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J. Phys. A: Math. Theor. 47 (2014) 015202 (34pp)

doi:10.1088/1751-8113/47/1/015202

An exact solution of two friendly interacting directed walks near a sticky wall

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Received 17 September 2013, revised 6 November 2013 Accepted for publication 9 November 2013 Published 3 December 2013

Abstract

We find the exact solution of two interacting friendly directed walks (modelling polymers) on the square lattice. These walks are confined to the quarter plane by a horizontal attractive surface, to capture the effects of DNA-denaturation and adsorption. We find the solution to the model's corresponding generating function by means of the *obstinate kernel method*. Specifically, we apply this technique in two different instances to establish partial solutions for two simplified generating functions of the same underlying model that ignore either surface or shared contacts. We then subsequently combine our two partial solutions to find the solution for the full generating function in terms of the two simpler variants. This expression guides our analysis of the model, where we find the system exhibits four phases, and proceed to delineate the full phase diagram, showing that all observed phase transitions are second-order.

Keywords: kernel method, interacting directed walks, polymer adsorption, DNA denaturation

PACS numbers: 05.50.+q, 05.70.fh, 61.41.+e

(Some figures may appear in colour only in the online journal)

1. Introduction

The adsorption of polymers both near a single surface, and confined between two interacting surfaces, has been the subject of continued interest [1-14]. This has been in part due to the advent of experimental techniques able to micro-manipulate single polymers [15-17] and the connection to modelling DNA denaturation [18-24]. In the pursuit of exact solutions, idealized two-dimensional directed walk models have been constructed to capture the effects

of adsorption, where a polymer grafts itself onto a surface at low temperature [1, 4, 10, 25]; as well as zipping, where two polymers are entwined with one another (again at low temperature) [26–28]. However, exact solutions of directed models that capture both phenomena remain elusive. Here we propose a system with both phenomena that translates to a model of two directed *friendly* walks confined to the quarter plane which allows the walks to touch but not cross one another. Now, while combinatorists have successfully tackled the non-interacting version of such a model (along with many other variants and extensions) by means of the Lindström–Gessel–Viennot lemma [29–35], the inclusion of multiple interaction parameters greatly affects the model's solvability. Even solutions of similar models that only include a single interaction term are in most instances not straight forward (if known), while it was only more recently that an exact solution of a two-friendly walker model in the quarter plane with *two* distinct adsorption parameters was found [12].

In this paper, we consider a two-dimensional model of DNA denaturation in the presence of an adsorbing wall consisting of two interacting upper and lower directed walks (polymers) near a horizontal sticky surface.

We begin in section 2 by constructing our model by first defining the combinatorial class of allowed configurations, and then introducing interaction parameters to assign our configurations with corresponding Boltzmann weights.

In section 3, we introduce two further variables that mark the final heights of both walks for any given configuration. These auxiliary variables, known as *catalytic* variables, are integral to solving our model. We then establish a mapping between our class of allowed paired walks onto itself which leads to a functional equation for the model's corresponding generating function that incorporates our added variables.

We then proceed in section 4 to determine an exact solution to the model's generating function by means of the *obstinate kernel method* [36]. While the beginnings of section 4 outline the precise steps undertaken, we briefly mention that this technique consists of generating a finite system of distinct functional equations by applying a set of different transformations to our original relation determined in section 3. We then subsequently collapse our system to construct a new refined functional equation which provides us (after some further work) with a solution to our generating function. Most importantly, we note in contrast to previous applications of the obstinate kernel method, we extend the process of this technique by establishing instead *two* independent systems of equations (and thus two distinct refined functional equations), which we then subsequently combine to arrive at our final solution. In particular, this allows us to express the generating function of our model as a relation between two simpler generating functions of the same underlying combinatorial class that ignore either polymer–surface or polymer–polymer interaction effects.

Equipped with our exact solution of the generating function, we analyse our model in section 5. Specifically, section 5.2 is devoted to determining the dominant singularity behaviour of the generating function over our parameter space. This then allows us in section 5.3 to identify four different phases of our system: a *free*, *adsorbed*, *zipped* and an *adsorbed-zipped* phase. We additionally specify the regions of the phases and plot the phase diagram, finding that all phases meet at a single critical point. Finally, in section 5.4 with the aid of our phase diagram, we are able to show that all phase transitions are second-order.

2. The model

Consider an upper and lower directed walk on the square integer lattice consisting of an equal number of pairwise steps. Both walks begin and end on a one-dimensional surface at y = 0 that restricts both walks to lie on or above the boundary of the upper half-plane, $\mathbb{Z} \times \mathbb{Z}_{\geq 0}$. Moreover,



Figure 1. An example of an allowed configuration with ten paired steps. Here, we have $m_a = 3$ surface visits (filled circles) and $m_c = 7$ shared contact sites (circles with filled inner circles). Thus, the overall Boltzmann weight for this configuration is a^3c^7 . Note that the final site of the configuration is both a surface visit and shared contact site.

walks only can take steps in either the north-east (1, 1) or south-east (1, -1) direction. Finally, steps of the lower walk can only either touch or lie below steps of the upper walk; with such objects typically referred to as (infinitely) *friendly* walks. Let $\widehat{\Omega}$ denote the class of allowed paired walks of *any* length. An example of an allowable configuration is given in figure 1.

For any configuration $\varphi \in \widehat{\Omega}$, we assign a weight *a* for each of the $m_a(\varphi)$ south-east *surface visit* steps of the lower walk that touch the surface at y = 0. Additionally, a weight *c* is assigned to each of the $m_c(\varphi)$ shared contact sites of the configuration where steps of the lower and upper walk share a vertex excepting the common initial vertex at the origin. Note that with this construction the trivial pair of walks of zero length has weight 1. With that in mind, the partition function for our model consisting of *L* paired steps is

$$Z_L(a,c) = \sum_{\varphi \in \widehat{\Omega}, |\varphi| = L} a^{m_a(\varphi)} c^{m_c(\varphi)}, \tag{1}$$

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

$$\kappa(a,c) = -\lim_{L \to \infty} \frac{1}{L} \log Z_L(a,c).$$
⁽²⁾

This thermodynamic quantity will be determined by solving for the model's generating function G(a, c; z), where

$$G(a, c; z) = \sum_{L=0}^{\infty} Z_L(a, c) z^L$$
(3)

and z is conjugate to the number of pairwise steps. Specifically, the relation between the free energy κ and the radius of convergence of G(a, c; z) is given by

$$\kappa(a,c) = \log z_s(a,c) \tag{4}$$

where $z_s(a, c)$ is the real and positive singularity of the generating function that is closest to the origin. Now, considering concatenations of paired walks of arbitrary positive length and recalling that these configurations must both start and end on the surface, it can be shown that for all $a, c \in \mathbb{R}_{>0}$, $\{Z_L\}_{L \ge 0}$ forms a positive *super-multiplicative* sequence—that is, that

$$Z_{N+M}(a,c) \ge Z_N(a,c)Z_M(a,c), \quad \forall N, M \in \mathbb{Z}_{\ge 0}.$$
(5)

Thus, a standard theorem on super-multiplicative functions due to Hille [37] (generalized in [38, 39]), shows that the limiting free energy $\kappa(a, c)$ in (2) exists. Moreover, by (4), this further implies that G(a, c; z) is analytic at z = 0 for all $a, c \in \mathbb{R}_{>0}$.

3. Constructing the functional equations

In section 2 we introduced the class of allowable configurations $\widehat{\Omega}$ with corresponding generating function G(a, c; z). We now want to establish a functional equation for G(a, c; z) by considering the effect of appending a pair of steps to the end of any given configuration $\varphi \in \widehat{\Omega}$. However, as paired walks in $\widehat{\Omega}$ both end on the surface, appending a step (which must be in the direction $(1, \pm 1)$) to each of the walks will result in a new configuration that is no longer in $\widehat{\Omega}$. Thus, our approach is to instead consider a larger combinatorial class containing $\widehat{\Omega}$ that allows us to append steps onto configurations while still remaining in our new, larger class.

First, we define the class of paired walks $\Omega(i, j)$ that consists of configurations with final lower walk height *i* and final distance between the two walks *j*, while still obeying the same friendly and surface constraints. Thus, we define our larger combinatorial class $\Omega(0^+, 0^+)$ as

$$\Omega(0^+, 0^+) \equiv \bigcup_{i \ge 0, j \ge 0} \Omega(i, j).$$
(6)

Note that our original class of walks in our model $\widehat{\Omega} \equiv \Omega(0, 0)$. Now, equipped with our larger combinatorial class, we can introduce its corresponding generating function F(a, c; z) that encodes information about the number of steps, surface visits and shared contacts for each configuration $\varphi \in \Omega(0^+, 0^+)$. However, determining whether appending a step-pair onto a given configuration φ results in a new and *allowable* configuration (i.e. φ remains in $\Omega(0^+, 0^+)$) further requires knowledge of the *final* step heights of both walks. Thus, solely for the purpose of establishing our functional equation for F(a, c; z), we additionally introduce two auxiliary (or so-called *catalytic*) variables *r* and *s* to construct the expanded generating function F(r, s, a, c; z) where

$$F(r, s, a, c; z) \equiv F(r, s) = \sum_{\varphi \in \Omega(0^+, 0^+)} z^{|\varphi|} r^{h(\varphi)} s^{d(\varphi)/2} a^{m_a(\varphi)} c^{m_c(\varphi)}$$
(7)

and again z is conjugate to the length $|\varphi|$ of a configuration $\varphi \in \Omega(0^+, 0^+)$, r is conjugate to the distance $h(\varphi)$ of the bottom walk from the surface and s is conjugate to half the distance $d(\varphi)$ between the final vertices of the two walks. Thus, for each $\varphi \in \Omega(0^+, 0^+)$, powers of r and s in F(r, s) track the final step heights of the bottom and top walk respectively. Note that due to the allowed step directions, $d(\varphi)$ must always be even, ensuring that F(r, s) contains only integer powers of s. Thus, we consider F(r, s) as an element of $\mathbb{Z}[r, s, a, c][[z]]$: the ring of formal power series in z with coefficients in $\mathbb{Z}[r, s, a, c]$.

We aim to solve $F(0, 0, a, c; z) \equiv G(a, c; z)$ by establishing a functional equation for F(r, s). Specifically, we construct a suitable mapping from $\Omega(0^+, 0^+)$ onto itself by considering the effect of appending an *allowable* step-pair onto a configuration, translating this map into its action on the generating function. Now, at the end of any given walk we can append a step $(1, \pm 1)$. Hence, for a pair of walks, there are a total of four possible combinations of paired steps that can be appended to a configuration. We denote the collection of allowable steps by the set S, where

$$S = \{\{(1, 1), (1, 1)\}, \{(1, -1), (1, 1)\}, \{(1, 1), (1, -1)\}, \{(1, -1), (1, -1)\}\}$$

$$= \{\uparrow \uparrow, \downarrow \uparrow, \uparrow \downarrow, \downarrow \downarrow\},$$
(8)

that alter the corresponding configuration weight by factors of zr, $\frac{zs}{r}$, $\frac{zr}{s}$ and $\frac{z}{r}$ respectively.

However, given the non-crossing constraint between the lower walk and the surface as well as between both walks, indeed not all four combinations of appended paired steps will necessarily result in allowable configurations. Additionally, surface and shared contact



Figure 2. The possible four ways of appending a pair of steps to an allowed configuration that results in no new surface or shared contacts.

interaction effects also need to be considered when attaching new steps. Thus, we identify ten distinct cases that capture all possible changes in weight that can arise from appending a pair of steps as seen in figures 2–4; allowing us to construct a functional equation for F(r, s), highlighting the underlying decomposition for $\Omega(0^+, 0^+)$.

We denote $\{\bullet\}$ as the trivial zero-length configuration and introduce the following shorthand notation

$$\Omega(n^+, j) \equiv \bigcup_{i \ge n} \Omega(i, j), \quad \Omega(i, m^+) \equiv \bigcup_{j \ge m} \Omega(i, j), \quad \Omega(n^+, m^+) = \bigcup_{i \ge n, j \ge m} \Omega(i, j), \tag{9}$$

while

$$\{s\} \cdot \Omega(i,j) \tag{10}$$



Figure 3. The two possible ways of appending a pair of steps to an allowed configuration that results in a surface (but not shared) contact.

represents the class of configurations formed by appending the step-pair $s \in S$ to the *end* of each pair of walks $\varphi \in \Omega(i, j)$. With that in mind, we can build up our functional equation F(r, s, a, c; z) by firstly establishing a relation for the non-interacting case F(r, s, 1, 1; z) and subsequently incorporating the effects of surface and shared contacts respectively. To do this, we consider the effect of appending a pair-step to a given configuration, making sure to eliminate newly formed paired walks that are no longer part of our allowable class $\Omega(0^+, 0^+)$. For F(r, s, 1, 1; z), we find

$$\begin{aligned} F(r, s, 1, 1; z) &= 1 & \Omega(0^+, 0^+) &= \{\bullet\} \\ &+ zrF(r, s) & \bigcup\{\uparrow\uparrow\} \cdot \Omega(0^+, 0^+), & \text{figure } 2(a) \\ &+ \frac{z}{r}(F(r, s) - [r^0]F(r, s)) & \bigcup\{\downarrow\downarrow\} \cdot \Omega(1^+, 0^+), & \text{figure } 2(b) \\ &+ \frac{zz}{s}(F(r, s) - [s^0]F(r, s)) & \bigcup\{\downarrow\uparrow\} \cdot \Omega(1^+, 0^+), & \text{figure } 2(c) \\ &+ \frac{zz}{s}(F(r, s) - [s^0]F(r, s)) & \bigcup\{\uparrow\downarrow\} \cdot \Omega(0^+, 1^+), & \text{figure } 2(d), \end{aligned}$$

where $[r^j]F(r, s), [s^k]F(r, s)$ and in general $[r^j s^k]F(r, s)$ denote the coefficients of r^j, s^k and $r^j s^k$ in the generating function F(r, s) respectively. Note, that thus

$$[r^{0}]F(r,s) = F(0,s),$$

$$[s^{0}]F(r,s) = F(r,0),$$

$$[r^{0}s^{0}]F(r,s) = F(0,0).$$
(12)

Next, we add surface interaction effects to (11) to get a functional equation for F(r, s, a, 1; z), with

$$F(r, s, a, 1; z) =$$
rhs of equation (11)

+
$$z(a-1)[r^1]F(r,s)$$
 { $\downarrow\downarrow$ } · $\Omega(1,0^+)$, figure 3(*a*)
+ $zs(a-1)[r^1]F(r,s)$ { $\downarrow\uparrow$ } · $\Omega(1,0^+)$, figure 3(*b*). (13)

Finally, we incorporate shared site contacts into (13) to get a functional equation for the full generating function $F(r, s, a, c; z) \equiv F(r, s)$ making sure we accommodate for the case



Figure 4. The four possible ways of appending a pair of steps to an allowed configuration that adds a new shared site contact. Note, that in (c) we add both a surface and shared site contact.

where two downward steps may add both a new surface and shared site contact. Thus, we have

F(r, s) = rhs of equation (13)

$$\begin{aligned} + zr(c-1)[s^{0}]F(r,s) & \{\uparrow\uparrow\} \cdot \Omega(0^{+},0), & \text{figure 4}(a) \\ + \frac{z(c-1)}{r}([s^{0}]F(r,s) - [r^{0}s^{0}]F(r,s)) & \{\downarrow\downarrow\} \cdot \Omega(1^{+},0), & \text{figure 4}(b) & (14) \\ + z(a-1)(c-1)[r^{1}s^{0}]F(r,s) & \{\downarrow\downarrow\} \cdot \Omega(1^{+},0), & \text{figure 4}(c) \\ + zcr[s^{1}]F(r,s) & \{\uparrow\downarrow\} \cdot \Omega(0^{+},2), & \text{figure 4}(d). \end{aligned}$$

By collecting terms we simply (14) down to

$$F(r,s) = 1 + z \left(r + \frac{1}{r} + \frac{s}{r} + \frac{r}{s}\right) F(r,s) - z \left(\frac{1}{r} + \frac{s}{r}\right) F(0,s) + z \left[(c-1)\left(r + \frac{1}{r}\right) - \frac{r}{s}\right] F(r,0) - \frac{z(c-1)}{r} F(0,0) + z(a-1)(s+1)[r^1]F(r,s) + zr(c-1)[s^1]F(r,s) + z(a-1)(c-1)[r^1s^0]F(r,s).$$
(15)

We can further refine (15) by eliminating the terms $[r^1]F(r, s)$, $[s^1]F(r, s)$ and $[r^1s^0]F(r, s)$. Specifically, we additionally construct a functional equation for F(0, 0)

$$F(0,0) = 1 + zac[r^{1}s^{0}]F(r,s) \qquad \Omega(0,0) = \{\bullet\} \bigcup \{\downarrow\downarrow\} \cdot \Omega(1,0)$$
(16)

along with an equation for F(0, s)

$$F(0, s) = 1 \qquad \Omega(0, 0^{+}) = \{\bullet\}$$

+ $za([r^{1}]F(r, s) - [r^{1}s^{0}]F(r, s)) \qquad \bigcup\{\downarrow\downarrow\} \cdot \Omega(1, 2^{+})$
+ $zac[r^{1}s^{0}]F(r, s) \qquad \bigcup\{\downarrow\downarrow\} \cdot \Omega(1, 0)$
+ $zas[r^{1}]F(r, s) \qquad \bigcup\{\downarrow\uparrow\} \cdot \Omega(1, 0^{+})$
(17)

and F(r, 0)

$$F(r, 0) = 1 \qquad \qquad \Omega(0^+, 0) = \{\bullet\}$$

$$+ zcrF(r, 0) \qquad \qquad \bigcup\{\uparrow\uparrow\} \cdot \Omega(0^+, 0)$$

$$+ \frac{zc}{r}(F(r, 0) - [r^0s^0]F(r, s) - r[r^1s^0]F(r, s)) \qquad \bigcup\{\downarrow\downarrow\} \cdot \Omega(2^+, 0) \qquad (18)$$

$$+ zac[r^1s^0]F(r, s) \qquad \qquad \bigcup\{\downarrow\downarrow\} \cdot \Omega(1, 0)$$

$$+ zcr[s^1]F(r, s) \qquad \qquad \bigcup\{\uparrow\downarrow\} \cdot \Omega(0^+, 2),$$

so that (15) simplifies to

$$K(r,s)F(r,s) = \frac{1}{ac} + \left(C - \frac{zr}{s}\right)F(r,0) + \left[A - \frac{z}{r}\left(s+1\right)\right]F(0,s) - ACF(0,0)$$
(19)

where

$$A \equiv \frac{a-1}{a}, \qquad C \equiv \frac{c-1}{c} \tag{20}$$

and the kernel K(r, s) is

$$K(r,s) \equiv K(r,s;z) = \left(1 - z \left[r + \frac{s}{r} + \frac{r}{s} + \frac{1}{r}\right]\right).$$
 (21)

The importance of the kernel in finding a solution to the generating function will be revealed in section 4.

4. Solution of the model

In section 3, we established functional equation (19) for our model containing the generating functions F(r, s), F(r, 0), F(0, s), F(0, 0) as well as the kernel K(r, s). Recall, that our ultimate goal is to find a solution to $F(0, 0) \equiv F(0, 0, a, c; z) \equiv G(a, c; z)$, and so ideally we would like to eliminate unknown terms from (19), which will be done by means of the *obstinate kernel method* [36]. We begin in section 4.1 by finding eight transformations that leave the kernel function (21) unchanged. Thus, substitution of these transformations into (19) results in a system of eight distinct equations, each of which contains the same unchanged kernel K(r, s).

In section 4.2 we utilize this fact by substituting in a root of the kernel with respect to s so that terms attached to K(r, s) vanish and then proceed to eliminate further terms by collapsing our system into a single refined functional equation. Specifically, this equation contains the unknowns F(r, 0), F(1/r, 0) and F(0, 0). We will also show that by using a different root of the kernel, now with respect to r, we can instead obtain an alternate equation consisting of the unknowns F(0, s), F(0, 1/s) and F(0, 0). The key point is that both of these equations now have generating functions containing powers of *only* one catalytic variable. Thus, as featured in previous applications of the obstinate kernel method [12, 35, 36, 40], the hope is that by extracting some carefully chosen coefficient of $[r^i]$ or $[s^j]$ from either of our functional equations, we can get a new relation solely in terms of $F(0, 0) \equiv G(a, c)$. Unfortunately, irrespective of which functional equation we choose, we find that we are unable to directly solve for the full generating function G(a, c) by the same process. However, in section 4.3 we will find that by setting c = 1, extracting the coefficient of s^1 from our equation containing F(0, s), F(0, 1/s) and F(0, 0) does allow us to solve for the simpler generating function G(a, 1) that ignores shared site contacts. Similarly, in section 4.4 by setting a = 1, we will make use of our other functional equation containing F(r, 0), F(1/r, 0) and F(0, 0), showing that by extracting the coefficient of r^1 we can instead solve for the generating function G(1, c)that ignores surface contacts.

Finally, in section 4.5 we make the surprising connection between the two refined functional equations that allows us to express G(a, c) solely in terms of G(a, 1) and G(1, c). Thus, our motivation for solving for these two simpler generating functions is additionally driven by the fact that we will also obtain an exact solution to the full generating function G(a, c).

4.1. Symmetries and roots of the kernel

Here, we follow the approach featured in [41]. Recalling the functional equation for F(r, s) in (19), we observe that the corresponding kernel function K(r, s) (21) is symmetric under the two transformations

$$\Phi: (r,s) \mapsto \left(r, \frac{r^2}{s}\right), \qquad \Psi: (r,s) \mapsto \left(\frac{s}{r}, s\right), \tag{22}$$

where both Φ and Ψ are involutions. These transformations generate a family of eight symmetries \mathcal{F} as seen in figure 5.

Now, considering K(r, s) as a polynomial in *s*, we find two roots \hat{s}_{\pm}

$$\hat{s}_{\pm}(r;z) = \frac{r-z-r^2z \pm \sqrt{(r^2z+z-r)^2 - 4r^2z^2}}{2z},$$

$$\hat{s}_{-}(r;z) = rz + (1+r^2)z^2 + O(z^3), \qquad \hat{s}_{+}(r;z) = \frac{r}{z} - (1+r^2) + O(z),$$
(23)

which when substituting into (19) sets the left-hand side of the functional equation to zero. The choice of which roots result in legitimate substitutions is justified by determining whether $F(r, \hat{s}_{\pm})$ remains in $\mathbb{Z}[r, a, c][[z]]$. In this instance, it suffices to check that F(0, s) remains formally convergent in this ring when substituting in either of the roots, which translates into ensuring that the coefficients of the truncated power series stabilize as polynomials in $\mathbb{Z}[r, a, c]$ as the length of the series grows. Recalling that *s* is conjugate to *half* the distance between the final heights of the upper and lower walks for any given configuration, we have

$$F(0, s; z) = \sum_{L \ge 0} \{ p_L(a, c) s^{\lfloor L/2 \rfloor} + o(s^{\lfloor L/2 \rfloor}) \} z^L, \qquad p_L(a, c) \in \mathbb{Z}[a, c],$$
(24)



Figure 5. The family of transformations \mathcal{F} that leave the kernel function $K(r, s; z) = (1 - z[r + \frac{s}{r} + \frac{r}{s} + \frac{1}{r}])$ invariant.

as the final distance between the upper and lower walks can only be at most L for any given configuration of length L. Substituting in the roots (23) we find

$$F(0, \hat{s}_{-}; z) = \sum_{L \ge 0} \{ p_L(a, c) r^{\lfloor L/2 \rfloor} z^{L + \lfloor L/2 \rfloor} + O(z^{L + \lfloor L/2 \rfloor}) \},$$

$$F(0, \hat{s}_{+}; z) = \sum_{L \ge 0} \{ p_L(a, c) r^{\lfloor L/2 \rfloor} z^{L - \lfloor L/2 \rfloor} + O(z^{L - \lfloor L/2 \rfloor}) \},$$
(25)

which implies

$$[z^{n}]F(0, \hat{s}_{-}; z) = \sum_{L=0}^{n} [z^{n}] \{ p_{L}(a, c) r^{\lfloor L/2 \rfloor} z^{L+\lfloor L/2 \rfloor} + O(z^{L+\lfloor L/2 \rfloor}) \},$$

$$[z^{n}]F(0, \hat{s}_{+}; z) = \sum_{L=0}^{2n} [z^{n}] \{ p_{L}(a, c) r^{\lfloor L/2 \rfloor} z^{L-\lfloor L/2 \rfloor} + O(z^{L-\lfloor L/2 \rfloor}) \}$$
(26)

and so both $F(0, \hat{s}_{\pm})$ are formally convergent in $\mathbb{Z}[r, a, c][[z]]$.

Of course, we can also treat the kernel as a polynomial in *r*, giving us roots $\hat{r}_{\pm}(s; z)$

$$\hat{r}_{\pm}(s;z) = \frac{s \pm \sqrt{s[s - 4(1 + s)^2 z^2]}}{2z(1 + s)},$$

$$\hat{r}_{-}(s;z) = (1 + s)z + \frac{(1 + s)^3}{s}z^3 + O(z^3), \qquad \hat{r}_{+}(s;z) = \frac{s}{(1 + s)z} - (1 + s) + O(1),$$
(27)

and again we determine which roots ensure that the generating function F(r, 0) is convergent where

$$F(r,0;z) = \sum_{L \ge 0} \{ b_L(a,c)r^L + o(r^L) \} z^L, \quad b_L(a,c) \in \mathbb{Z}[a,c],$$
(28)

recalling that *r* is conjugate to the final height of the lower walk above the surface. Substituting the roots $\hat{r}_{\pm}(s; z)$ into (28) we find

$$F(\hat{r}_{-}, 0; z) = \sum_{L \ge 0} \{ b_L(a, c)(1+s)^L z^{2L} + O(z^{2L+1}) \},$$

$$F(\hat{r}_{+}, 0; z) = \sum_{L \ge 0} \left\{ b_L(a, c) \left(\frac{s}{1+s} \right)^L + O(z) \right\},$$
(29)

and so while $F(\hat{r}_{-}, 0)$ is formally convergent, it is clear that for each $n \in \mathbb{Z}_{\geq 0}$, $[z^n]F(\hat{r}_{+}, 0)$ cannot be determined by truncating the corresponding series in (29).

However, we note that while we are free to substitute the roots \hat{s}_{\pm} and \hat{r}_{-} into (19), we in fact find that it suffices to only consider \hat{s}_{-} and \hat{r}_{-} . Thus, for the remainder of this paper, we define $\hat{s}(r; z) \equiv \hat{s}_{-}(r; z)$ and $\hat{r}(s; z) \equiv \hat{r}_{-}(s; z)$. Finally, when the kernel (21) K(r, s) = 0 we have

$$rs = z(1+s)(r^2+s)$$
(30)

and thus by Lagrange inversion [42], we have

$$\hat{r}(s;z)^{k} = \sum_{n=k}^{\infty} \frac{k}{n} [u^{n-k}] \left\{ \frac{(1+s)^{n} (u^{2}+s)^{n}}{s^{n}} \right\} z^{n}, \quad k > 0$$
$$= \sum_{n=k}^{\infty} \frac{k}{2n+k} {2n+k \choose n} \frac{(1+s)^{2n+k}}{s^{n}} z^{2n+k}, \tag{31a}$$

$$\hat{s}(r;z)^{k} = \sum_{n=k}^{\infty} \frac{k}{n} [t^{n-k}] \left\{ \frac{(1+t)^{n} (r^{2}+t)^{n}}{r^{n}} \right\} z^{n}, \quad k > 0$$
$$= \sum_{n=k}^{\infty} \frac{k}{n} \left\{ \sum_{j=0}^{n-k} \binom{n}{j} \binom{n}{k+j} r^{2(k+j)-n} \right\} z^{n}, \quad (31b)$$

giving us explicit series representations for positive integer powers of the roots \hat{r} and \hat{s} , which will later be utilized in finding a explicit solution to the generating function.

4.2. Using the symmetries of the kernel

Equipped with the roots \hat{s} and \hat{r} as well as the family of symmetries \mathcal{F} that leave the kernel invariant, we can now apply the obstinate kernel method. Specifically, we substitute $(r, s) \mapsto (r, \hat{s})$ and $(r, s) \mapsto (\hat{r}, s)$ into the simplified functional equation (19), subsequently applying a subset of transformations from \mathcal{F} to generate a system of new functional equations. With that in mind, mapping $(r, s) \mapsto (r, \hat{s})$ we have the system

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

(r, s) \mapsto (r, \hat{s}) (32a)

$$0 = \frac{\hat{s}}{ac} + \left(C\hat{s} - \frac{z\hat{s}}{r}\right)F\left(\frac{\hat{s}}{r}, 0\right) + [A\hat{s} - zr(\hat{s} + 1)]F(0, \hat{s})$$
$$-AC\hat{s}F(0, 0), \quad (r, s) \mapsto \left(\frac{\hat{s}}{r}, \hat{s}\right)$$
(32b)

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$$0 = \frac{\hat{s}}{acr^2} + \left(\frac{C\hat{s}}{r^2} - \frac{z\hat{s}}{r}\right)F\left(\frac{\hat{s}}{r}, 0\right) + \left[\frac{A\hat{s}}{r^2} - \frac{z}{r}\left(\frac{\hat{s}}{r^2} + 1\right)\right]F\left(0, \frac{\hat{s}}{r^2}\right) - \frac{AC\hat{s}}{r^2}F(0, 0), \quad (r, s) \mapsto \left(\frac{\hat{s}}{r}, \frac{\hat{s}}{r^2}\right)$$
(32c)

$$0 = \frac{\hat{s}}{acr^2} + \left(\frac{C\hat{s}}{r^2} - \frac{z\hat{s}}{r}\right)F\left(\frac{1}{r}, 0\right) + \left[\frac{A\hat{s}}{r^2} - \frac{z\hat{s}}{r}\left(\frac{\hat{s}}{r^2} + 1\right)\right]F\left(0, \frac{\hat{s}}{r^2}\right) - \frac{AC\hat{s}}{r^2}F(0, 0), \quad (r, s) \mapsto \left(\frac{1}{r}, \frac{\hat{s}}{r^2}\right),$$
(32d)

where the chosen subset of transformations guarantee that each functional equation (32a)–(32d) only contain non-negative powers of \hat{s} and thus the generating functions are formally convergent in $\mathbb{Q}[a, c, r, \bar{r}, s, \bar{s}][[z]]$. Now, considering the system of equations (32a)–(32d), we can eliminate $F(0, \hat{s})$ by

$$0 = [\text{coeff. of } F(0, \hat{s}) \text{ in } (32b)] \times [\text{rhs of } (32a)] - [\text{coeff. of } F(0, \hat{s}) \text{ in } (32a)] \times [\text{rhs of } (32b)] = [A\hat{s} - zr(\hat{s} + 1)][\text{rhs of } (32a)] - \left[A\hat{s} - \frac{z\hat{s}}{r}(\hat{s} + 1)\right][\text{rhs of } (32b)].$$
(33)

In a similar vein we can eliminate $F(0, \frac{\hat{s}}{r^2})$ from the system by

$$0 = \left[\text{coeff. of } F\left(0, \frac{\hat{s}}{r^2}\right) \text{ in } (32d) \right] \times [\text{rhs of } (32c)] - \left[\text{coeff. of } F\left(0, \frac{\hat{s}}{r^2}\right) \text{ in } (32c) \right] \times [\text{rhs of } (32d)] = \left[\frac{A\hat{s}}{r^2} - \frac{z\hat{s}}{r} \left(\frac{\hat{s}}{r^2} + 1\right) \right] [\text{rhs of } (32c)] - \left[\frac{A\hat{s}}{r^2} - \frac{z}{r} \left(\frac{\hat{s}}{r^2} + 1\right) \right] [\text{rhs of } (32d)]$$
(34)

and combining (33) with (34) we can further eliminate $F(0, \frac{s}{r^2})$

$$0 = \left[\text{coeff. of } F\left(0, \frac{\hat{s}}{r^2}\right) \text{ in (34)} \right] \times [\text{rhs of (33)}] \\ - \left[\text{coeff. of } F\left(0, \frac{\hat{s}}{r^2}\right) \text{ in (33)} \right] \times [\text{rhs of (34)}],$$
(35)

yielding a functional equation solely in terms of the generating functions F(r, 0), $F(\frac{1}{r}, 0)$ and F(0, 0). Specifically, we have

$$N_1(r;z)F(1/r,0) + N_2(r;z)F(r,0) = [M(r;z) - aH(r;z)]\left(\frac{1}{ac} - ACF(0,0)\right)$$
(36)

where

$$N_{1}(r; z) = (cr - r - cz)(r - ar + az - ar^{2}z + a^{2}r^{2}z),$$

$$N_{2}(r; z) = r(1 - c + crz)(r - ar - az + a^{2}z + ar^{2}z),$$

$$M(r; z) \equiv M(r, a, c; z) = -ac(a + c - 2)r(r^{2} - 1)z,$$

$$H(r; z) \equiv H(r, c; z) = (c - 2)c^{2}(r^{4} - 1)z^{2} + O(z^{2}).$$
(37)

Note, that H(r, c; z) in (36) is an algebraic function *independent* of the surface contact weight *a*. This observation will be integral to establishing a solution to the full generating function G(a, c) in section 4.5.

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Alternatively, by an identical process, we can instead use the root \hat{r} along with a subset of transformations in \mathcal{F}

$$(\hat{r}, s) \mapsto (\hat{r}, s), \left(\hat{r}, \frac{\hat{r}^2}{s}\right), \left(\frac{\hat{r}}{s}, \frac{\hat{r}^2}{s}\right), \left(\frac{\hat{r}}{s}, \frac{1}{s}\right)$$
(38)

that contain positive powers of \hat{r} to yield an alternate refined functional equation

$$N_1^{\star}(s; z)F(0, 1/s) + N_2^{\star}(s; z)F(0, s) = [M^{\star}(s) - c^2 H^{\star}(s; z)] \left(\frac{1}{ac} - ACF(0, 0)\right),$$
(39)

where

$$N_{1}^{\star}(s; z) = (-1+c)s(-1+(-1+c)s) + c^{2}(1+s)z^{2},$$

$$N_{2}^{\star}(s; z) = \frac{s(1-a+s)((-1+c)^{2}+s-cs+c^{2}s(1+s)z^{2})}{s(a-1)-1},$$

$$M^{\star}(s) \equiv M^{\star}(s, a, c) = \frac{a(-1+c)c(-1+s)(1+s)}{s(-1+(-1+a)s)},$$

$$H^{\star}(s; z) \equiv H^{\star}(s, a; z) = \frac{a(-1+s)(1+s)(1-(-2+a)s+s^{2})z^{2}}{s^{2}(-1+(-1+a)s)} + O(z^{2}).$$
(40)

Again, we note that $H^*(s; z)$ is an algebraic function *independent* of the shared contact weight c, while $M^*(s)$ is a rational function solely in terms of s, a and c.

Overall, by using the symmetries of the kernel we have established two new refined functional equations (36) and (39), containing unknown generating functions in only one catalytic variable (either in r or s respectively). As mentioned at the beginning of section 4, the potential benefit of these new equations is that by extracting the coefficients of r^i or s^j for some choice of *i* or *j* (depending on which of the functional equations we consider), we hope to arrive at a relation solely in terms of $F(0, 0) \equiv G(a, c)$. Unfortunately, we find that while coefficient extraction is able to further refine our equations, we are unable to solve for the full generating function. However, by setting either c = 1 or a = 1, we will find that both of (36) and (39) can be utilized to solve for G(a, 1) and G(1, c), which we indeed proceed to do in sections 4.3 and 4.4 respectively. Keep in mind that we are ultimately leading up to section 4.5 where we establish a relation that expresses G(a, c) in terms of G(a, 1) and G(1, c). Thus, to solve for our full generating function G(a, c), we do indeed need to first determine solutions to the two simpler generating functions.

4.3. Solving the simplified generating function: c = 1

Our aim now is to utilize the refined functional equations that were established in section 4.2. Specifically, for functional equation (39) that contains powers of s, we find extracting the coefficient of s^1 gives us

$$(-1+a)(a(-1+c)^{2}+c(1+c(-1+z^{2})))F(0,0) + (-1+a)(-1+c)^{2}[s^{1}]F(0,s)$$

= $([s^{1}]M^{\star}(s) - c^{2}[s^{1}]H^{\star}(s;z))\left(\frac{1}{ac} - ACF(0,0)\right)$ (41)

and subsequently setting c = 1,

$$(a-1)z^{2}G(a,1) = -\frac{1}{a}[s^{1}]H^{\star}(s;z)$$

= $[s^{1}]\frac{(1-s)(1+s)(1-(-2+a)s+s^{2})z^{2}}{s^{2}(-1+(-1+a)s)}.$ (42)

Thus, we have related G(a, 1) to coefficients of s^1 of the algebraic function $H^*(s; z)$. However, while (41) will be important in solving the full generating function G(a, c), thankfully, at this point we do not need to attempt to further refine our equation, as an exact solution for G(a, 1) has already been determined in [43] and [12]. Specifically, we have

$$G(a,1) = 1 + \sum_{i=1}^{\infty} z^{2i} \sum_{m=1}^{i} a^m \frac{m(m+1)(m+2)}{(i+1)^2(i+2)(2i-m)} {2i \choose i} {2i-k \choose i}.$$
 (43)

In section 4.4, a solution for the simplified generating function G(1, c) is found by employing the same method featured in [12] that was used to solve for G(a, 1) (43).

4.4. Solving the simplified generating function: a = 1

To establish a relation for the alternate simplified model that instead weighs only shared site contacts, we consider functional equation (36) containing powers of r. By extracting the coefficient of r^1 we find

$$z[a(a-2) - c(1 + a(a-3))]F(0,0) - (a-1)(acz^{2} + c - 1)[r^{1}]F(r,0) + az(a-1)(c-1)[r^{2}]F(r,0) = ([r^{1}]M(r;z) - a[r^{1}]H(r;z))\left(\frac{1}{ac} - ACF(0,0)\right),$$
(44)

which when setting a = 1 simplifies to

$$G(1,c) = [r^1]R(r,c;z) \equiv [r^1]\frac{\hat{s}(r^2-1)[r-cr+cz(1+r^2-\hat{s})]}{(c-1)(\hat{s}-c\hat{s}+crz)},$$
(45)

where we recall that G(a, c) = F(0, 0, a, c; z). Thus, our generating function is expressed in terms of coefficients of r^1 contained in the algebraic function R(r, c; z). Following a similar approach to [12], we begin by expanding R(r, c; z) as a power series in c, so that (45) becomes

$$G(1,c) = \sum_{m=0}^{\infty} [r^1] c^m \frac{(r^2 - 1)(r^2 - \hat{s})(\hat{s} - 1)\left(1 - \frac{rz}{\hat{s}}\right)^m}{r}.$$
(46)

Therefore, if we can find a series representation for $(1 - \frac{rz}{s})^m$ in z and r, then extracting the coefficients of our sum in (46) becomes a fairly straightforward (though time-consuming) task. With that in mind, we have

$$\left(1 - \frac{rz}{\hat{s}}\right)^m = \sum_{k=0}^m \binom{m}{k} (-1)^k \left(\frac{rz}{\hat{s}}\right)^k,\tag{47}$$

which implies that we need to determine an expansion for \hat{s}^{-k} . Recall in section 4.1, we gave a series representation for positive powers of $\hat{s}(z)$ by means of Lagrange inversion which utilized the relation

$$\hat{s}(z) = \frac{z}{r}(1+s)(r^2 + \hat{s}(z))$$
(48)

that was determined by setting the kernel (21) to zero. Now, for an arbitrary function H(u), a more generalized form of the Lagrange Inversion Theorem [42] gives us

$$[z^{n}]H(\hat{s}(r;z)) = \frac{1}{n} [u^{n-1}] \left(H'(u) \frac{1}{r^{n}} (u+1)^{n} (u+r^{2})^{n} \right).$$
(49)

Thus, in particular, when $H(u) = u^{-k}$ for $k \in \mathbb{N}^+$, we find

$$[z^{n}]\hat{s}(r;z)^{-k} = -\frac{k}{nr^{n}}[u^{n-k}]\frac{(u+1)^{n}(u+r^{2})^{n}}{u^{k+1}},$$
(50)

which with some work gives us

$$\hat{s}(r;z)^{-k} = -\left\{\sum_{n=k}^{\infty} \frac{k}{n} \sum_{j=0}^{n-k} \binom{n}{j} \binom{n}{k+j} r^{2j-n} z^n \right\} + (-1)^k \left(1 + \frac{1}{r^{2k}}\right) \\ + \left\{\sum_{n=1}^k \frac{k}{n} (-1)^{k-n} \sum_{j=0}^{k-n} \binom{n+j-1}{j} \binom{k-j-1}{n-1} r^{n-2k+2j} z^{-n} \right\}.$$
(51)

`

Substituting (51) into (47), we are now in a position to extract coefficients of *r* for the expression $\left(1 - \frac{rz}{s}\right)^m$. For instance, one can show that

$$[r^{0}]\left(1 - \frac{rz}{\hat{s}}\right)^{m} = \left\{\sum_{k=1}^{m} (-1)^{k+1} \binom{m}{k} \sum_{p=0}^{\infty} \frac{k}{2p+k} \binom{2p+k}{p} \binom{2p+k}{p+k} z^{2p+2k} \right\} + \left\{\sum_{k=2}^{m} \binom{m}{k} \sum_{p=1}^{\lfloor\frac{k-1}{2}\rfloor} \frac{k}{k-2p} (-1)^{k} \binom{k-p-1}{p} \binom{k-p-1}{k-2p-1} z^{2p} \right\}.$$
 (52)

Returning to our expression for G(1, c) at (46), we partition the coefficients of c^m into common powers of r, \hat{s} and $\left(1 - \frac{r_2}{\hat{s}}\right)^m$ so that

$$[c^{m}]G(1,c) = ([r^{0}] - [r^{-2}])\left(1 - \frac{rz}{\hat{s}}\right)^{m} + ([r^{-2}] - [r^{2}])\hat{s}\left(1 - \frac{rz}{\hat{s}}\right)^{m} + ([r^{2}] - [r^{0}])\hat{s}^{2}\left(1 - \frac{rz}{\hat{s}}\right)^{m}.$$
(53)

Therefore, along with $[r^0] \left(1 - \frac{rz}{s}\right)^m$ found in (52), there remain five other components in (53) whose series representation can be determined in the same fashion. Finally, we change the order of summation to get terms that are power series in z (all negative powers of z vanish after coefficient extraction) and with the aid of Maple³ to combine our sums we find the exact solution for G(1, c) to be

$$G(1, c; z) = 1 + c^{2}z^{2} + c^{3}(1 + 2z)z^{4} + \sum_{i=3}^{\infty} z^{2i} \sum_{m=3}^{2i} c^{m} \sum_{k=3}^{m} (-1)^{k+1} \times \frac{k(k-1)(k-2)(2i-k+1)(i-k+2)}{i^{2}(i-1)^{2}(i+1)(i-2)} {m \choose k} {2i-k \choose i-2} {2i-k-1 \choose i-3}.$$
 (54)

The above expression is more complicated than the double sum expression for G(a, 1) given in (43). We were unable to refine the triple sum expression into a double sum.

4.4.1. Finding a differential equation: a = 1. In section 4.4, G(1, c) was solved by explicitly finding the series representation of the algebraic function R(r, c; z) (45) and subsequently extracting coefficients. As an alternative approach, one can employ an algorithm due to Almkvist and Zeilberger [44] that involves differentiating *hyperexponential* functions under the integral sign to instead establish a homogeneous linear differential equation solved by $[r^1]R(r, c; z)$.

We begin by noting that a general multivariable function $g(\mathbf{x}) \equiv g(x_1, \ldots, x_n)$ is *hyperexponential* if for each $i = 1, \ldots, n$, the logarithmic derivative $(\partial/\partial_{x_i}g(\mathbf{x}))/g(\mathbf{x})$ is a rational function in $\mathbb{C}(x_1, \ldots, x_n)$. For further details about the underlying theory and innards of the algorithm, we direct the reader to [44] and [45] respectively. Utilizing the

³ Maplesoft: a division of Waterloo Maple Inc. Maple 14 (software package).

Maple package DETools which implements the so-called fast Zeilberger algorithm applicable to hyperexponential functions, we find the linear differential operator \mathcal{L} to be

$$\mathcal{L} = [(236544c^{19} + \dots + 88704c^{16})z^{27} + \dots + (-140c^{11} + \dots + 560)z^5](\partial/\partial_{x_i})^5 + [(2838528c^{19} + \dots + 1064448c^{16})z^{26} + \dots + (-1960c^{11} + \dots + 7840)z^4](\partial/\partial_{x_i})^4 + \dots + [(13824c^{15} + \dots + 14515200)z^2 + \dots - 322560c^{11} + \dots + 1290240], (55)$$

satisfying the equation

$$\mathcal{L}[r^1]R(r,c;z) = 0.$$
 (56)

In section A.2 of the appendix, we explicitly write out the leading polynomial coefficient of (55), which will prove to be useful in our analysis of G(1, c) in section 5.1. Note, that naively attempting to solve differential equation (56) using Maple was unsuccessful. However, as we have already established an exact solution to G(1, c) by alternate means, no attempt was made to further refine the linear operator \mathcal{L} in (55) in the hope that a solution to our differential equation (56) could be computed.

Overall, it should not be concluded that finding the differential equation satisfied by $[r^1]R(r, c; z)$ was a fruitless exercise. Firstly, we highlight that this approach is a far less laborious and error-prone process than that of finding the series representation and then subsequently extracting the coefficients of R(r, c; z). Thus, at a minimum, one should be encouraged to employ this algorithm as a means of confirming the correctness of a given solution. More importantly, as our differential equation solely contains polynomial coefficients in z and c, one can easily determine both the singularities and coefficient asymptotics of G(1, c; z), which indeed we proceed to do in section 5.1.

4.5. Solution of the full model G(a, c)

In sections 4.3 and 4.4 we solved for the two simpler generating functions G(a, 1) and G(1, c) respectively. In particular we made use of the two refined equations that were established in section 4.2—(36) that contains the unknowns F(r, 0), F(1/r, 0) and F(0, 0); as well as (39) that contains F(0, s), F(0, 1/s) and F(0, 0). We are now in a position to connect these two refined equations which will ultimately allow us to express G(a, c) in terms of G(a, 1) and G(1, c).

Recall, when solving for G(1, c) in section 4.3 we utilized functional equation (41) which when setting c = 1, gave us (42)

$$(a-1)z^2G(a,1) = -\frac{1}{a}[s^1]H^*(s,a;z).$$
(57)

Now, solving (57) for $[s^1]H^*(s, a; z)$ which is *independent* of *c*, and substituting into (41) gives

$$(-1+a)(a(-1+c)^{2}+c(1+c(-1+z^{2})))G(a,c)+(-1+a)(-1+c)^{2}[s^{1}]F(0,s)$$

= $([s^{1}]M^{\star}(s,a,c)+a(a-1)c^{2}z^{2}G(a,1))\left(\frac{1}{ac}-ACG(a,c)\right),$ (58)

leaving us with a relation containing G(a, c), G(a, 1) and the boundary term $[s^1]F(0, s)$. Similarly, when solving for G(a, 1) in section 4.4 we employed functional equation (44) and when setting a = 1 gave us

$$z(c-1)G(1,c) = \frac{1}{c}([r^1]M(r,1,c;z) - [r^1]H(r,c;z)).$$
(59)



Figure 6. The three possible ways of appending a pair of steps to an allowed configuration so that both walks end at a height 1 above the surface $(\Omega(1, 0))$: (*a*) $\Omega(0, 0) \cdot \uparrow \uparrow (b) \Omega(2, 0) \cdot \downarrow \downarrow (c) \Omega(0, 1) \cdot \uparrow \downarrow$.

In this instance, we solve for $[r^1]H(r, c; z)$ in (59), which is independent of *a*, and substitute into (44). Finally, as M(r, a, c; z) is a polynomial in *r* and *z*, we find

$$z[a(a-2) - c(1 + a(a-3))]G(a, c) - (a-1)(acz^{2} + c - 1)[r^{1}]F(r, 0) + az(a-1)(c-1)[r^{2}]F(r, 0) = [c(-1+c+a(-2+a+c))z + zac(c-1)G(1, c)]\left(\frac{1}{ac} - ACG(a, c)\right), (60)$$

giving us a relation containing G(a, c), G(1, c), $[r^1]F(r, 0)$ and $[r^2]F(r, 0)$.

Our aim now is to combine equations (58) and (60) to express G(a, c) solely in terms of the simpler generating functions G(a, 1) and G(1, c). Thus, to do this, we need to eliminate the lingering boundary terms $[s^1]F(0, s)$, $[r^1]F(r, 0)$ and $[r^2]F(r, 0)$. Firstly, we will require the previously established relation (16) that relates G(a, c) and $[r^1]F(r, 0)$. Now, we can construct an additional relevant relation by considering the combinatorial decomposition for $\Omega(1, 0)$ —the class of allowed paired walks that *both* end at a height one above the surface. Specifically, we have

$$\Omega(1,0) = \{\Omega(0,0) \cdot \uparrow \uparrow\} \bigcup \{\Omega(2,0) \cdot \downarrow \downarrow\} \bigcup \{\Omega(0,1) \cdot \uparrow \downarrow\},$$
(61)

as highlighted schematically in figure 6. Translating the decomposition in terms of weights gives us

$$[r^{1}]F(r,0) = zc\left(G(a,c) + [r^{2}]F(r,0) + [s^{1}]F(0,s)\right),$$
(62)

equipping us with another relation that contains G(a, c) along with the boundary terms $[r^1]F(r, 0), [r^2]F(r, 0)$ and $[s^1]F(0, s)$.

Finally, combining the four equations (58), (60), (16) and (62) gives the desired expression

$$G(a, c; z) = \frac{1}{(a-1)(c-1)} \left[1 + \frac{p_0(a, c; z)}{G_b(a, c; z)} \right]$$
(63)

where

 $\begin{aligned} G_b(a,c;z) &\equiv p_1(a,c,z)G(a,1;z) + p_2(a,c,z)G(1,c;z) + p_3(a,c,z), \\ p_0(a,c;z) &= (a-1)(c-1)^2(a-c)(ac-c-a) \\ &- (c-1)(2a-a^2+3c-3ac+a^2c-2)a^2c^2z^2 - (a-1)a^2c^4z^4, \end{aligned}$

$$p_1(a, c; z) = (a - 1)a^2c^3(1 - a - c + ac)z^4,$$

$$p_2(a, c; z) = (a - 1)a(c - 1)^3c^2z^2,$$

$$p_3(a, c; z) = (a - 1)(c - 1)^2(a - c) - a^2(c - 1)c^2[1 + c(a - 2)]z^2 + (a - 1)a^2c^4z^4.$$
 (64)

We have not been able to find a more direct combinatorial proof for (63). It is certainly not immediately obvious how one can express a given configuration from our underlying class of allowed paired walks as a combination of configurations whose corresponding weights ignore either surface or shared surface contacts.

5. Phase structure and transitions

In section 4.5 we found an exact solution for our model, expressing in (64) the generating function $G(a, c; z) \equiv G(a, c)$ in terms of the two simpler generating function $G(a, 1; z) \equiv G(a, 1)$ and $G(1, c; z) \equiv G(1, c)$. In particular, the decomposition of G(a, c) highlights that the dominant singularity $z_s(a, c)$ of the full generating function is determined for any $a, c \ge 0$ by considering the dominant singularity of G(a, 1), the dominant singularity of G(1, c) and the roots of G_b (defined in (64)) that give rise to poles of the generating function. Recall that $z_s(a, c)$ dictates the reduced free energy $\kappa(a, c)$, and thus phases of the model. With that in mind, we begin in section 5.1 by determining the dominant singularities and phases of our two simpler generating functions G(a, 1) and G(1, c). In section 5.2, we will then use our results from section 5.1 to describe the dominant singularity structure of the full generating function G(a, c), allowing us to subsequently construct the phase diagram of our model. Finally, in section 5.4 we determine the order and behaviour of all exhibited phase transitions.

5.1. Transitions and asymptotics of G(a, 1) and G(1, c)

For the generating function G(a, 1; z), it was found in [43] that the dominant singularity $z_s(a, 1)$ is given as

$$z_{s}(a,1) = \begin{cases} z_{b} \equiv 1/4, & a \leq 2\\ z_{a}(a) \equiv \frac{\sqrt{a-1}}{2a}, & a > 2. \end{cases}$$
(65)

Introducing the order parameter $\mathcal{A}(a, c)$ the limiting average surface contacts as

$$\mathcal{A}(a,c) = \lim_{L \to \infty} \frac{\langle m_a \rangle}{L} = a \frac{\partial \kappa}{\partial a},\tag{66}$$

we say that the system is in a *desorbed* phase when

$$\mathcal{A} = 0, \tag{67}$$

while an *adsorbed* phase is observed when

$$\mathcal{A} > 0. \tag{68}$$

Thus, by use of (65), we have

$$\mathcal{A}(a,1) = \begin{cases} 0, & a \leq 2\\ \frac{a-2}{2(a-1)}, & a > 2, \end{cases}$$
(69)

highlighting that the singularities z_b and $z_a(a)$ correspond to a desorbed and adsorbed phase respectively, with the model exhibiting a second-order adsorption phase transition as is seen in figure 7(*a*).



Figure 7. (*a*) The limiting average number of visit sites $\mathcal{A}(a)$ for the adsorption-only model with generating function G(a, 1; z). (*b*) The limiting average number of shared site contacts $\mathcal{C}(c)$ for the friendly interaction-only model with generating function G(1, c; z).

For the generating function G(1, c), $z_s(1, c)$ can be determined from the linear homogeneous differential equation obtained in section 4.4. Specifically, the differential equation (55) only contains polynomial coefficients in z, which by standard results in the theory of linear differential equations [42, p 519] implies that the singularities of G(1, c; z)are given by the zeroes of the leading polynomial (which can be found in the appendix). Thus, we find the *dominant* singularity $z_s(1, c)$ to be

$$z_{s}(1,c) = \begin{cases} z_{b} \equiv 1/4, & c \leq 4/3\\ z_{c}(c) \equiv \frac{1-c+\sqrt{c^{2}-c}}{c}, & c > 4/3. \end{cases}$$
(70)

In a similar fashion to G(a, 1), we introduce an appropriate order parameter C(a, c) the limiting average shared site contacts as

$$C(a,c) = \lim_{L \to \infty} \frac{\langle m_c \rangle}{L} = c \frac{\partial \kappa}{\partial c},$$
(71)

and say that the system is in a *unzipped* phase when

$$\mathcal{C} = 0, \tag{72}$$

while a *zipped* phase is observed when

$$C > 0. \tag{73}$$

Considering the singularity structure (70), we thus find

$$\mathcal{C}(1,c) = \begin{cases} 0, & c \leq 4/3\\ \frac{c-2+\sqrt{c(c-1)}}{2(c-1)}, & c > 4/3, \end{cases}$$
(74)

and so for the model that only weights shared contacts we observe a second-order *zipping* transition as is seen in figure 7(b).

Finally, to determine the singularity structure $z_s(a, c)$ of the full generating function in section 5.3, we will require knowledge of the asymptotics of the two simpler generating functions which we now proceed to calculate. For the generating function G(a, 1; z), we know from [12] that the singular part of the generating function near its radius of convergence behaves as

$$G(a, 1; z) \sim \begin{cases} A_{-}(1 - 4z)^{4} \log(1 - 4z), & a < 2, \\ A_{0}(1 - 4z)^{2} \log(1 - 4z), & a = 2, \\ A_{+}(1 - z/z_{a}(a))^{1/2}, & a > 2. \end{cases}$$
(75)

We compute the asymptotics of G(1, c; z) from the differential equation satisfied by the generating function which was found in section 4.4.1. Specifically, substituting into (55) the general power series solution

$$G(1, c; z) = \sum_{n \ge 0} Z_n z^n, \tag{76}$$

we can establish a recurrence for the coefficients $Z_n \equiv Z_n(1, c)$ of G(1, c; z). With the assistance of the Maple package Gfun [46] we find

$$16c^{8}n(7c-6)(n-4)(n-2)(n+1)(n+3)Z_{n+10} +q_{2}(c,n)Z_{n+8}+q_{3}(c,n)Z_{n+6}+q_{4}(c,n)Z_{n+4}+q_{5}(c,n)Z_{n+2} +2(c-1)^{4}(2c^{2}-3+)(n+6)(n+8)(n+10)^{2}(n+12)Z_{n}=0, q_{i=2,...,5}(c,n) \in \mathbb{Z}[c,n],$$
(77)

giving us a tenth-order homogeneous linear recurrence equation with polynomial coefficients in *n*. Note that the explicit expression for the recurrence can be found in the appendix. The growth of Z_n can be directly determined from recurrence (77) by appealing to the method of Wimp and Zeilberger [47], showing the existence and specific form of a basis set of asymptotic solutions for any given linear recurrence which, in particular, contains rational coefficients (in *n*). In this instance, we substitute into (77) the ansatz

$$Z_n = \mu^n n^{\gamma - 1} (b_0 + b_1/n + b_2/n^2 + O(1/n^3)), \quad b_0 \neq 0$$
(78)

where $\mu, \gamma, b_{i \ge 0} \in \mathbb{R}$. By collecting dominant powers of *n* and equating their corresponding coefficients to zero we can solve for μ , γ as well as an arbitrary number of correction coefficients $b_{i \ge 1}$ (as factors of b_0). In doing so we find

$$Z_n \equiv Z_n(1, c)$$

$$= \begin{cases} B_-4^n n^{-5} \left(1 + \frac{5(16 - 24c + c^2)}{2n(4 - 3c)^2} + O(1/n^2) \right), & c < 4/3, \\ B_04^n n^{-3} (1 + 9/2n + O(1/n^2)), & c = 4/3, \\ B_+z_c(c)^{-n} n^{-3/2} & (c < 4/3, -24/2) + 20(c - 20) \end{pmatrix}$$

$$\left| \times \left(1 + \frac{3}{2n(4-3c)^2} \left(24 + c(11c - 30) - \frac{(98c^3 - 313c^2 + 296c - 80)}{4\sqrt{c(c-1)}} \right) + O(1/n^2) \right), \ c > 4/3,$$
(79)

which implies that the singular part of the generating function near the radius of convergence behaves as

$$G(1, c; z) \sim \begin{cases} B_{-}(1 - 4z)^{4} \log(1 - 4z), & c < 4/3, \\ B_{0}(1 - 4z)^{2} \log(1 - 4z), & c = 4/3, \\ B_{+}(1 - z/z_{c}(c))^{1/2}, & c > 4/3. \end{cases}$$
(80)

5.2. Singularities of the full model

We now want to describe the dominant singularity $z_s(a, c)$ for all a, c > 0. For $c \le 1$, the coefficients of G(a, c; z) grow at the same exponential rate as G(a, 1; z). This can be seen from the expression (63) noting the denominator is never zero in this region. Thus, in this region, the dominant singularities of these two generating functions, G(a, c; z) and G(a, 1; z), are equivalent and so from section 5.1 we have

$$z_{s}(a,c) = \begin{cases} z_{b} \equiv 1/4, & a \leq 2, c \leq 1\\ z_{a}(a) \equiv \frac{\sqrt{a-1}}{2a}, & a > 2, c \leq 1. \end{cases}$$
(81)

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By a similar argument, we can additionally conclude that for $a \leq 1$

$$z_s(a,c) = \begin{cases} z_b \equiv 1/4, & c \leq 4/3, a \leq 1\\ z_c(c) \equiv \frac{1-c+\sqrt{c^2-c}}{c}, & c > 4/3, a \leq 1. \end{cases}$$
(82)

We now show that

$$z_s(a,c) = z_b \equiv 1/4 \quad \text{for all} \quad 1 \leqslant a \leqslant 2, \quad 1 \leqslant c \leqslant 4/3.$$
(83)

Note, within this region the coefficients of G(a, c) cannot grow more slowly than those of either G(a, 1) or G(1, c), implying that $z_s(a, c) \leq \min(z_s(a, 1), z_s(1, c)) = z_b$. Thus, it suffices to show that $G(2, 4/3; z_b)$ is convergent as $G(a, c; z_b)$ would additionally be convergent for any $1 \leq a \leq 2, 1 \leq c \leq 4/3$. With that in mind, we begin by recalling the decomposition of G(a, c) in (63)

$$G(a, c; z) = \frac{1}{(a-1)(c-1)} \left[1 + \frac{p_0(a, c; z)}{G_b(a, c; z)} \right]$$
(84)

where

$$G_b(a, c; z) \equiv p_1(a, c, z)G(a, 1; z) + p_2(a, c, z)G(1, c; z) + p_3(a, c, z)$$
(85)

and $p_{i=0,1,2,3}(a, c; z)$ are polynomials in z. Moreover, we denote the smallest positive root of G_b to be $z_{ac}(a, c)$. We find that $p_0(2, 4/3; 1/4) = 0$, while using our exact solutions to our two generating function we find

$$G(2, 1; 1/4) = 8 - \frac{64}{3\pi}, \qquad G(1, 4/3; 1/4) = \frac{32}{\pi} - 9,$$
 (86)

which when subsequently substituting into the denominator (84) gives $G_b(2, 4/3; z_b) = 0$. Now, picking z < 1/4 and expanding G_b around $z_b \equiv 1/4$ (recall that $z_a(2) = z_c(4/3) = 1/4$) we find

$$G_{b}(2, 4/3; z) = \frac{1}{243} [-96(1 - 4z) + G(1, 4/3; 1/4)(1 - 4z) + 2A_{0}(1 - 4z)^{2} \log(1 - 4z) + 3G(2, 1; 1/4)(1 - 4z) + 3B_{0}(1 - 4z)^{2} \log(1 - 4z)] + O(1 - 4z)^{3} = \frac{16(9\pi - 32)}{243\pi} (1 - 4z) + \frac{1}{243} (2A_{0} + 3B_{0})(1 - 4z)^{2} \times \log(1 - 4z) + O(1 - 4z)^{3}$$
(87)

where we have used the asymptotic behaviour of the singular parts of G(a, 1) and G(1, c) near $z_a(2)$ and $z_c(4/3)$ respectively found in section 5.1 to make the substitutions

$$G(2, 1; z) \sim G(2, 1; 1/4) + A_0(1 - 4z)^2 \log(1 - 4z),$$

$$G(1, 4/3; z) \sim G(1, 4/3; 1/4) + B_0(1 - 4z)^2 \log(1 - 4z).$$
(88)

Moreover, from the explicit definition of $p_0(a, c; z)$ in (64) we have

$$p_0(a,c;z) = -\frac{256}{81}(1-4z)^2 + O(1-4z)^3.$$
(89)

Thus, overall our expansion of G(2, 4/3) becomes

$$G(2, 4/3; z) \sim 3 \left[1 - \frac{\frac{256}{81}(1 - 4z)^2}{\frac{16(9\pi - 32)}{243\pi}(1 - 4z) + \frac{1}{243}(2A_0 + 3B_0)(1 - 4z)^2\log(1 - 4z)} \right] \\ \sim 3 \left[1 - \frac{48\pi}{9\pi - 32}(1 - 4z) + \frac{3\pi^2(2A_0 + 3B_0)}{(9\pi - 32)^2}(1 - 4z)^2\log(1 - 4z) \right].$$
(90)

In particular, the singular part of G(2, 4/3; z) is then given as

$$G(2, 4/3; z)_{\text{singular}} \sim \frac{3\pi^2 (2A_0 + 3B_0)}{(9\pi - 32)^2} (1 - 4z)^2 \log(1 - 4z)$$
(91)



Figure 8. An example of an allowed configuration where the lower walk has a maximal number of surface contacts, while the upper walk is free to make arbitrary excursions above the lower walk.

which implies that $G(2, 4/3; z_b \equiv 1/4)$ is convergent, with

$$G(2, 4/3; 1/4) = 3. (92)$$

Now we argue that

$$z_s(a,c) = z_{ac}(a,c) \quad \text{for all} \quad a \ge 2, c \ge 4/3.$$
(93)

We begin, by noting that wherever the smallest root $z_{ac}(a, c)$ of G_b is defined, we must have

$$z_{ac}(a,c) \leqslant \min(z_a(a), z_c(c), z_b).$$
(94)

If we instead assume the converse, then either $G(a, 1; z_{ac})$ and/or $G(1, c; z_{ac})$ would be divergent, which from (85) further implies that G_b diverges and thus z_{ac} could not be a root for the expression.

It is straightforward to argue that for large *a* and *c* that $z_s(a, c) = z_{ac}(a, c)$ by considering a subset of configurations of the model. Specifically, let $G^{\Delta}(a, c; z)$ be the generating function for the sub-class of allowed configurations where the lower walk permanently zig-zags along the surface, while the upper walk is free to make arbitrary excursions as seen in figure 8. Thus, we essentially have a single adsorbing Dyck path model whose generating function is known (see [48]), where the upper walk 'adsorbs' (with weight *c*) onto the peaks of the lower walk. In this instance, the generating function $G^{\Delta}(a, c; z)$ is given as

$$G^{\Delta}(a,c;z) = 1 + \frac{2acz^2}{2 - c - 2ac^2 z^2 + c\sqrt{1 - 4az^2}},$$
(95)

which has smallest positive root $z_u(a, c)$

$$z_u(a,c) = \left(\frac{1-c+\sqrt{(c-1)(3+c)}}{2ac^2}\right)^{1/2}$$
(96)

for all a > 2, c > 4/3. Moreover, as G^{Δ} is counting a subset of configurations from our original model, we know $z_s(a, c) \leq z_u(a, c)$ for all a, c > 1. Now, one can show that $z_u(a, c)$ is monotonically decreasing in c and a at a faster rate to $z_c(c)$ and $z_a(a)$ respectively, implying that for large a^*, c^*

$$z_u(a,c) < \min(z_c(c), z_a(a)), \qquad c > c^*, a > a^*.$$
 (97)

But because the radius of convergence of the full generating function $z_s(a, c) \leq z_u(a, c)$, the only remaining possibility is that additionally

$$z_{ac}(a,c) \leq z_u(a,c) < \min(z_c(c), z_a(a)), \quad c > c^*, \quad a > a^*.$$
 (98)



Figure 9. An example of an allowed configuration where all sites are shared contacts, so that the paired walks are in effect a single adsorbing Dyck path.

By considering the denominator on the rhs of equation (63) it can be seen numerically that $z_s(a, c) = z_{ac}(a, c)$ extends to the region $a \ge 2$, $c \ge 4/3$. Once this is conjectured one can prove that for all a > 2 and small c the system has $z_s(a, c) = z_a(a)$, while for large c the system has $z_s(a, c) = z_{ac}(a, c)$. Moreover there is a single change of dominant singularity on increasing c at a point $c = \alpha(a)$ where $1 < \alpha(a) < 4/3$. Similarly, one can show that for all c > 4/3 and small a the system has $z_s(a, c) = z_c(c)$ and on increasing a the system has a single change of dominant singularity at $a = \gamma(c)$ to $z_s(a, c) = z_{ac}(a, c)$ for large a.

We can now fully describe the dominant singularity $z_s(a, c)$ of the generating function G(a, c; z) as

$$z_{s}(a,c) = \begin{cases} z_{b} \equiv 1/4, & a \leq 2, c \leq 4/3, \\ z_{a}(a) \equiv \frac{\sqrt{a-1}}{2a}, & a > 2, c \leq \alpha(a) \\ z_{c}(c) \equiv \frac{1-c+\sqrt{c^{2}-c}}{c}, & a \leq \gamma(c), c > 4/3 \\ z_{ac}(a,c), & a > \gamma(c), c > \alpha(a). \end{cases}$$
(99)

Now, while we cannot locate the boundaries $\alpha(a)$ and $\gamma(c)$ explicitly, we can employ lowtemperature arguments to describe their asymptotic behaviour. Specifically, considering first the z_c -to- z_{ac} boundary $\gamma(c)$, as $c \to \infty$, G(a, c; z) is dominated by those configurations where both the upper and lower walk *always* share a common site for each pairwise step as seen in figure 9. Thus, the two-walker model simplifies into a single adsorbing Dyck path model whose generating function is known (see [49]) and we have

$$G(a, c; z) \sim \frac{2}{2 - a(1 - \sqrt{1 - 4c^2 z^2})}, \quad c \to \infty.$$
 (100)

Equating the two singularities of the limiting generating function implies that

$$\gamma(c) \sim 2, \quad c \to \infty.$$
 (101)

By a similar low-temperature approximation argument, as $a \to \infty$, G(a, c; z) is now dominated by configurations where the lower walk permanently zig-zags along the surface, while the upper walk is free to make arbitrary excursions, whose corresponding generating function $G^{\Delta}(a, c; z)$ is at (95). Thus, in this instance, the limiting generating function becomes

$$G(a, c; z) \sim G^{\Delta}(a, c; z) = 1 + \frac{2acz^2}{2 - c - 2ac^2z^2 + c\sqrt{1 - 4az^2}}, \quad a \to \infty$$
(102)

and equating the two found singularities, we find

$$\alpha(a) \sim \sqrt{5} - 1 \approx 1.2306, \quad a \to \infty , \tag{103}$$

and we observe that

$$\sqrt{5} - 1 < \alpha(a) < 4/3 . \tag{104}$$

In section 5.5, more refined asymptotic expansions for the boundaries $\alpha(a)$ and $\gamma(c)$ will be established.

5.3. Phases and phase diagram of full model

With the dominant singularity structure of G(a, c) established in section 5.2, we can now introduce the phases of our model using the same order parameters \mathcal{A} and \mathcal{C} that were introduced in section 5.1. Specifically, we say that the system is in a *free* (desorbed and unzipped) phase when

$$\mathcal{A} = \mathcal{C} = 0, \tag{105}$$

while an *adsorbed* (adsorbed and unzipped/a-rich) phase is observed when

$$\mathcal{A} > 0, \quad \mathcal{C} = 0, \tag{106}$$

a zipped (desorbed and zipped/c-rich) phase is observed when

$$\mathcal{A} = 0, \quad \mathcal{C} > 0, \tag{107}$$

and finally an *adsorbed-zipped* (ac-rich) phase occurs when

$$\mathcal{A} > 0, \quad \mathcal{C} > 0. \tag{108}$$

Now, the dominant singularity $z_s(a, c)$ at (99) as well as our analysis of the two simpler generating functions G(a, 1) and G(1, c) in section 5.2 allow us to conclude that the singularities z_b , $z_a(a)$ and $z_c(c)$ correspond to the *free*, *adsorbed* and *zipped* phases respectively. Moreover, in section 5.4, we will additionally show, rather unsurprisingly, that $z_{ac}(a, c)$ corresponds to the *adsorbed-zipped* phase of our system.

Finally, we plot the full phase diagram in figure 10, estimating the boundaries *adsorbed* to *adsorbed-zipped* $\alpha(a)$ and *zipped* to *adsorbed-zipped* $\gamma(c)$ where $z_{ac}(a, c)$ coincides with $z_a(a)$ and $z_c(c)$ respectively. Specifically, to estimate $\gamma(c)$, we begin by picking an a > 0, c > 4/3 and use the exact solutions of our generating functions to evaluate truncated estimates of G(a, 1) and G(1, c) when $z = z_c(c)$. Next, we employ a technique featured in [12] of accelerating the convergence of our estimate for $G(1, c; z_c(c))$ whose terms $c_n z_c(c)^n$ grow as $n^{-3/2}$ (see section 5.1). Now, as

$$G(1, c; z_c(c)) = G_N(1, c; z_c(c)) + G_{N+1,\infty}(1, c; z_c(c))$$
(109)

where

$$G_N(1,c;z) = \sum_{n=0}^{N} c_n z^n, \quad G_{N+1,\infty}(1,c;z) = \sum_{n=N}^{\infty} c_n z^n,$$
(110)

by the Euler–Maclaurin asymptotic expansion of a sum [42] we thus have

$$G_{N,\infty}(1,c;z_c(c)) \sim \sum_{n=N+1}^{\infty} Bn^{-3/2} \sim B \int_{N+1}^{\infty} n^{-3/2} dn = B (N+1)^{-1/2}, \quad N \to \infty$$
(111)

and so by considering the system of equations

$$G(1, c; z_c(c)) = G_N(1, c; z_c(c)) + B(N+1)^{-1/2}$$

$$G(1, c; z_c(c)) = G_{N-1}(1, c; z_c(c)) + BN^{-1/2},$$
(112)



Figure 10. The phase diagram of our model. All transitions are second-order while the critical point where all boundaries meet (filled circle) occurs when a = 2 and c = 4/3. Additionally, the vertical and horizontal dashed lines show the asymptotic estimates of the boundaries $\alpha(a) \sim \sqrt{5} - 1$ and $\gamma(c) \sim 2$ as $a \to \infty$ and $c \to \infty$ respectively.

Table 1. The growth rates of the coefficients $Z_n(a, c)$ modulo the amplitudes of the full generating function G(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	$z_{ac}(a,c)^{-n}n^{-n}$

we can solve for the non-zero constant *B*, and thus subsequently $G(1, c; z_c(c))$. Equipped with the estimates, we can then finally check whether $G_b(a, c; z_c(c)) = 0$ to determine whether $z_c(c) = z_{ac}(a, c)$ for our chosen *a* and c > 4/3. We follow the same process to estimate the adsorbed to adsorbed-zipped $\alpha(a)$ boundary, with the exception that now $z = z_a(a)$. As seen in figure 10, we find that the asymptotic behaviour of both estimated boundaries as either $a \to \infty$ or $c \to \infty$ agrees with our low-temperature approximations from section 5.2. Overall, in table 1 we summarize the growth rate of the coefficients $Z_n \equiv Z_n(a, c)$ of the full generating function G(a, c) along the entire phase space. Note, that along the boundaries $\alpha(a)$ and $\gamma(c)$ the sub-exponential behaviour of our growth rates are estimates that are deduced from the nature of the corresponding dominant singularities in the surrounding adsorbed-zipped (simple pole) and adsorbed/zipped regions (convergent square-root singularity). In particular, this restricts the possible behaviour of Z_n that may be observed on the boundaries. Moreover, by generating the sequence $\{Z_{n+1}/Z_n\}$ for large *n* for fixed points *a*,*c* along $\alpha(a)$ and then $\gamma(c)$, fitting the coefficients into a equivalent ansatz form as in (78) and solving for the unknown exponents, we can conclude that along both boundaries, the dominant singularity behaves as a divergent square-root singularity.

5.4. Transitions of the full model

In section 5.3 we associated phases of our system to the different singularities of the generating function G(a, c) dependent on our choice of a, c > 0. In particular, we found that lying in a *free* phase implies $z_s(a, c) = z_b$, an *adsorbed* phase implies $z_s(a, c) = z_a(a)$, while a *zipped* phase implies $z_s(a, c) = z_c(c)$. Thus, moving from a free to an adsorbed (zipped) phase we observe the same critical behaviour in our full model as with the c = 1 (a = 1) subcases, which from our analysis in section 5.1, implies the system similarly exhibits a second-order adsorption (zipping) phase transition.

What remains is to describe the critical behaviour of our model as we move across the adsorbed to adsorbed-zipped $\alpha(a)$ and zipped to adsorbed-zipped $\gamma(c)$ boundaries. Considering first the former case, picking a > 2, we know from section 5.3 that z_{ac} is given implicitly in (64) as the smallest positive root of $G_b(a, c, z)$, where

$$G_b(a, c; z) = p_1(a, c, z)G(a, 1; z) + p_2(a, c, z)G(1, c; z) + p_3(a, c, z),$$
(113)

with each of p_1 , p_2 and p_3 polynomials in z. Thus, if we consider the expression

$$G_b(a, \alpha(a); z_a) - G_b(a, c; z_{ac}) = 0,$$
(114)

and expand z_a around z_{ac} we have

$$G_b(a, \alpha(a); z_{ac}) + G'_b(a, \alpha(a); z_{ac})(z_a - z_{ac}) - G_b(a, c; z_{ac}) + O(z_c - z_{ac})^2 = 0.$$
(115)

From (113), this expansion is implicitly an expansion of both $G(a, 1; z_a)$ and $G(1, \alpha(a); z_a)$. In the former case, we know from section 5.1 that for a > 2 and $z_{ac} \approx z_a$

$$G(a, 1; z_{ac}) \sim G(a, 1; z_a) + A_+(a)(z_a - z_{ac})^{1/2}.$$
(116)

Now, in section 5.3, a low-temperature approximation argument showed that $\alpha(a) \rightarrow \sqrt{5}-1 \approx 1.2306 < 4/3$. Moreover, as we expect the order of the transition to remain unchanged along the boundary for all a > 2, we are justified in assuming $\alpha(a) < 4/3$ within this region. Thus, we can conclude that the radius of convergence of $G(1, \alpha(a))$ is greater than that of G(a, 1). Moreover, as the polynomials p_1 and p_2 in (113) contain constant terms independent of z, our expansion (115) as $z_{ac} \rightarrow z_a$ becomes

$$F(a,c)[c-\alpha(a)] \approx (z_a - z_{ac})^{1/2}$$
 (117)

where F(a, c) is a non-zero algebraic function, which solving for z_{ac} gives us

$$z_{ac}(a,c) \approx z_a(a) + F(a,c)^2 [c - \alpha(a)]^2,$$
 (118)

which implies we have a second-order *adsorbed* to *adsorbed-zipped* phase transition, as there is a finite-jump discontinuity in the second-derivative (with respect to *c*) in the free energy $\kappa(a, c) = \log z_{ac}$.

We now move on to the transition from across the zipped to adsorbed-zipped boundary $\gamma(c)$ which can be analysed by a similar process, only now the leading behaviour of $G_b(a_c, c; z_c)$ near z_{ac} is dictated instead by $G(1, c; z_{ac})$ as

$$G(1, c; z_{ac}) \sim G(1, c; z_c) + C_+(c)(z_c - z_{ac})^{1/2},$$
(119)

for c > 4/3 and $z_c \approx z_{ac}$. The remainder of the argument follows exactly from the adsorbed to adsorbed-zipped transition case, and so we conclude that as we move from a zipped to

adsorbed-zipped phase, we again observe a *second-order* phase transition with a finite-jump discontinuity in the second-derivative of the free energy.

Thus, overall, all phase transitions are second-order and moreover as alluded to in section 5.3, the singularity $z_{ac}(a, c)$ corresponds to our system lying in an *adsorbed-zipped* phase where both $\mathcal{A}, \mathcal{C} > 0$.

5.5. Asymptotics of the boundaries α (a) and γ (c)

In section 5.2, by means of a low-temperature approximation argument, we found that the zipped to adsorbed-zipped critical boundary $\gamma(c)$ behaves as

$$\gamma(c) \sim 2, \quad c \to \infty,$$
 (120)

while the adsorbed to adsorbed-zipped boundary $\alpha(a)$ behaves as

$$\alpha(a) \sim \sqrt{5} - 1 \approx 1.2306, \quad a \to \infty.$$
(121)

However, by employing a similar approach seen in [12], we can obtain more accurate asymptotics of both these boundaries. Beginning with $\gamma(c)$ where the singularities $z_c(c)$ and $z_{ac}(a, c)$ coincide, we know from (64) that

$$G_b(a, c; z_c) \equiv p_1(a, c, z_c) G(a, 1; z_c) + p_2(a, c, z_c) G(1, c; z_c) + p_3(a, c, z_c) = 0, \quad (122)$$

with each of p_1 , p_2 and p_3 polynomials in *z* also defined in (64). Now, note that the coefficients $Z_n(a, 1)$ are independent of *c* and moreover that

$$z_c(c) \sim \frac{1}{2c}, \quad c \to \infty.$$
 (123)

Thus, the dominant asymptotic behaviour of $G(a, 1; z_c)$ with respect to c is captured by the initial terms of our generating function

$$G(a, 1; z) = 1 + az^{2} + a(2a+1)z^{4} + a(5a^{2}+6a+3)z^{6} + O(z^{6}),$$
(124)

by setting $z = z_c$ and expanding to give

$$G(a, 1; z_c) \sim 1 + \frac{a}{4c^2} - \frac{a}{8c^3} + \frac{a(8a+1)}{64c^4} - \frac{a(16a+11)}{128c^5}.$$
 (125)

Unfortunately, we cannot compute the asymptotics of $G(1, c; z_c)$ in the same manner as our coefficients $Z_n(1, c)$ are no longer independent of c. Moreover, despite being equipped with a solution for G(1, c), the general form of the coefficients $Z_n(1, c)$ further makes it difficult to find an explicit expansion. This is in contrast to [12], where the simpler form of the coefficients $Z_n(a, 1)$ allowed them to proceed analytically to determine the asymptotic expansion of the corresponding critical boundary. Instead, we assume the ansatz for the asymptotic expansion of $G(1, c; z_c(c))$

$$G(1, c; z_c(c)) \sim y_0 + \frac{y_1}{c} + \frac{y_2}{c^2} + \dots + \frac{y_5}{c^5}, \quad y_i \in \mathbb{R}$$
(126)

and aim to conjecture a solution for each y_i . Specifically, we consider the truncated series of $G(1, c; vz_c(c))$, where the auxiliary variable v is introduced to guide our estimates of the coefficients y_i . Specifically, for $[c^0]G(1, c; vz_c(c))$ we find

$$[c^{0}]G(1,c;vz_{c}) = 1 + \frac{v^{2}}{4} + \frac{v^{4}}{8} + \frac{5v^{6}}{64} + \frac{7v^{8}}{128} + \frac{21v^{10}}{512} + \frac{33v^{12}}{1024} + O(v^{12}).$$
(127)

By inspection, our coefficients in (127) appear to follow the sequence

$$\left\{\frac{C_n}{4^n}\right\} = \left\{\frac{1}{4^n(n+1)} \binom{2n}{n}\right\},\tag{128}$$

$$[c^{0}]G(1,c;vz_{c}) = 1 + \sum_{n \ge 1} \frac{C_{n}}{4n} v^{2n} = \frac{2(1-\sqrt{1-v^{2}})}{v^{2}}.$$
(129)

Moreover, we can further test our computation for $[c^0]G(1, c; vz_c)$ by employing a technique of rationalizing the generating function seen in [50] and [6]. Specifically, if we perform the substitution

$$v \mapsto \frac{2q}{q^2 + 1} \tag{130}$$

then

$$\sqrt{1 - v^2} \mapsto \frac{1 - q^2}{1 + q^2}, \quad 0 \leqslant q \leqslant 1$$
(131)

and so the conjectured generating function $[c^0]G(1, c; vz_c)$ becomes

$$[c^{0}]G\left(1,c;\frac{2q}{q^{2}+1}z_{c}\right) = 1+q^{2}.$$
(132)

Thus, if our computation for $[c^0]G(1, c; (2q/q^2 + 1)z_c)$ is correct, our truncated series expansion should stabilize to $1 + q^2$ irrespective of how many correction terms (with respect to *v* before our substitution) we include. Indeed, this is precisely what we observe. Therefore, overall, setting the auxiliary variable v = 1 in (129), we conclude that

$$y_0 \equiv [c^0]G(1, c; z_c) = 2.$$
 (133)

Next, finding y_1 , we first look at the truncated series $[c^{-1}]G(1, c; vz_c(c))$ where

$$[c^{-1}]G(1,c;vz_c) = -\left(\frac{v^2}{8} + \frac{v^4}{16} + \frac{5v^6}{128} + \frac{7v^8}{256} + \frac{21v^{10}}{1024} + \frac{33v^{12}}{2048}\right) + O(v^{12}).$$
 (134)

In this instance, we cannot directly guess the general form of the coefficients by inspection. However, if we make substitution (130) we find

$$[c^{-1}]G\left(1,c;\frac{2q}{q^2+1}z_c\right) = -\frac{q^2}{2} + O(q^{12}),\tag{135}$$

which once again suggests that our coefficients follow a modified Catalan sequence. Thus, setting q = 1 (and thus v = 1) in (135), we can conclude that

$$y_1 \equiv [c^{-1}]G(1, c; z_c) = -\frac{1}{2}.$$
 (136)

As far as we have observed, we are able to repeat this process for subsequent coefficients $y_{i>1}$, giving us

$$G(1,c;z_c(c)) \sim 2 - \frac{1}{2c} - \frac{5}{8c^2} - \frac{7}{16c^3} - \frac{29}{128c^4} - \frac{5}{256c^5}, \quad c \to \infty, \ (137)$$

where our truncated expansion contains the first six dominant terms.

We are now in a position to improve upon the asymptotics of $\gamma(c)$. By substituting (125), (137) along with the ansatz

$$a = \gamma(c) \sim 2 + \frac{x_1}{c} + \frac{x_2}{c^2} + \ldots + \frac{x_5}{c^5}, \quad x_i \in \mathbb{R},$$
 (138)

into the asymptotic expansion of (122) $G_b(a, c; z_c) = 0$, our aim is to equate coefficients in *c* to zero and solve for each x_i . For instance, we have

$$[c^{-2}]G_b(a,c;z_c) = \frac{1}{4}(2x_1+1) = 0,$$
(139)



Figure 11. Numerical (solid line) against asymptotic (dashed line) estimates of the critical boundaries (*a*) γ (*c*) and (*b*) α (*a*) respectively. Note, that both the origin and axis scales differ between the two figures.

and thus $x_1 = -1/2$. By repeating this process and incrementally eliminating coefficients, overall we find

$$\gamma(c) \sim 2 - \frac{1}{2c} + \frac{3}{8c^2} - \frac{3}{16c^3} + \frac{51}{128c^4} - \frac{65}{256c^5}, \quad c \to \infty.$$
 (140)

Finding the asymptotic behaviour for the boundary $\alpha(a)$ follows the exact some procedure as for $\gamma(c)$. However, as seen in [12], in this instance one can use the series solution of G(a, 1; z) to explicitly calculate the coefficients of the asymptotic expansion $G(a, 1; z_a(a))$, giving us

$$G(a, 1; z_a) \sim 2 - \frac{2}{a} + \frac{1}{a^3} + \frac{5}{4a^4} + \frac{15}{16a^5}, \quad a \to \infty.$$
 (141)

Thus, using expansions of both $G(a, 1; z_a)$ and $G(1, c; z_a)$, we find

$$\alpha(a) \sim \sqrt{5} - 1 + \left(5 - \frac{11}{\sqrt{5}}\right) \frac{1}{a} + \left(-39 + \frac{437}{5\sqrt{5}}\right) \frac{1}{a^2} + \left(\frac{673}{2} - \frac{37611}{50\sqrt{5}}\right) \frac{1}{a^3} + \left(-\frac{24\,861}{8} + \frac{1389\,823}{200\sqrt{5}}\right) \frac{1}{a^4} + \left(\frac{961\,077}{32} - \frac{1343\,139\,703}{20\,000\sqrt{5}}\right) \frac{1}{a^5}, \quad a \to \infty.$$
(142)

Note, that our improved asymptotics of both $\gamma(c)$ and $\alpha(a)$ correspond closely to our numerical estimates of the boundaries for large *c* and *a* as seen in figures 11(*a*) and (*b*) respectively.

5.6. Physical models

In section 2 we described our model combinatorially by associating weights *a* and *c* with the different types of interactions in our model. Let us now translate our findings into the more physical language of energies and temperature. We first define energies associated with visits to the surface $-\varepsilon_a$ and contacts shared between the polymers $-\varepsilon_c$ so that

$$a \equiv e^{\varepsilon_a k_B/T}$$
 and $c \equiv e^{\varepsilon_c k_B/T}$ (143)

where *T* is the temperature and k_b is Boltzmann's constant. If both energies are positive (that is, ε_a , $\varepsilon_c < 0$ and so a, c < 1) so that the interactions are repulsive the system will stay in the free phase for all temperatures. If either one of the energies is negative so that the interaction is attractive there will be a single phase transition on lowering the temperature; an adsorption transition if $\varepsilon_a > 0$ and alternatively a zipping transition if $\varepsilon_c > 0$.

Let us now consider a family of models where the ratio of the energies is held fixed: we define

$$r = \frac{\varepsilon_c}{\varepsilon_a} \tag{144}$$

in a similar approach featured in [12] and let us examine ε_a , $\varepsilon_c > 0$ so that both interactions are attractive and $0 < r < \infty$. At high temperatures the system is in the free phase. At very low temperatures where both *a* and *c* are large the system is in the adsorbed-zipped phase. The intermediate behaviour of the system depends on the size of *r*. There is a special value of *r* we call r_{\star} defined via

$$r_{\star} \equiv \frac{\log 2}{\log 4/3} \approx 2.4092. \tag{145}$$

For $0 < r < r_{\star}$ there are two second-order phase transitions on lowering the temperature; firstly a zipping transition from the free to the zipped phase and then another second-order adsorption transition at a lower temperature occurs to the adsorbed-zipped phase. Conversely, for $r > r_{\star}$ there are two second-order phase transitions on lowering the temperature; firstly an adsorption transition from the free to the adsorbed phase and again another second-order zipping transition at a lower temperature occurs to the adsorbed-zipped phase. When $r = r_{\star}$ precisely there is only one second-order pause transition on lowering the temperature directly from the high temperature free phase to the low temperature adsorbed-zipped phase.

6. Conclusion

We have solved exactly a model of two interacting friendly directed walks near an attractive surface, as a means of simultaneously capturing the effects of DNA denaturation and polymer adsorption. By means of the obstinate kernel method, we established two distinct systems of functional equations that correspond to the two auxiliary (catalytic) variables that were introduced within our model. Ultimately, this allowed us to express the full generating function G(a, c; z) in terms of the two simpler generating functions G(a, 1; z) and G(1, c; z) whose underlying models ignore either shared or surface contacts respectively. We are not aware of a similar decomposition in the literature. Thus, we consider our approach an extension of the traditional obstinate kernel method.

Our decomposition for G(a, c; z) highlighted that the dominant singularity structure of the generating function and thus phases of the system for the full model are strongly influenced by the two simpler variants. Specifically, we found *free, adsorbed* and *zipped* phases which correspond to the dominant singularity behaviours of G(a, 1; z) and G(1, c; z); while the full model further introduces an additional *adsorbed-zipped* phase that arises from the smallest positive pole in our expression for G(a, c; z) in terms of two simpler generating functions. We found that all four phases coincide when a = 2, c = 4/3, with G(2, 4/3; 1/4) = 3where the radius of convergence of the generating function when a = 2, c = 4/3 is z = 1/4. We have described the phase regions of each of the phases: we have established the exact region of the free phase, while the adsorbed to adsorbed-zipped boundary located at $\alpha(a)$ and zipped to adsorbed-zipped boundary located at $\gamma(c)$ were estimated and bounds on the location of these boundaries established. Low-temperature approximation arguments were employed to show that $\alpha(a) \sim \sqrt{5} - 1$ as $a \to \infty$, while $\gamma(c) \sim 2$ as $c \to \infty$. We showed that all observed phase transitions (including across the $\alpha(a)$ and $\gamma(c)$ boundaries) were second-order.

Acknowledgments

Financial support from the Australian Research Council via its Discovery Projects scheme and the Centre of Excellence for Mathematics and Statistics of Complex Systems is gratefully acknowledged by the authors. One of the authors, RT, acknowledges financial support from the University of Melbourne via its Melbourne Research Scholarships scheme. Additionally, RT and ALO thank the Department of Mathematics, University of British Columbia, for hospitality. AR thanks the Department of Mathematics and Statistics, The University of Melbourne, for the office space and coffee.

Appendix. G(1, c): differential equation and recurrence

A.1. G(1, c): linear recurrence

The following is the explicit linear homogeneous recurrence (77) satisfied by the *even* coefficients $Z_n \equiv Z_n(1, c)$ of the generating function G(1, c; z). Note that $Z_n = 0$ for *n* odd as we are counting paired walks that begin and end on the surface.

$$\begin{split} 16c^8(-6+7c)(-4+n)(-2+n)n(1+n)(3+n)Z_n \\ &-c^6(-2+n)n(-67776+144\,672c-91\,872c^2+14\,784c^3 \\ &-42\,560n+90\,032cn-57\,168c^2n+9688c^3n \\ &-8768n^2+19\,552cn^2-13\,980c^2n^2+3206c^3n^2 \\ &-704n^3+1872cn^3-1734c^2n^3+567c^3n^3)Z_{n+2} \\ &+(-1+c)c^4n(6+n)(-33\,344-45\,888c+180\,384c^2 \\ &-114\,880c^3+12\,992c^4+16\,640n-127\,216cn \\ &+212\,920c^2n-118\,628c^3n+16\,464c^4n+8768n^2-43\,392cn^2 \\ &+63\,900c^2n^2-34\,388c^3n^2+5194c^4n^2+1024n^3 \\ &-4304cn^3+5852c^2n^3-3049c^3n^3+483c^4n^3)Z_{n+4} \\ &-(-1+c)^2c^2(6+n)(8+n)(43\,200-136\,800c+79\,200c^2 \\ &+64\,800c^3-50\,400c^4+19\,520n-62\,320cn \\ &+27\,288c^2n+50\,464c^3n-35\,668c^4n+1176c^5n+576n^2 \\ &-4512cn^2+156c^2n^2+10\,542c^3n^2-6970c^4n^2+364c^5n^2 \\ &-320n^3+496cn^3-480c^2n^3+701c^3n^3-414c^4n^3+28c^5n^3)Z_{n+6} \\ &-(-1+c)^3(6+n)(8+n)(10+n) \\ \times\,(3360-3360c-480c^2-480c^3-720c^4+1440c^5+1152n \\ &-1152cn-732c^2n+552c^3n-194c^4n+304c^5n+96n^2 \\ &-96cn^2-84c^2n^2+75c^3n^2-15c^4n^2+16c^5n^2)Z_{n+8} \\ &+2(-1+c)^4(-3+2c^2)(6+n)(8+n)(10+n)^2(12+n)Z_{n+10}=0. \quad (A.1) \end{split}$$

A.2. G(1, c): leading coefficient of the differential equation

The following is the leading polynomial coefficient of the linear homogeneous differential equation (55) satisfied by the generating function G(1, c; z).

$$z^{5}(-1+4z)(1+4z)(1-c+2cz-2c^{2}z+c^{2}z^{2})^{2}(1-c-2cz+2c^{2}z+c^{2}z^{2})^{2} \times (-560+4480c-15820c^{2}+32340c^{3}-42140c^{4}+36260c^{5})$$

$$\begin{aligned} &-20\,580c^{6}+7420c^{7}-1540c^{8}+140c^{9}-4200z^{2}+40\,040cz^{2}\\ &-160\,114c^{2}z^{2}+345\,440c^{3}z^{2}-414\,018c^{4}z^{2}\\ &+207\,596c^{5}z^{2}+128\,868c^{6}z^{2}-296\,520c^{7}z^{2}+229\,292c^{8}z^{2}-96\,072c^{9}z^{2}\\ &+21\,934c^{10}z^{2}-2328c^{11}z^{2}+94c^{12}z^{2}-12c^{13}z^{2}+8400cz^{4}\\ &-61\,260c^{2}z^{4}+155\,932c^{3}z^{4}-81\,895c^{4}z^{4}-389\,563c^{5}z^{4}+913\,048c^{6}z^{4}\\ &-798\,289c^{7}z^{4}+106\,647c^{8}z^{4}+385\,054c^{9}z^{4}-355\,360c^{10}z^{4}+144\,267c^{11}z^{4}\\ &-31\,086c^{12}z^{4}+5151c^{13}z^{4}-1214c^{14}z^{4}+168c^{15}z^{4}-3528c^{2}z^{6}\\ &+25\,892c^{3}z^{6}-65\,610c^{4}z^{6}+113\,279c^{5}z^{6}-452\,377c^{6}z^{6}+1604\,730c^{7}z^{6}\\ &-3132\,720c^{8}z^{6}+3491\,487c^{9}z^{6}-2261\,166c^{10}z^{6}+815\,117c^{11}z^{6}\\ &-153\,244c^{12}z^{6}+25\,566c^{13}z^{6}-7909c^{14}z^{6}+105c^{15}z^{6}+378c^{16}z^{6}-952c^{4}z^{8}\\ &+23\,928c^{5}z^{8}-326\,754c^{6}z^{8}+1729\,550c^{7}z^{8}-4451\,154c^{8}z^{8}+6199\,103c^{9}z^{8}\\ &-4695\,975c^{10}z^{8}+1694\,292c^{11}z^{8}-128\,480c^{12}z^{8}-26\,317c^{13}z^{8}-15\,393c^{14}z^{8}\\ &-6636c^{15}z^{8}+4788c^{16}z^{8}-15\,056c^{6}z^{10}+390\,272c^{7}z^{10}-2033\,138c^{8}z^{10}\\ &+4222\,649c^{9}z^{10}-3643\,316c^{10}z^{10}+306\,799c^{11}z^{10}+1382\,539c^{12}z^{10}\\ &-613\,766c^{13}z^{10}+9191c^{14}z^{10}-36\,666c^{15}z^{10}+30\,492c^{16}z^{10}\\ &-177\,136c^{8}z^{12}+805\,704c^{9}z^{12}-922\,558c^{10}z^{12}-631\,258c^{11}z^{12}\\ &+1751\,964c^{12}z^{12}-764\,416c^{13}z^{12}-88\,058c^{14}z^{12}-68\,742c^{15}z^{12}\\ &+94\,500c^{16}z^{12}+11\,928c^{10}z^{14}-153\,124c^{11}z^{14}+393\,492c^{12}z^{14}\\ &-207\,968c^{13}z^{14}-142\,020c^{14}z^{14}+6132c^{15}z^{14}+91\,728c^{16}z^{14}\\ &+5544c^{12}z^{16}-8976c^{13}z^{16}-14\,916c^{14}z^{16}+14\,784c^{15}z^{16})^{2}. \end{aligned}$$

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