

Exact solution of asymmetric gelation between three walks on the square lattice

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Abstract

We find and analyse the exact solution of a model of three different polymers with asymmetric contact interactions in two dimensions, modelling a scenario where there are different types of polymers involved. In particular, we find the generating function of three directed osculating walks in star configurations on the square lattice with two interaction Boltzmann weights, so that there is one type of contact interaction between the top pair of walks and a different interaction between the bottom pair of walks. These osculating stars are found to be the most amenable to exact solution using functional equation techniques in comparison to the symmetric case where three friendly walks in watermelon configurations were successfully solved with the same techniques. We elucidate the phase diagram, which has four phases, and find the order of all the phase transitions between them. We also calculate the entropic exponents in each phase.

Keywords: exact solution, directed walks, osculating walks, gelation, zipping

1. Introduction

Models of polymer gelation have received interest over an extended period of time based upon understanding the phase behaviour of systems of multiple polymers [1]. Models of a small fixed number of polymers have been studied in their own right for various reasons. For example, models of the unzipping of DNA which naturally lead to the study of two polymers with interpolymer interactions have been a research focus [2–10]. Two varieties of models have the two polymers modelled via either self-avoiding or directed walk systems on lattices in two and three dimensions with various types of contact interactions. The exact solution of directed so-called friendly walkers, which can share edges and sites, on the square lattice with

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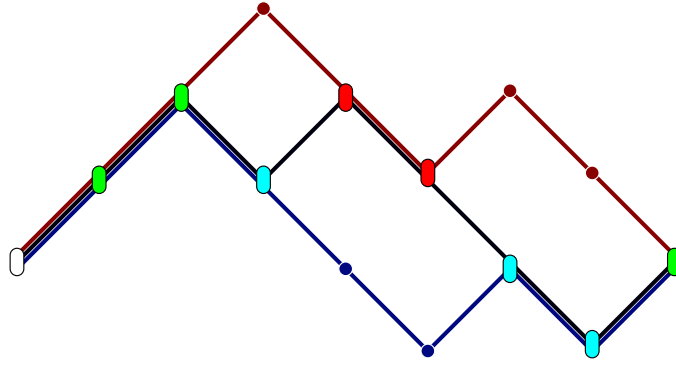


Figure 1. Three friendly walks in a watermelon configuration as considered previously. Reproduced from [12]. © IOP Publishing Ltd. All rights reserved.

such interactions [9, 10] has led to the extension of a key combinatorial technique for lattice paths, the *obstinate kernel method* [11]. More generally the binding of multiple polymers have been studied for some time [12–19].

The modelling of three polymers has considered in the context of polymer binding/zippering [12]. One source of motivation was the search for models of Efimov-like states in triple stranded DNA [20, 21]. In [12] an exact solution was found for three interacting friendly directed walks on the square lattice in the bulk. Two distinct interaction parameters were introduced: one that acts on pairs of walks and one that acts when all three walks comes together. The exact solution was found by the analysis of functional equations for the model’s corresponding generating function by means of the obstinate kernel method. Without the triple walk interaction the model exhibits two phases which can be classified as free and gelated (or zipped), with the system exhibiting a second-order phase transition between these phases. The interactions between the different pairs of polymers were identical, modelling the situation where the homopolymers are all of the same type. It is of general interest then to consider a generalisation where the polymers may be different from one another so that the pairwise interaction may differ. It is such a model we consider in the work.

In [12] the directed walk system consisted of three friendly walks (see figure 1) in which the walks may share sites and edges though are considered never to cross. They were specifically considered to start and end together. In our preliminary attempts to analyse a problem where the interactions between different pairs of walks were different we were unable to solve the corresponding functional equations as the breaking of the symmetry meant it appeared we lacked sufficient equations to solve the model. Moreover, the D-finite nature of the generating function in the symmetric case meant we were unable to guess a solution in the more general case.

We turned to the study of other varieties of configuration in the hope that there may be a more amenable type whilst still allowing the required interactions. We noticed that both two and three osculating walks, where walks may share vertices but not edges, in star configurations (see figure 2) and the final endpoints are summed over gave algebraic solutions for the generating functions. As such it pointed to the idea that considering the asymmetric version of a similar three walk system would be a prudent line of attack. It turned out to be so and although we did not use the kernel method to solve the problem it was feasible to find the algebraic equation satisfied by the solution. Along the way we could elucidate the solution, provide the exact phase diagram and calculate all important exponents.

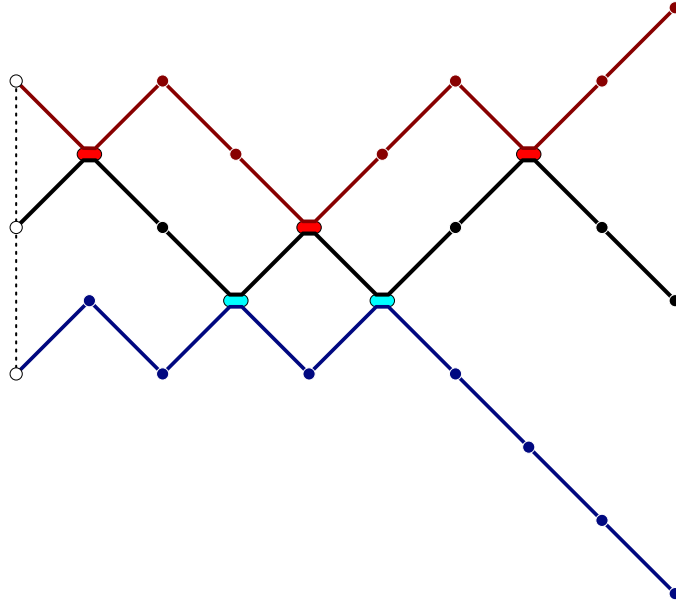


Figure 2. Three osculating walks in a star configuration as considered in this work. An example of an allowed configuration of length $n = 9$. The walks start one lattice spacing apart (distance two) at coordinates $(0, 0)$, $(0, 2)$ and $(0, 4)$, and end at $x = n$ with any allowed y . In this configuration the upper two walks end (rightmost) two lattice spacing (distance four) apart whilst the bottom two walks end three lattice spacings (distance six) apart. Here, we have $m_a = 3$ shared sites between the upper two walks and $m_b = 2$ shared sites between the lower two walks. Thus, the overall Boltzmann weight for this configuration is $a^3 b^2$.

2. Three osculating stars

2.1. Model definition

In the Euclidean plane with coordinates x and y consider three directed walks on the square integer lattice which has been rotated by 45° . The lattice has sites at coordinates $(x, y) = (2i, 2j)$ and $(2i + 1, 2j + 1)$ for $i, j \in \mathbb{Z}$. A square of the lattice is defined by the quartet of coordinates $(2i, 2j)$, $(2i + 1, 2j + 1)$, $(2i + 1, 2j - 1)$ and $(2i + 2, 2j)$. The three directed walks consisting of an equal number of steps n so that the total number of steps in a configuration is $3n$. All walks begin at $x = 0$ with $y = 0, 2, 4$, and end at $x = n$ with any heights. Walks do not cross. Moreover, walks only can take steps in either the north-east $(1, 1)$ or south-east $(1, -1)$ direction along edges of the squares. Finally, any pair of walks may share common site, however none of the walks are able to share common edges. Such walks are typically referred to as *osculating* walks. This contrasts to the model considered in [12] where (infinitely) *friendly* walks were considered where walks may share edges and sites without restriction, but may not cross. The other difference between the models is that in [12] the walks always ended at the same site (or otherwise close by at a fixed distance), known as a watermelon configuration; here we consider *stars* where we sum over all possible end points. Let Ω_3 denote the class of allowed triple walks of *any* length. An example of an allowable configuration is given in figure 2. 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

$$Z_n(a, b) = \sum_{\varphi \in \Omega_3, |\varphi|=n} a^{m_a(\varphi)} b^{m_b(\varphi)}, \quad (2.1)$$

where $|\varphi|$ denotes the length of the configuration φ . The reduced free energy $\kappa(a, b)$ is given by

$$\kappa(a, b) = - \lim_{n \rightarrow \infty} \frac{1}{n} \log Z_n(a, b). \quad (2.2)$$

And generating function $G_3(a, b; z)$ for three walks is defined as

$$G_3(a, b; z) = \sum_{n=0}^{\infty} Z_n(a, b) z^n. \quad (2.3)$$

In the usual manner, where z is conjugate to the length of the configuration. Importantly, the relation between the free energy κ and the radius of convergence of $G(a, b; z)$ is given by

$$\kappa(a, b) = \log z_s(a, b), \quad (2.4)$$

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 as

$$Z_n(a, b) \sim A(a, b) \mu(a, b)^n n^{\gamma-1}. \quad (2.5)$$

Which defines the standard polymer exponent known as the *entropic* exponent γ , the value of which is expected to depend upon the phase or phase boundary at which the partition function is evaluated [22–24]. The *growth rate* μ is a function of a and b and is given by

$$\mu(a, b) = z_s(a, b)^{-1} = e^{-\kappa(a, b)}. \quad (2.6)$$

From the generating function solution we will find the location of the singularity $z_s(a, b)$ which then effectively gives us the growth rate μ and free energy κ .

We show that there are four possible natural phases in our system which we will fully delineate in our analysis below. The phases are characterised by canonical order parameters related to the number of contacts between the walks and conjugate to the Boltzmann weights a and b . So, as such, we introduce the order parameters $\mathcal{A}(a, b)$ and $\mathcal{B}(a, b)$ being the limiting average density of contacts between the top two and bottom two walks respectively as

$$\mathcal{A}(a, b) = \lim_{n \rightarrow \infty} \frac{\langle m_a \rangle}{n} = a \frac{\partial \kappa}{\partial a}, \quad (2.7)$$

and

$$\mathcal{B}(a, b) = \lim_{n \rightarrow \infty} \frac{\langle m_b \rangle}{n} = b \frac{\partial \kappa}{\partial b}. \quad (2.8)$$

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

$$\mathcal{A} = \mathcal{B} = 0. \quad (2.9)$$

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

$$\mathcal{A} > 0 \text{ with } \mathcal{B} = 0. \quad (2.10)$$

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

$$\mathcal{B} > 0 \text{ with } \mathcal{A} = 0. \quad (2.11)$$

When both

$$\mathcal{B} > 0 \text{ and } \mathcal{A} > 0. \quad (2.12)$$

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

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 standard polymer exponent α [24, 25] as related to the non-analyticity in the free energy κ^{non} as

$$\kappa^{\text{non}} \sim K t^{2-\alpha} \text{ as } t \rightarrow 0, \quad (2.13)$$

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

$$\mathcal{M} \sim M t^{1-\alpha} \text{ as } t \rightarrow 0^+. \quad (2.14)$$

A standard scaling argument [24, 25] connects this to the scaling of the number of contacts evaluated exactly at the transition

$$\langle m_{a,b} \rangle(n) \sim C n^\phi, \quad (2.15)$$

where

$$\phi = 2 - \alpha. \quad (2.16)$$

Here which contact number m_a or m_b is considered is related to the order parameter(s) that are changing from zero to a non-zero value as the phase transition point is traversed.

3. Functional equations for the generating function

We can establish a functional equation for $G(a, b; z)$ by considering the effect of appending a triplet of steps to the end of any given configuration $\varphi \in \Omega_3$. To begin, we define $\Omega_3(i, j)$ to be the class of triple osculating walks that consists of configurations with final top to middle walk distance i and middle to bottom distance j , that still obey the osculating constraints. The full combinatorial class Ω_3 is then the union

$$\Omega_3 \equiv \bigcup_{i \geq 0, j \geq 0} \Omega_3(i, j). \quad (3.1)$$

Equipped with our refined combinatorial classes we can introduce its corresponding generating function $G(a, b; z)$ that encodes information about the number of steps and shared contacts for each configuration $\varphi \in \Omega_3$. However, determining whether appending a triple-step onto a given configuration φ results in a new and *allowable* configuration (i.e. φ remains in Ω_3) further requires knowledge of the *final* step distances between the three walks. Hence, solely for the purpose of establishing our functional equation for $G(a, b; z)$, we additionally introduce two catalytic variables r and s to construct the expanded generating function $F(r, s, a, b; z)$ where

$$F(r, s, a, b; z) \equiv F(r, s) = \sum_{\varphi \in \Omega_3} z^{|\varphi|} r^{h(\varphi)/2} s^{f(\varphi)/2} a^{m_a(\varphi)} b^{m_b(\varphi)}. \quad (3.2)$$

And again z is conjugate to the length $|\varphi|$ of a configuration $\varphi \in \Omega_3$, 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. For each $\varphi \in \Omega_3$, powers of r and s in $F(r, s)$ track the final step distances between the three walks. Due to the allowed step directions, both $h(\varphi)$ and $f(\varphi)$ must always be even, ensuring that $F(r, s)$ contains only integer powers of r and s . Thus, we consider $F(r, s)$ as an element of $\mathbb{Z}[r, s, a, b][[z]]$: the ring of formal power series in z with coefficients in $\mathbb{Z}[r, s, a, b]$.

We aim to solve $F(1, 1, a, b; z) \equiv G_3(a, b; z)$ by establishing a functional equation for $F(r, s)$. Specifically, we construct a suitable mapping from Ω_3 onto itself by considering the effect of appending an *allowable* triple-step onto a configuration, translating this map into its action on the generating function.

We then follow the procedure suitably modified found in [12] to construct the functional equation:

$$\begin{aligned} K(r, s)F(r, s) = rs - \left(\frac{(1+r)(r+s+rs)z}{rs} + \frac{1-b}{b} \right) F(r, 0) \\ - \left(\frac{(1+s)(r+s+rs)z}{rs} + \frac{1-a}{a} \right) F(0, s), \end{aligned} \quad (3.3)$$

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

$$K(r, s) \equiv K(r, s; z) = 1 - \frac{z(r+1)(s+1)(r+s)}{rs}. \quad (3.4)$$

4. Exact solution of osculating stars

4.1. Two interacting osculating star walks

We start by reproducing the solution for two osculating walks with contact interaction [19, 26, 27]. Analogous to our definitions for the generating function of three walks we have the extended generating function

$$F(s, a; z) \equiv F(s) = \sum_{\varphi \in \Omega_2} z^{|\varphi|} s^{d(\varphi)/2} a^{m(\varphi)}, \quad (4.1)$$

where $m(\varphi)$ counts the number of contacts between the two walks and $d(\varphi)$ the distance between the final vertices of the two walks. We want the generating function for star configurations given by $G_2(a, z) = F(1, a; z)$. Here Ω_2 denote the class of allowed pairs of walks of *any* length.

The functional equation for $F(s)$ is

$$(1 - z(s + 2 + 1/s))F(s) = s + \left(\frac{a-1}{a} - z(2 + 1/s) \right) F(0), \quad (4.2)$$

where s is now conjugate to the distance between the endpoints of the two walks. Note that the walks start 1 lattice spacing apart.

This equation can be solved using the now fairly standard approach of the kernel-method. Solving the kernel gives two roots

$$s = \sigma_{\pm}(z) = \frac{1 - 2z \pm \sqrt{1 - 4z}}{2z}. \quad (4.3)$$

Table 1. 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

Of which only one, $\sigma_-(z)$, is combinatorial (being analytic at zero). Substituting this into the functional equation then eliminates the unknown $F(s)$ leaving a single equation for $F(0)$, which yields:

$$F(0; a, z) = \frac{a\sigma_-(z)^2}{az + \sigma_-(z)(1 - a(1 - 2z))}. \quad (4.4)$$

Back substitution into equation (4.2) and setting $s = 1$ then gives

$$G_2(a, z) = \frac{1 + (3z - 1)a}{2z(1 + a(2z - 1) + z^2a^2)\sqrt{1 - 4z}} - \frac{1 + a(3z - 1) + 2z^2a^2}{2z(1 + a(2z - 1) + z^2a^2)}. \quad (4.5)$$

This generating function has two physical singularities; a square-root singularity when $z = 1/4$ and a simple pole when $z = \frac{\sqrt{a-1}}{a}$. These meet at $a = 4$ and the singularities coalesce giving

$$G_2(4, z) = \frac{16z}{(3 + 4z)(1 - 4z)} - \frac{3}{2z(3 + 4z)\sqrt{1 - 4z}} - \frac{3}{2z(3 + 4z)}. \quad (4.6)$$

And the behaviour is dominated by a simple pole at $z = 1/4$ with a confluent one-on-square-root singularity. The asymptotic behaviour of $m(a)$ the average number of contacts between the two walks as a function of a is given explicitly by

$$m(a) = \langle m \rangle = \begin{cases} \frac{a}{(4-a)} + O(n^{-1}) & a < 4 \\ \frac{1}{\sqrt{\pi}} \cdot \sqrt{n} + O(1) & a = 4 \\ \frac{a-\sqrt{a-2}}{2(a-1)} \cdot n + O(1) & a > 4. \end{cases} \quad (4.7)$$

Hence the associated order parameter

$$\mathcal{M}(a) = \lim_{n \rightarrow \infty} \frac{\langle m \rangle}{n} = a \frac{\partial \kappa}{\partial a}, \quad (4.8)$$

is given by

$$\mathcal{M}(a) = \begin{cases} 0 & a \leq 4 \\ \frac{a-\sqrt{a-2}}{2(a-1)} & a > 4. \end{cases} \quad (4.9)$$

This implies that for $a < 4$ there is a free phase where the two walks do not share a macroscopic number of sites whilst they are zipped together for $a > 4$ sharing a non-zero macroscopic density of sites. Our generating function leads us to provide the table of entropic exponents in table 1.

Finally, we note that 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 $a = 4$.

4.2. Three walks: symmetric interactions $a = b$

We can explicitly solve the functional equation (3.3) for three osculating walks when $a = b$ following the same method applied by Bousquet-Mélou [11, 18]. This reproduces the results found by Essam [16]. When $a = b$ the physical variable conjugate to a counts the total number of shared sites between pairs of osculating walks in three walk stars.

The kernel $K(r, s)$ does not depend explicitly on a and b whilst the function equation is

$$K(r, s)F(r, s) = r^2 - \left(\frac{(1+r)(r+s+rs)z}{rs} + \frac{1-a}{a} \right) F(r, 0) - \left(\frac{(1+s)(r+s+rs)z}{rs} + \frac{1-a}{a} \right) F(0, s). \quad (4.10)$$

We immediately notice the symmetry $r \leftrightarrow s$, which facilitates the solution and that this symmetry is broken when $a \neq b$.

The generating function $G_3(a, a; z) = F(1, 1, a, a, z)$ is

$$G_3(a, a; z) = \frac{(6az - a + 1)(az + 1)(az - 1)}{4z^2(a^2z - a + 2)(4a^2z^2 + 4az - a + 1)} \cdot \sqrt{1 - 4z} + \frac{-8a^4z^4 + 2a^2(a - 20)z^3 + a(a + 7)(a - 4)z^2 + (10a - 4)z - a + 1}{4z^2(a^2z - a + 2)(4a^2z^2 + 4az - a + 1)}. \quad (4.11)$$

We immediately notice that this is an algebraic function and this contrasts to the D-finite non-algebraic solution for the generating function for three friendly walks in a watermelon configuration found in [12]. This provides a pointer to why we could extend the current model to the asymmetric solution below whilst could not similarly extend the work in [12].

The analysis of this generating function is very similar to that of the two-walk problem. When a is small, the asymptotics are dominated by the square-root singularity at $z = 1/8$. When a is large, the problem is dominated by a simple pole at $z = \frac{a-2}{a^2}$. We note that there is an additional pole at $z = \frac{\sqrt{a}-1}{2a}$ but it is dominated by the other. All three singularities coalesce when $a = 4$ and the generating function simplifies to

$$G_3(4, 4; z) = \frac{1}{1 - 8z} + \frac{3(1 - 4z)(4z + 1)}{8z^2(8z + 3)\sqrt{1 - 8z}} - \frac{3(8z^2 + 4z + 1)}{8z^2(8z + 3)}. \quad (4.12)$$

And the system is dominated by a simple pole at $z = 1/8$. Hence the singularity closest to the origin is given by

$$z_c = \begin{cases} \frac{1}{8} & a \leq 4 \\ \frac{a-2}{a^2} & a > 4. \end{cases} \quad (4.13)$$

The asymptotic behaviour of average total number of contacts $m(a)$ between pairs of osculating walks as a function of a is given by

$$m(a) = \begin{cases} \frac{a(192 - 8a - a^2)}{(4-a)(64-a^2)} + O(n^{-1}) & a < 4 \\ \frac{3}{\sqrt{\pi}} \cdot \sqrt{n} + O(1) & a = 4 \\ \frac{a-4}{a-2} \cdot n + O(1) & a > 4. \end{cases} \quad (4.14)$$

Hence the associated order parameter is given by

$$\mathcal{M}(a) = \begin{cases} 0 & a \leq 4 \\ \frac{a-4}{a-2} & a > 4. \end{cases} \quad (4.15)$$

Table 2. 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

Once again 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. Our generating function leads us to provide the table of entropic exponents in table 2.

4.3. Three walks: asymmetric interactions for stars $r = s = 1$

We have not been able to use the kernel method to directly solve the above equation (3.3) for the watermelon case, namely $r = s = 0$, nor for general r, s by using any variant of the kernel method. We believe that this is due to the breaking of the $r \leftrightarrow s$ symmetry when $a \neq b$. We were, however, able to determine a quartic equation satisfied by the generating function of the star case, namely $r = s = 1$ by analytically guessing the solution and then confirming that it is indeed the solution. Given the solution of the symmetric problem is algebraic, and, in particular quadratic, there is some hope that the solution of the asymmetric problem might satisfy a low degree algebraic equation. We note that this is precisely the case for a related problem—Kreweras walks—in which the symmetric problem satisfies a polynomial of degree 6 [28] and the asymmetric problem satisfies a polynomial of degree 12 [28–30]. Consequently we searched for low degree algebraic equations.

We note that Bousquet-Mélou [18] derived a quadratic solution in the non-interacting case $r = s = a = b = 1$. We found that for $r = s = 1$ and general $a = b$ the generating function also satisfied a quadratic. 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 [31] 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. We give the quartic Equation in the appendix for the generating function $G \equiv G_3(a, b; z)$: it is of the standard form

$$\sum_{j=0}^4 c_j(a, b; z) G^j = 0, \quad (4.16)$$

where the coefficients $c_j(a, b; z)$ are polynomials in a, b and z . Hence we could write a closed form solution for $G_3(a, b; z)$ in terms of the classical solution of a quartic. It would be unwieldy and we can provide the asymptotic results required by directly analysing the quartic. Important in this regard is that the coefficient of G^4 is

$$c_4(a, b; z) = 4z^6 (4b^2 z^2 + 4bz - b + 1) (4a^2 z^2 + 4az - a + 1) \times (a^2 b^2 z^2 + 2abz - ab + a + b)^2. \quad (4.17)$$

5. Phase diagram and exponents

As described in the definition of the model, its natural quantities, the two candidate order parameters, point to four possible phases depending on whether those two order parameters are non-zero or not.

Given that non-analyticities in the free energy are governed by the change of singularities closest to the origin of the generating function the location of those possible singularities are central to delineating the possible phases. Since we know the quartic satisfied by the generating function, we can, in principle, compute the generating function in closed form. Unfortunately, that proves to be rather unwieldy for general a, b , but is useful for confirming the location of singularities for particular fixed choices of a, b . Instead, we locate possible singularities by examining its discriminant 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 find four independent singularities ($z_{\text{free}}, z_{\text{top}}, z_{\text{bottom}}, z_{\text{fully}}$) of the generating function which correspond to these four phases when they are the singularity closest to the origin at some value of a and b :

$$z_c = \begin{cases} z_{\text{free}} = \frac{1}{8} \\ z_{\text{top}} = \frac{\sqrt{a}-1}{2a} \\ z_{\text{bottom}} = \frac{\sqrt{b}-1}{2b} \\ z_{\text{fully}} = \frac{-1 + \sqrt{(a-1)(b-1)}}{ab} \end{cases} \quad (5.1)$$

Notice that when $b = a$ we recover the results in equation (4.13). Additionally, note that $z_{\text{free}}, z_{\text{top}}, z_{\text{bottom}}$ are precisely half the critical point of the two-walk model; this is commensurate with adding a third (effectively) non-interacting directed walk to the system.

From this we can find the phase boundaries by looking where the singularities above are equal.

- The singularities z_{free} and z_{top} meet when $\frac{1}{8} = \frac{\sqrt{a}-1}{2a}$ which happens at $a = 4$ and $b \leq 4$, which we shall label t_1 ;
- The singularities z_{free} and z_{bottom} meet when $\frac{1}{8} = \frac{\sqrt{b}-1}{2b}$ which happens at $b = 4$ and $a \leq 4$, which we shall label t_2 ;
- The singularities z_{top} and z_{fully} meet, which we shall label t_t , when

$$\frac{\sqrt{a}-1}{2a} = \frac{-1 + \sqrt{(a-1)(b-1)}}{ab} \quad (5.2)$$

Which happens along the curve

$$a = \frac{b^2}{(b-2)^2} \quad \text{for } b < 4; \quad (5.3)$$

- The singularities z_{bottom} and z_{fully} meet, which we shall label t_b , when

$$\frac{\sqrt{b}-1}{2b} = \frac{-1 + \sqrt{(a-1)(b-1)}}{ab} \quad (5.4)$$

Which happens along the curve

$$b = \frac{a^2}{(a-2)^2} \quad \text{for } a < 4. \quad (5.5)$$

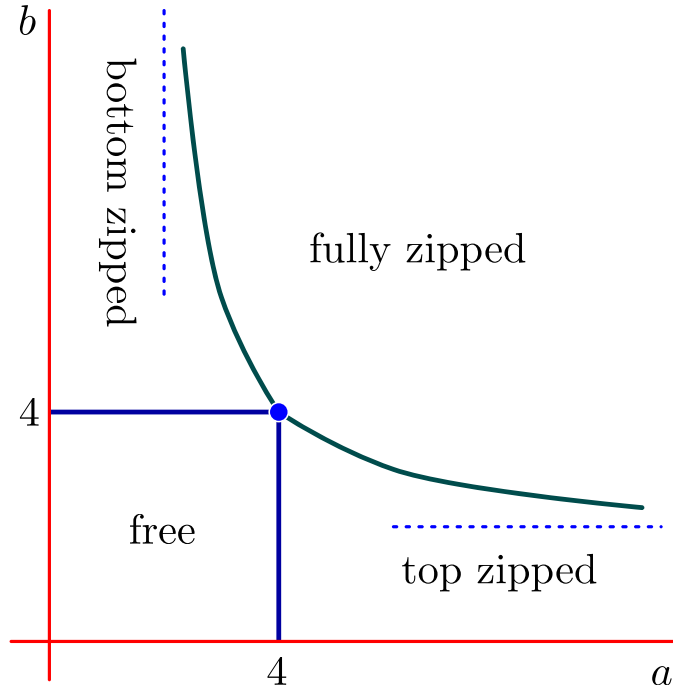


Figure 3. The phase diagram of our model. The dashed lines indicate the asymptotes of the phase boundaries along $b = 2$ for large a and $a = 2$ for large b .

We note that for large a the transition boundary t_t is asymptotic to the line $b = 2$ and so there is utility in inverting the curve $a = \frac{b^2}{(b-2)^2}$ as

$$b_c(a) = \frac{2\sqrt{a}}{\sqrt{a}-1} \quad \text{for } a > 4. \quad (5.6)$$

Similarly, the phase transition boundary t_b occurs when

$$a_c(b) = \frac{2\sqrt{b}}{\sqrt{b}-1} \quad \text{for } b > 4. \quad (5.7)$$

Hence we deduce that the closest singularity to the origin is given by

$$z_c(a, b) = \begin{cases} z_{\text{free}} = \frac{1}{8} & \text{when } a < 4 \text{ and } b < 4 \\ z_{\text{top}}(a) = \frac{\sqrt{a}-1}{2a} & \text{when } a > 4 \text{ and } 0 \leq b < \frac{2\sqrt{a}}{\sqrt{a}-1} \\ z_{\text{bottom}}(b) = \frac{\sqrt{b}-1}{2b} & \text{when } 0 \leq a < \frac{2\sqrt{b}}{\sqrt{b}-1} \text{ and } b > 4 \\ z_{\text{fully}}(a, b) = \frac{-1 + \sqrt{(a-1)(b-1)}}{ab} & \text{otherwise.} \end{cases} \quad (5.8)$$

These give us the growth constant μ and free energy κ in each phase. Given these singularities we can now analysis the scaling of the generating function/ partition function and the two types of contact (hence the order parameters). Our phase diagram in figure 3 is derived from the singularity structure given in equation (5.8) and our analysis below

5.1. 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

$$Z_n \sim 8^n n^{-3/2}. \quad (5.9)$$

Leading to $\mu = 8$ and $\gamma = -1/2$.

In this phase we have calculated that

$$\begin{aligned} m_a(a, b) &= \frac{a(ab + 8b - 192)}{2(4 - a)(ab - 64)} + O(n^{-1}), \\ m_b(a, b) &= \frac{b(ab + 8a - 192)}{2(4 - b)(ab - 64)} + O(n^{-1}). \end{aligned} \quad (5.10)$$

So that

$$\mathcal{A} = \mathcal{B} = 0 \text{ when } a < 4 \text{ and } b < 4. \quad (5.11)$$

Which could be deduced by the constancy of the free energy in this region. So we label this as a *Free* phase where the three walks are effectively repulsive and share few (a finite number) sites with one another. Notice that when $b = a$ we recover the $a < 4$ case in equation (4.14).

5.2. Partially zipped phase: top zipped

The singularity in this phase arises from the factor of $(a^2 z^2 + 2az - a + 1)$ in the coefficient c_4 of G^4 in the quartic. In the region ($a > 4$ and $0 \leq b < \frac{2\sqrt{a}}{\sqrt{a}-1}$) where $z_{\text{top}} = \frac{\sqrt{a}-1}{2a}$ dominates we have a phase where the free energy is independent of b so $\mathcal{B} = 0$ but

$$\mathcal{A} = \frac{a}{z_{\text{top}}(a)} \frac{\partial z_{\text{top}}(a)}{\partial a} = \frac{a - \sqrt{a} - 2}{2(a - 1)}. \quad (5.12)$$

So in this phase we expect the top two walks share a macroscopic number of sites osculating frequently effectively zipped together whilst the bottom walk is repelled from the upper two walks. We refer to this phase as *Top Zipped*.

In this region we find that

$$Z_n \sim z_{\text{top}}^{-n} n^{-1/2}. \quad (5.13)$$

Leading to

$$\mu = \frac{1}{z_{\text{top}}} = \frac{2a}{\sqrt{a} - 1} \quad (5.14)$$

and $\gamma = 1/2$.

In this region we have

$$\begin{aligned} m_a(a, b) &= \frac{a - \sqrt{a} - 2}{2(a - 1)} \cdot n + o(n), \\ m_b(a, b) &= O(1). \end{aligned} \quad (5.15)$$

We expect that $m_b(a, b) = \text{const} + o(1)$ in this region, however we have not been able to compute more precise value of this statistic. Although there is no theoretical impediment to this calculation, we have found that various computer algebra systems have been unable to expand $G_3(a, b; z)$ about $z = z_{\text{top}}(a)$. Despite this we were able to guess the expressions but it is so convoluted it appears that they are too complicated to be manipulated readily.

5.3. Partially zipped phase: bottom zipped

In the region ($0 \leq a < \frac{2\sqrt{b}}{\sqrt{b}-1}$ and $b > 4$) where z_{bot} dominates we have a phase where the free energy is independent of a so $\mathcal{A} = 0$ but

$$\mathcal{B} = \frac{b}{z_{\text{bot}}(b)} \frac{\partial z_{\text{bot}}(b)}{\partial b} = \frac{b - \sqrt{b} - 2}{2(b-1)}. \quad (5.16)$$

So in this phase we expect the bottom two walks share a macroscopic number of sites osculating frequently effectively zipped together whilst the top walk is repelled from the lower two walks. We refer to this phase as *bottom zipped*.

In this region we find that

$$Z_n \sim z_{\text{bot}}^{-n} n^{-1/2}. \quad (5.17)$$

Leading to

$$\mu = \frac{1}{z_{\text{bot}}} = \frac{2b}{\sqrt{b}-1} \quad (5.18)$$

and $\gamma = 1/2$.

In this region we have

$$\begin{aligned} m_a(a, b) &= O(1), \\ m_b(a, b) &= \frac{b - \sqrt{b} - 2}{2(b-1)} \cdot n + o(n). \end{aligned} \quad (5.19)$$

Again, we expect that $m_a(a, b) = \text{const} + o(1)$ in this region, but we have been unable to further elucidate the value of this statistic simply.

5.4. Fully zipped

Finally, when both a, b are large there is a simple pole and it is given by a zero of the leading coefficient in the algebraic equation; namely,

$$0 = a^2 b^2 z^2 + 2abz - ab + a + b, \quad (5.20)$$

which gives

$$z_c = z_{\text{fully}} = \frac{-1 + \sqrt{(a-1)(b-1)}}{ab}. \quad (5.21)$$

And, moreover, the simple pole in the generating function results in the scaling of the partition function as

$$Z_n \sim z_{\text{fully}}^n. \quad (5.22)$$

Leading to

$$\mu(a, b) = \frac{1}{z_{\text{fully}}(a, b)} \quad (5.23)$$

and $\gamma = 1$.

Finally, we calculate 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*:

$$\begin{aligned}\mathcal{A}(a, b) &= \frac{a}{z_{\text{top}}(a)} \frac{\partial z_{\text{top}}(a)}{\partial a} = \frac{1}{2(a-1)} \left(a - 2 + \frac{a}{1 + \sqrt{(a-1)(b-1)}} \right), \\ \mathcal{B}(a, b) &= \frac{b}{z_{\text{bot}}(b)} \frac{\partial z_{\text{bot}}(b)}{\partial b} = \frac{1}{2(b-1)} \left(b - 2 + \frac{b}{1 + \sqrt{(a-1)(b-1)}} \right).\end{aligned}\quad (5.24)$$

Notice that $\mathcal{A}(a, a) + \mathcal{B}(a, a) = \frac{a-4}{a-2}$ and so recovers the large a behaviour given in equation (4.14).

5.5. Phase transition boundary scaling

We have also calculated the scaling of the number of the two types of contacts on each of the phase boundaries.

- For the phase boundary t_1 , when $a = 4$ and $b < 4$ we have

$$\begin{aligned}Z_n &\sim 8^n n^{-3/4}, \\ m_a &\sim \frac{\pi\sqrt{2}}{4\Gamma(3/4)^2} \cdot \sqrt{n} + O(n^{-1/2}), \\ m_b &\sim \frac{b(40-b)}{2(4-b)(16-b)} + O(n^{-1}).\end{aligned}\quad (5.25)$$

Which implies that $\mu = 8$, $\gamma = 1/4$ and $\phi = 1/2$,

- For the phase boundary t_2 , when $a < 4$ and $b = 4$ we have

$$\begin{aligned}Z_n &\sim 8^n n^{-3/4}, \\ m_a &\sim \frac{a(40-a)}{2(4-a)(16-a)} + O(n^{-1}), \\ m_b &\sim \frac{\pi\sqrt{2}}{4\Gamma(3/4)^2} \cdot \sqrt{n} + O(n^{-1/2}),\end{aligned}\quad (5.26)$$

which implies that $\mu = 8$, $\gamma = 1/4$ and $\phi = 1/2$,

- For the phase boundary t_t , when $b = \frac{2\sqrt{a}}{\sqrt{a}-1}$ and $a > 4$ we have

$$\begin{aligned}Z_n &\sim \left(\frac{2a}{\sqrt{a}-1} \right)^n n^0, \\ m_a &\sim \frac{a - \sqrt{a} - 2}{2(a-1)} \cdot n + O(1), \\ m_b &\sim O(\sqrt{n}) + O(n^{-1/2}).\end{aligned}\quad (5.27)$$

Which implies that $\mu = \frac{2a}{\sqrt{a}-1}$ and $\gamma = 1$. As before, we have not been able to compute more detailed asymptotics for m_b along this boundary.

Table 3. The growth rates (growth rates give the free energies) 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

- For the phase boundary t_b , when $a = \frac{2\sqrt{b}}{\sqrt{b}-1}$ for $b > 4$ we have

$$\begin{aligned}
 Z_n &\sim \left(\frac{2b}{\sqrt{b}-1} \right)^n n^0, \\
 m_a &\sim O(\sqrt{n}) + O(n^{-1/2}), \\
 m_a &\sim \frac{b - \sqrt{b} - 2}{2(b-1)} + O(1).
 \end{aligned} \tag{5.28}$$

Which implies that $\mu = \frac{2b}{\sqrt{b}-1}$ and $\gamma = 1$. As before, we have not been able to compute more detailed asymptotics for m_a along this boundary.

- For special critical point at $a = b = 4$ we have

$$\begin{aligned}
 Z_n &\sim 8^n n^0, \\
 m_a &\sim \frac{3}{2\sqrt{\pi}} \cdot \sqrt{n} + O(n^{-1/2}), \\
 m_b &\sim \frac{3}{2\sqrt{\pi}} \cdot \sqrt{n} + O(n^{-1/2}).
 \end{aligned} \tag{5.29}$$

Which implies that $\mu = 8$ and $\gamma = 1$ with $\phi = 1/2$. Notice that $m_a + m_b$ gives the $a = 4$ result in (4.14).

5.6. Results summary

The phase diagram is delineated by equation (5.8). We report that all of the phase transitions between these phases in our model are second-order with $\alpha = 0$ and $\phi = 1/2$. We then summarise the growth rates/free energy and entropic exponents in tables 3:

6. Conclusion

We have ascertained the exact solution of a model of three directed osculating walks with asymmetric contact interactions in star configurations. We expect that similar models such as friendly walks and watermelon configurations will behave similarly with similar phase diagrams though the entropic exponents will differ for watermelon type configurations. We have delineated the order of the transitions and the associated exponents, especially the entropic exponents at all points in the phase diagram. We note that the values of $1/4$ on two of the phase boundaries are somewhat novel. At high temperatures the system is in a free state where the three polymers repel each other. At low temperatures the system is in a bound state where all three polymers are bound together. Given any asymmetry there is a state at intermediate temperatures where two of the polymers are bound whilst the third polymer is repelled by the other pair. Regarding the method of exact solution of the model considered we note that we moved to the osculating case after not being able to solve the friendly model with asymmetric interaction though the symmetric model can be solved. A further understanding of the reasons for this and why the watermelon configuration is less amenable to solution would be most interesting.

Data availability statement

No new data were created or analysed in this study.

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Appendix. Equation for asymmetric stars

The following is the quartic we found to be satisfied by the generating function $G \equiv G_3(a, b; z)$.

$$\begin{aligned}
0 = & G^4 \cdot 4z^6(4b^2z^2 + 4bz - b + 1)(4a^2z^2 + 4az - a + 1)(a^2b^2z^2 + 2abz - ab + a + b)^2 \\
& + G^3 \cdot 8z^4(4b^2z^2 + 4bz - b + 1)(4a^2z^2 + 4az - a + 1) \\
& \cdot (a^2b^2z^2 + 2abz - ab + a + b)(a^2b^2z^3 + 5abz^2 - abz + 2az + 2bz - 1) \\
& + G^2 \cdot z^2(96a^6b^6z^{10} + 48a^5b^5(2a + 2b + 23)z^9 \\
& - 4a^4b^4(6a^2b + 6ab^2 - 6a^2 + 41ab - 6b^2 - 378a - 378b - 600)z^8 \\
& - 4a^3b^3(9a^2b^2 + 120a^2b + 120ab^2 - 172a^2 - 99ab - 172b^2 - 1080a - 1080b)z^7 \\
& + a^2b^2(5a^3b^3 + 51a^3b^2 + 51a^2b^3 - 160a^3b - 679a^2b^2 - 160ab^3 + 104a^3 - 1732a^2b \\
& - 1732ab^2 + 104b^3 + 2904a^2 + 6040ab + 2904b^2)z^6 \\
& + 2ab(71a^3b^3 + 109a^3b^2 + 109a^2b^3 - 592a^3b - 1845a^2b^2 - 592ab^3 + 432a^3 + 1402a^2b \\
& + 1402ab^2 + 432b^3)z^5 \\
& + (-11a^4b^4 - 4a^4b^3 - 4a^3b^4 + 127a^4b^2 + 987a^3b^3 + 127a^2b^4 - 208a^4b - 1579a^3b^2 \\
& - 1579a^2b^3 - 208ab^4 + 96a^4 + 432a^3b + 452a^2b^2 + 432ab^3 + 96b^4)z^4 \\
& - 4ab(32a^2b^2 - 77a^2b - 77ab^2 + 50a^2 - 12ab + 50b^2 + 52a + 52b)z^3 \\
& + (7a^3b^3 - 25a^3b^2 - 25a^2b^3 + 34a^3b - 97a^2b^2 + 34ab^3 - 16a^3 + 194a^2b \\
& + 194ab^2 - 16b^3 - 48a^2 - 112ab - 48b^2)z^2 \\
& + (22a^2b^2 - 46a^2b - 46ab^2 + 24a^2 + 30ab + 24b^2 - 4a - 4b)z \\
& - (b - 1)(a - 1)(ab - a - b - 4) \\
& + G^1 \cdot (a^2b^2z^3 + 5abz^2 - abz + 2az + 2bz - 1) \cdot (32a^4b^4z^8 + 32a^4b^3z^7 + 32a^3b^4z^7 \\
& - 8a^4b^3z^6 - 8a^3b^4z^6 + 400a^3b^3z^7 + 8a^4b^2z^6 - 68a^3b^3z^6 + 8a^2b^4z^6 - 4a^3b^3z^5 \\
& + 520a^3b^2z^6 + 520a^2b^3z^6 + a^3b^3z^4 - 160a^3b^2z^5 - 160a^2b^3z^5 + 15a^3b^2z^4 + 224a^3bz^5 \\
& + 15a^2b^3z^4 + 484a^2b^2z^5 + 224ab^3z^5 - 48a^3bz^4 - 215a^2b^2z^4 - 48ab^3z^4 + 32a^3z^4 \\
& + 32a^2b^2z^3 + 112a^2bz^4 + 112ab^2z^4 + 32b^3z^4 - 2a^2b^2z^2 - 24a^2bz^3 - 24ab^2z^3 + 2a^2bz^2 + 2ab^2z^2 \\
& - 32abz^3 + 42abz^2 - 12abz - 16az^2 - 16bz^2 + ab + 8az + 8bz - a - b - 4z + 1) \\
& + (4a^6b^6z^{10} + 4a^5b^5(a + b + 25)z^9 - a^4b^4(a^2b + ab^2 - a^2 + 21ab - b^2 - 130a - 130b - 625)z^8 \\
& + a^3b^3(a^2b^2 - 41a^2b - 41ab^2 + 56a^2 - 187ab + 56b^2 + 1000a + 1000b)z^7 \\
& + 4a^2b^2(a^3b^2 + a^2b^3 - 3a^3b + 4a^2b^2 - 3ab^3 + 2a^3 - 109a^2b - 109ab^2 \\
& + 2b^3 + 150a^2 + 250ab + 150b^2)z^6 - ab(a^3b^3 - 77a^3b^2 - 77a^2b^3 + 216a^3b + 397a^2b^2 \\
& + 216ab^3 - 160a^3 - 220a^2b - 220ab^2 - 160b^3)z^5
\end{aligned}$$

$$\begin{aligned}
& + \left(-5a^4b^3 - 5a^3b^4 + 21a^4b^2 + 48a^3b^3 + 21a^2b^4 - 32a^4b \right. \\
& + 17a^3b^2 + 17a^2b^3 - 32ab^4 + 16a^4 - 48a^3b - 162a^2b^2 - 48ab^3 + 16b^4 \Big) z^4 \\
& + \left(-a^3b^3 - 23a^3b^2 - 23a^2b^3 + 48a^3b + 139a^2b^2 + 48ab^3 - 16a^3 - 72a^2b - 72ab^2 - 16b^3 \right) z^3 \\
& + \left(2a^3b^2 + 2a^2b^3 - 6a^3b - 24a^2b^2 - 6ab^3 + 4a^3 + 22a^2b + 22ab^2 + 4b^3 - 4a^2 - 4b^2 \right) z^2 \\
& + \left(a^2b^2 - a^2b - ab^2 - 7ab + 4a + 4b \right) z + (b-1)(a-1).
\end{aligned}$$

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