$$\mathcal{B} > 0 \text{ with } \mathcal{A} = 0.$$

When both

$$\mathcal{B} > 0 \text{ and } \mathcal{A} > 0$$

all three walks are bound, which we refer to as *fully zipped*.

Phase Transitions

Phase transitions are defined by non-analytic behaviour of the free energy and so are indicated by a non-analytic change in the singularity of the generating function. It is usual to define the exponent α as related to the non-analyticity in the free energy κ^{non} as

$$\kappa^{non} \sim K\, t^{2-\alpha} \text{ as } t \to 0, \tag{1}$$

where t measures in Boltzmann weights a and b (or temperature) the distance to the phase transition and K is a constant. This implies that the associated order parameter $\mathcal{M} = \mathcal{A}, \mathcal{B}$ behaves as

$$\mathcal{M} \sim M\, t^{1-\alpha} \text{ as } t \to 0^+. \tag{2}$$

A standard scaling argument connects this to the scaling of the number of contacts evaluated exactly at the transition

$$\langle m_{a,b} \rangle (n) \sim C\, n^{\phi}, \tag{3}$$

where

$$\phi = 2 - \alpha. \tag{4}$$

Functional Equation

$$F(r,s,a,b;z) \equiv F(r,s) = \sum_{\varphi \in \Omega_3} z^{|\varphi|} r^{h(\varphi)/2} s^{f(\varphi)/2} a^{m_a(\varphi)} b^{m_b(\varphi)},$$

$$K(r,s)F(r,s) = rs - \left(\frac{(1+r)(r+s+rs)z}{rs} + \frac{1-b}{b} \right) F(r,0) - \left(\frac{(1+s)(r+s+rs)z}{rs} + \frac{1-a}{a} \right) F(0,s),$$

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

$$K(r,s) \equiv K(r,s;z) = 1 - \frac{z(r+1)(s+1)(r+s)}{rs}.$$

Want 'stars' with $r = s = 1$

$$G_3(a,b;z) = F(1,1,a,b;z)$$

Still not clear we have enough equations ...

Two interacting osculating star walks

Two walks have previously been studied[1]. The generating function is a quadratic algebraic equation

$$G_2(a,z) = \frac{1+(3z-1)a}{2z(1+a(2z-1)+z^2a^2)\sqrt{1-4z}} - \frac{1+a(3z-1)+2z^2a^2}{2z(1+a(2z-1)+z^2a^2)}.$$

The asymptotic behaviour of the average number of contacts, $m(a)$, is

$$m(a) = \langle m \rangle = \begin{cases} \frac{a}{(4-a)} + O(n^{-1}) & a < 4 \\ \frac{1}{\sqrt{\pi}} \cdot \sqrt{n} + O(1) & a = 4 \\ \frac{a-\sqrt{a}-2}{2(a-1)} \cdot n + O(1) & a > 4. \end{cases}$$

The associated order parameter

$$\mathcal{M}(a) = \lim_{n\to\infty} \frac{\langle m \rangle}{n} = a\frac{\partial \kappa}{\partial a} = \begin{cases} 0 & a \le 4 \\ \frac{a-\sqrt{a}-2}{2(a-1)} & a > 4. \end{cases}$$

[1] *Fisher* J. Stat. Phys 34: 667 1984, *Katori and Inui*, Trans. Mat. Res. Soc.- Japan, 26: 405, 2001, *Guttmann and Vöge*, J. Stat. Plan. Inf 10: 107 2002

Two interacting osculating star walks

The phase transition is a continuous one with $\alpha = 0$ (the order parameter decays linearly on approaching the transition) and $\phi = 1/2$. There is a jump in the specific heat on traversing the transition at $a = 4$.

Table: The growth rate and entropic exponent for two walk stars.

Phase region	μ	γ
Free	4	1/2
Zipped	$\frac{a}{\sqrt{a}-1}$	1
Free to Zipped transition	4	1

Three symmetric osculating star walks

For $r = s = 1$ (stars) and general $a = b$ (symmetric case) the generating function is quadratic.

$$G_3(a, a; z) = \frac{(6az - a + 1)(az + 1)(az - 1)}{4z^2 (a^2 z - a + 2)(4a^2 z^2 + 4az - a + 1)} \cdot \sqrt{1 - 4z}$$
$$+ \frac{-8a^4 z^4 + 2a^2 (a - 20) z^3 + a(a + 7)(a - 4) z^2 + (10a - 4) z - a + 1}{4z^2 (a^2 z - a + 2)(4a^2 z^2 + 4az - a + 1)}.$$

The asymptotic behaviour of the average number of contacts, $m(a)$, is

$$m(a) = \begin{cases} \frac{a(192-8a-a^2)}{(4-a)(64-a^2)} + O(n^{-1}) & a < 4 \\ \frac{3}{\sqrt{\pi}} \cdot \sqrt{n} + O(1) & a = 4 \\ \frac{a-4}{a-2} \cdot n + O(1) & a > 4. \end{cases}$$

The associated order parameter is given by

$$\mathcal{M}(a) = \begin{cases} 0 & a \leq 4 \\ \frac{a-4}{a-2} & a > 4. \end{cases}$$

PHASE DIAGRAM

The transition is continuous with $\alpha = 0$ and $\phi = 1/2$. Also, as with two walk stars when $a < 4$ there is a free phase where the none of the pairs of walks share a macroscopic number of sites whilst they are all zipped together (fully zipped) for $a > 4$ sharing a non-zero macroscopic density of sites.

Table: The growth rates and entropic exponents for three walk stars with symmetric interactions.

Phase region	μ	γ
Free	8	$-1/2$
Fully Zipped	$\frac{a^2}{a-2}$	1
Free to Fully Zipped	8	1

ASYMMETRIC SOLUTION

For particular values of $a \neq b$ (for example $(a, b) = (1, 2), (2, 3), (2, 4), (3, 4)$ and so on) we generated long series and were able to guess quartic equations using the Ore Algebras package[2] for the Sage computer algebra system. By computing these quartics at sufficient particular values of $a \neq b$ we were able to construct the general $a \neq b$ equation.

$$\sum_{j=0}^{4} c_j(a, b; z) G^j = 0,$$

where the coefficients $c_j(a, b; z)$ are polynomials in a, b and z.

$$c_4(a, b; z) = 4z^6(4b^2z^2 + 4bz - b + 1)(4a^2z^2 + 4az - a + 1)(a^2b^2z^2 + 2abz - ab + a + b)^2.$$

[2] *Kauers, Jaroschek, and Johansson*. In Computer Algebra and Polynomials: Applications of Algebra and Number Theory, pages 105–125. Springer, 2015)

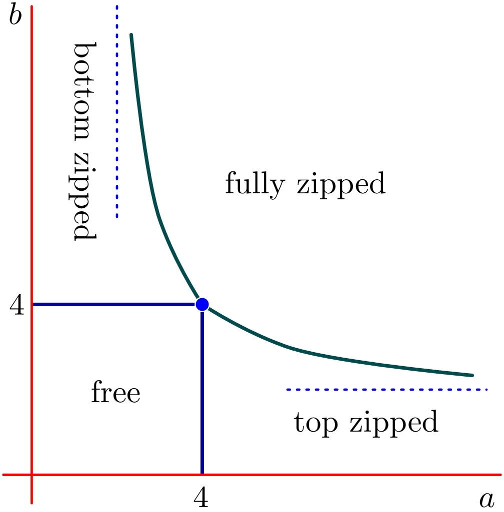
SINGULARITIES

We located possible singularities by examining its discriminant of the quartic and the zeros of the leading coefficient. We can also locate potential singularities by converting the algebraic equation to a (second order) linear differential equation and examining the zeros of its highest order term. In so doing, we found four independent singularities $(z_{\text{free}}, z_{\text{top}}, z_{\text{bottom}}, z_{\text{fully}})$ of the generating function

$$z_c(a = a, b) = \begin{cases} z_{\text{free}} = \frac{1}{8} & \text{when } a < 4 \text{ and } b < 4 \\ z_{\text{top}}(a) = \frac{\sqrt{a}-1}{2a} & \text{when } a > 4 \text{ and } 0 \le b < \frac{2\sqrt{a}}{\sqrt{a}-1} \\ z_{\text{bottom}}(b) = \frac{\sqrt{b}-1}{2b} & \text{when } 0 \le a < \frac{2\sqrt{b}}{\sqrt{b}-1} \text{ and } b > 4 \\ z_{\text{fully}}(a, b) = \frac{-1+\sqrt{(a-1)(b-1)}}{ab} & \text{otherwise.} \end{cases} \tag{5}$$

Phase boundaries were found by looking where the singularities are equal.

Phase diagram



FREE PHASE

For low a, b when $a < 4, b < 4$ the dominant singularity is $z_c = z_{\text{free}} = \frac{1}{8}$. In this region we find that

$$Z_n \sim 8^n \, n^{-3/2}.$$

Leading to $\mu = 8$ and $\gamma = -1/2$.
In this phase we have calculated that

$$m_a(a,b) = \frac{a(ab + 8b - 192)}{2(4-a)(ab-64)} + O(n^{-1}),$$
$$m_b(a,b) = \frac{b(ab + 8a - 192)}{2(4-b)(ab-64)} + O(n^{-1}).$$

so that

$$\mathcal{A} = \mathcal{B} = 0 \text{ when } a < 4 \text{ and } b < 4,$$

Partially zipped phases

For top zipped

$$Z_n \sim z_{\text{top}}^{-n} \, n^{-1/2}.$$

Leading to

$$\mu = \frac{1}{z_{top}} = \frac{2a}{\sqrt{a} - 1}$$

and $\gamma = 1/2$.
In this region we have

$$m_a(a, b) = \frac{a - \sqrt{a} - 2}{2(a-1)} \cdot n + o(n),$$
$$m_b(a, b) = O(1).$$

For bottom zipped b replaces a.

Fully Zipped

$$Z_n \sim z_{\text{fully}}^n.$$

Leading to

$$\mu(a,b) = \frac{1}{z_{\text{fully}}(a,b)} = \frac{ab}{-1+\sqrt{(a-1)(b-1)}}$$

and $\gamma = 1$.

The order parameters, both of which are non-zero which implies that all three walks are zipped together as hence we refer to this phase a *Fully Zipped*:

$$\mathcal{A}(a,b) = \frac{a}{z_{\text{top}}(a)} \frac{\partial z_{\text{top}}(a)}{\partial a} = \frac{1}{2(a-1)} \left(a - 2 + \frac{a}{1+\sqrt{(a-1)(b-1)}} \right),$$

$$\mathcal{B}(a,b) = \frac{b}{z_{bot}(b)} \frac{\partial z_{bot}(b)}{\partial b} = \frac{1}{2(b-1)} \left(b - 2 + \frac{b}{1+\sqrt{(a-1)(b-1)}} \right).$$

Summary of Results

Table: The growth rates and entropic exponent for three walk stars with asymmetric interactions. In the top part of the table each of the primary phases are listed whilst in the bottom part of the table the phases boundaries are listed.

Phase regions	μ	γ
free	8	$-1/2$
partially zipped (top)	$\frac{2a}{\sqrt{a}-1}$	$1/2$
partially zipped (bottom)	$\frac{2b}{\sqrt{b}-1}$	$1/2$
fully zipped	$\frac{ab}{\sqrt{(a-1)(b-1)}-1}$	1
Phase boundaries	μ	γ
free to partially zipped (top)	8	$1/4$
free to partially zipped (bottom)	8	$1/4$
free to fully zipped	8	1
partially zipped (top) to fully zipped	$\frac{2a}{\sqrt{a}-1}$	1
partially zipped (bottom) to fully zipped	$\frac{2b}{\sqrt{b}-1}$	1

Conclusion

- Model of asymmetric gelation with three osculating walks on the square lattice has been solved
- Solution is a algebraic and, in particular, quartic as opposed to symmetric case which is quadratic
- Focus was on osculating stars since friendly watermelons proved more difficult to analyse (D-Finite not algebraic)
- Found solution my using Sage package at a number of fixed integer values of the parameters
- Current writing up work on four walks

Owczarek and Rechnitzer, arXiv:2507.17111 ('25)