Adsorbing staircase polygons subject to a force

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Abstract
We study several models of staircase polygons on the $45^\circ$ rotated square lattice, which interact with an impenetrable surface while also being pushed towards or pulled away from the surface by a force. The surface interaction is governed by a fugacity $a$ and the force by a fugacity $y$. Staircase polygons are simplifications of more general self-avoiding polygons, a well-studied model of interacting ring polymers. For this simplified case we are able to exactly determine the limiting free energy in the full $a$-$y$ plane, and demonstrate that staircase polygons exhibit four different phases, including a ‘mixed’ adsorbed-ballistic phase.

Keywords: polymers, adsorption, lattice paths, polygons

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

1. Introduction
The study of lattice walks as models of polymers in solution has a rich history—see [22] for a thorough treatment. One particular scenario that has yielded many results is that of a polymer adsorbing onto an impenetrable surface. This can be elegantly modelled by a self-avoiding walk in a half-space of a lattice, with a temperature-dependent fugacity (Boltzmann weight) associated with points at which the walk touches the boundary of the half-space. A variety of exact [5, 13] and numerical [4, 11, 23, 16] results have been found, particularly regarding the location and nature of the adsorption phase transition.

A related scenario is that of a long polymer tethered to a surface, with a pulling force applied to part of polymer at some angle to the surface. Atomic force microscopy [14] has allowed for such experiments in the laboratory. Lattice models are again a useful tool for investigating such systems [2, 11, 24, 15]. Many of these and other studies have considered polymer models incorporating both interactions with the surface and a pulling force, and the phase diagrams that result from the interplay between the two.
Instead of linear polymers, in nature there also exist ring polymers, which have a natural circular structure. The relevant lattice objects are then self-avoiding polygons, rather than walks. It is again possible to investigate adsorption [19, 20, 26], pulling forces [1, 3, 25], and both [12].

With some exceptions (e.g. [2, 5]), most exact quantitative results regarding interacting self-avoiding walks and polygons are non-rigorous, and typically depend on assumptions about the scaling limit of the model. For this reason (and others), there has been considerable attention given to subclasses, which often allow for exact solutions for various thermodynamic quantities. Some of the simplest models which still display rich physical behaviour include directed paths (see [21] for a thorough review) and polygons [18].

1.1. Interacting self-avoiding walks and polygons

In the most general model, we let \( p_n(v, h) \) be the number of self-avoiding polygons of length \( n \) on \( \mathbb{Z}^d \), counted up to translation, with

- all vertices having nonnegative \( x_v \)-coordinate,
- \( v > 0 \) vertices lying in the hyperplane \( x_v = 0 \), and
- \( h \) being the maximal \( x_v \)-coordinate among all vertices.

(Note that \( p_n(v, h) \) > 0 only if \( n \) is even.) Then define the partition function

\[
P_n(a, y) = \sum_{v, h} p_n(v, h) a^v y^h.
\]

Here we interpret \( a = \exp(-\alpha/kT) \) and \( y = \exp(f/kT) \), where \( \alpha \) is the energy associated with a single surface contact, \( f \) is the pulling force, \( T \) is absolute temperature, and \( k \) is Boltzmann’s constant. When \( \alpha < 0 \), adsorption may occur for sufficiently small \( T \). Likewise, for sufficiently large \( f \), the polygons may become ballistic, and reach vertices at distance \( O(n) \) above the surface.

For all \( d \geq 2 \) and \( a, y \geq 0 \), it is known [25, 26] that the limiting free energies

\[
\kappa_0(a) := \lim_{n \to \infty} \frac{1}{2n} \log P_{2n}(a, 1) \quad \text{and} \quad \lambda_0(y) := \lim_{n \to \infty} \frac{1}{2n} \log P_{2n}(1, y)
\]

exist. They are convex functions of \( \log a \) (resp. \( \log y \)), and are thus continuous and almost-everywhere differentiable. It is also known [26] that \( \kappa_0(a) \) has a point of non-analyticity at some \( d^*_0 > 1 \), separating the desorbed (free) phase \( a < d^*_0 \) (where \( \kappa_0(a) = \kappa \), the connective constant of the lattice) and the adsorbed phase \( a > d^*_0 \) (where \( \kappa_0(a) > \kappa \)). Likewise, \( \lambda_0(y) \) has a point of non-analyticity at \( y^*_0 = 1 [2, 12, 25] \), separating the free phase (where \( \lambda_0(y) = \kappa \)) and the ballistic phase (where \( \lambda_0(y) > \kappa \)).

In \( d \geq 3 \) dimensions, it has also been shown [12] that the two-parameter free energy

\[
\psi_0(a, y) := \lim_{n \to \infty} \frac{1}{2n} \log P_n(a, y)
\]

exists for all \( a, y > 0 \). Moreover

\[
\psi_0(a, y) = \max \{ \kappa_0(a), \lambda_0(y) \}.
\]

The relation (2) completely (qualitatively) characterises the phase diagram for \( d \geq 3 \), showing that there are three phases: free (when \( a < d^*_0 \) and \( y < 1 \)), adsorbed (when \( a > d^*_0 \) and \( \kappa_0(a) > \lambda_0(y) \)) and ballistic (when \( y > 1 \) and \( \lambda_0(y) > \kappa_0(a) \)). The model has two natural order parameters: the limiting density of surface visits...
\[ V := \lim_{n \to \infty} \frac{1}{n} \langle v \rangle = a \frac{\partial}{\partial a} \psi_0(a, y), \]

where the expectation is taken with respect to the Boltzmann distribution on polygons of length \( n \); and the limiting ‘density’ of the height

\[ H := \lim_{n \to \infty} \frac{1}{n} \langle h \rangle = y \frac{\partial}{\partial y} \psi_0(a, y). \]

Then in the free phase \( V = H = 0 \), while in the adsorbed phase \( V > 0 \) and in the ballistic phase \( H > 0 \).

In \( d = 2 \) dimensions less is known. In particular it has not been proved that the limit (1) exists; instead, only bounds on the lim inf and lim sup have been established [12]. It is also not known whether there are only three phases as in \( d \geq 3 \), or whether there are one or more additional, ‘mixed’ phases, where the free energy depends on both \( a \) and \( y \) and in which the polygons are both adsorbed and ballistic.

1.2. Outline of the paper

In this paper we investigate a directed version of the adsorbing and pulled/pushed polygons discussed above. In particular, our goal is to find and study a simple two-dimensional model which displays a mixed adsorbed and ballistic phase. To this end we employ staircase polygons, for which a number of existing enumerative results are already known.

In section 2 we define interacting staircase polygons and two main subclasses which will be of use in our investigation, and also state our main theorems. In section 3 we make use of well-known results which relate staircase polygons to pairs of nonintersecting paths, in order to exactly enumerate one of our subclasses. The asymptotic behaviour of these enumerations is covered in section 4, leading to a complete phase diagram. In sections 5 and 6 we find lower and upper bounds respectively for all staircase polygons, with one proof for the lower bound being deferred to the appendix. In section 7 we offer some closing remarks.

2. The model: staircase polygons

2.1. Binomial paths

Let \( L \) be a square lattice which has been rotated \( 45^\circ \) from the usual orientation and scaled by \( \sqrt{2} \), so that all vertices have integer coordinates (in particular, all integer points \( (x, y) \) with \( x \equiv y \pmod{2} \) are vertices). A binomial path \( \omega \) on \( L \) is a sequence of vertices \( (\omega_0, \omega_1, \ldots, \omega_n) \) such that \( \omega_i - \omega_{i-1} \in \{(1, 1), (1, -1)\} \) for all \( i = 1, \ldots, n \). That is, \( \omega \) is a path comprising \((1, 1)\) (‘up’ or ‘north-east’) steps and \((1, -1)\) (‘down’ or ‘south-east’) steps. Probably the most famous type of binomial paths are Dyck paths, which start and end with vertices on the line \( y = 0 \) and remain in the half-space \( y \geq 0 \) at all times.

We will first briefly review some known results about the physics of adsorbing and pulled binomial paths. Let \( L^+ \subset L \) be the subspace defined by \( y \geq 0 \), and define \( c_n(v, h) \) to be the number of \( n \)-step binomial paths \( \omega \) in \( L^+ \) which begin at vertex \((0, 0)\) and finish at vertex \((n, h)\), and which contain \( v \) vertices in the line \( y = 0 \). (Note then that \( c_n(v, 0) \) counts interacting Dyck paths.) Define the partition function

\[ C_n(a, y) = \sum_{h,v} c_n(v, h) a^v y^h. \]
and the generating function
\[ C(t; a, y) = \sum_{n,h,v} c_n(v,h)t^n a^v y^h = \sum_n c_n(a, y)t^n. \]

Then [22, equation (5.47)]
\[ C(t; a, y) = \frac{2a \left( 1 - 2t^2 + \sqrt{1 - 4t^2} \right)}{\left( 1 - 2ta + \sqrt{1 - 4t^2} \right) \left( 1 - 2ty + \sqrt{1 - 4t^2} \right)}. \]  
(3)

(Note that we are associating a weight \( a \) with the first vertex of a path, while this is not the case in [22].)

It is a central principle of enumerative combinatorics that the dominant singularity (i.e. the one closest to the origin) of a generating function determines the asymptotic behaviour of the coefficients (see e.g. [9]). Viewing \( C(t; a, y) \) as a Taylor series in \( t \) with coefficients \( C_n(a, y) \in \mathbb{Z}[a, y] \), we can then examine the generating function for various \( a, y \geq 0 \) in order to find the dominant singularity. Denoting this quantity by \( t_c(a, y) \), we have
\[ t_c(a, y) = \min \left\{ \frac{1}{2}, \frac{y}{y^2 + 1}, \frac{\sqrt{a - 1}}{a} \right\} \]
\[ = \begin{cases} \frac{1}{2} & a \leq 2 \text{ and } y \leq 1 \\ \frac{y}{y^2 + 1} & y > 1 \text{ and } a < y^2 + 1 \\ \frac{\sqrt{a - 1}}{a} & a > 2 \text{ and } y < \sqrt{a - 1}. \end{cases} \]  
(4)

It follows that
\[ \psi^P(a, y) := \lim_{n \to \infty} \frac{1}{n} \log C_n(a, y) = \max \left\{ \lambda^P(y), \kappa^P(a) \right\} \]  
(5)

where
\[ \lambda^P(y) = \begin{cases} \log 2 & y \leq 1 \\ \log(y^2 + 1) - \log y & y > 1 \end{cases} \]
and
\[ \kappa^P(a) = \begin{cases} \log 2 & a \leq 2 \\ \log a - \frac{1}{2} \log(a - 1) & a > 2. \end{cases} \]

2.2. Staircase polygons

A staircase polygon (also known as a parallelogram polygon) \( \pi \) is a pair \((\pi^+, \pi^-)\) of two binomial paths \( \pi^+ = (\pi^+_0, \ldots, \pi^+_n) \) and \( \pi^- = (\pi^-_0, \ldots, \pi^-_n) \) with
\[ \pi^+_0 = \pi^-_0, \quad \pi^+_n = \pi^-_n, \quad \text{and} \quad \pi^+_i > \pi^-_i \text{ for } i = 1, \ldots, n - 1. \]
That is, \( \pi \) consists of two binomial paths \( \pi^+ \) and \( \pi^- \) which start and end at the same points, but otherwise with \( \pi^+ \) strictly above \( \pi^- \). If the two paths each have \( n \) steps then we say that \( \pi \) has length \( 2n \).

Let \( P^S_{2n} \) be the set of staircase polygons of length \( 2n \) which
\[ \bullet \text{ lie entirely within } \mathbb{L}^+, \]
\[ \bullet \text{ contain at least one vertex in the line } y = 0, \text{ and} \]
\[ \bullet \text{ have their leftmost vertex in the line } x = 0. \]
The last condition is equivalent to saying that polygons in $P_{2n}^S$ are considered modulo translation in the $\pm x$ directions.) Let $p_{2n}^S = |P_{2n}^S|$. For a staircase polygon $\pi \in P_{2n}^S$, let $v(\pi)$ be the number of vertices of $\pi$ in the line $y = 0$. Such vertices will be called visits. Let $h(\pi)$ be the $y$-coordinate of $\pi_{\lfloor n/2 \rfloor}$. This will be called the height of $\pi$. See figure 1. For $a, y \in \mathbb{R}^+$ we then define the partition function

$$P_{2n}^S(a,y) := \sum_{\pi \in P_{2n}^S} a^{v(\pi)} y^{h(\pi)}.$$  

(6)

(Note the difference between the weight $y$ and the ordinate $y$ of a lattice point.)

We define the limiting free energy to be

$$\psi_{2n}^S(a, y) := \lim_{n \to \infty} \frac{1}{2n} \log P_{2n}^S(a, y).$$  

(7)

At this point it is not immediately obvious that this limit should even exist. In theorem 3 we will prove its existence and give its value for all $a$ and $y$. Before stating that theorem, however, we will introduce two subsets of staircase polygons, for which certain calculations will be easier.

2.3. Grafted staircase polygons

We will say a polygon $\pi \in P_{2n}^S$ is grafted if

- the leftmost vertex of $\pi$ has $y$-coordinate 1, and
  - if $n$ is even, the rightmost vertex of $\pi$ has $y$-coordinate 1, or
  - if $n$ is odd, the rightmost vertex of $\pi$ has $y$-coordinate 2.

See figure 2. If $n$ is even, note that by removing the two leftmost and two rightmost edges (whose locations and directions are completely fixed), a grafted polygon can be decomposed into two nonintersecting binomial paths: the lower path starting and ending on the $x$-axis (i.e., a Dyck path), and the upper path starting and ending on the line $y = 2$ (a Dyck path shifted up by 2 units). If $n$ is odd, then doing the same almost gives two Dyck paths—each path will end one unit higher than where it started.

Let $P_{2n}^G$ be the set of grafted polygons of length $2n$. Similarly to (6), we have the partition function

Figure 1. A half-space staircase polygon of length 32, with 3 visits and height 7.
\begin{align*}
\psi_G(a, y) &= \lim_{n \to \infty} \frac{1}{2n} \log P_G^{2n}(a, y). \quad (9)
\end{align*}

We will prove the following theorem.

**Theorem 1.** The free energy \( \psi_G(a, y) \) exists for all \( a, y \in \mathbb{R}^+ \). Moreover, it is given by

\begin{align*}
\psi_G(a, y) &= \frac{1}{2} \lambda^P \left( \sqrt{y} \right) + \frac{1}{2} \kappa^P (a) \quad (10)
\end{align*}

and free energy

\begin{align*}
\psi_G(a, y) &= \frac{1}{2} \log 2 + \frac{1}{2} \log a - \frac{1}{2} \log(a - 1) \quad a \leq 2 \text{ and } y \leq 1
\end{align*}

\begin{align*}
&= \frac{1}{2} \log 2 + \frac{1}{2} \log(y + 1) - \frac{1}{2} \log y \quad a > 2 \text{ and } y \leq 1
\end{align*}

\begin{align*}
&= \frac{1}{2} \log a - \frac{1}{2} \log(a - 1) + \frac{1}{2} \log(y + 1) - \frac{1}{2} \log y \quad a \leq 2 \text{ and } y > 1
\end{align*}

\begin{align*}
&= \frac{1}{2} \log a - \frac{1}{2} \log(a - 1) + \frac{1}{2} \log(y + 1) - \frac{1}{2} \log y \quad a > 2 \text{ and } y > 1. \quad (11)
\end{align*}

We will denote the four regions in the \((a, y)\)-quarter-plane as \( G_I, G_{II}, G_{III} \) and \( G_{IV} \) respectively. These correspond to free (\( V = H = 0 \)), adsorbed (\( V > 0 \)), ballistic (\( H > 0 \)) and 'mixed' (\( V > 0, H > 0 \)) phases respectively.

**2.4. Centred staircase polygons**

We will say that a polygon \( \pi \in \mathcal{P}_G^{2n} \) is centred if the vertex \( \pi_{n/2} \) has \( y \)-coordinate 0. See figure 3. Let \( \mathcal{P}_C^{2n} \) be the set of centred polygons of length \( 2n \). We again have a partition function

\begin{align*}
P_C^{2n}(a, y) := \sum_{\pi \in \mathcal{P}_C^{2n}} a^{v(\pi)} y^{h(\pi)} \quad (12)
\end{align*}

and free energy

\begin{align*}
\psi_C(a, y) &= \lim_{n \to \infty} \frac{1}{2n} \log P_C^{2n}(a, y). \quad (13)
\end{align*}
Theorem 2. The free energy $\psi^C(a, y)$ exists for all $a, y \in \mathbb{R}^+$. Moreover, it is given by

$$\psi^C(a, y) = \frac{1}{2} \lambda^P(\sqrt{y}) + \frac{1}{2} \max\left\{ \lambda^P(\sqrt{y}), \kappa^P(a) \right\}$$

(14)

$$= \begin{cases} \log 2 & a \leq 2 \text{ and } y \leq 1 \\ \frac{1}{2} \log 2 + \frac{1}{2} \log a - \frac{1}{4} \log(a - 1) & a > 2 \text{ and } y \leq 1 \\ \log(y + 1) - \frac{1}{2} \log y & y > 1 \text{ and } a \leq y + 1 \\ \frac{1}{2} \log a - \frac{1}{4} \log(a - 1) + \frac{1}{2} \log(y + 1) - \frac{1}{4} \log y & y > 1 \text{ and } a > y + 1. \end{cases}$$

(15)

We will denote these four regions in the $(a, y)$-quarter-plane as $C_I, C_{II}, C_{III}$ and $C_{IV}$ respectively. Note that $C_I = G_I$ and $C_{II} = G_{II}$.

The main theorem of this paper is the following, which essentially says that the restriction from staircase polygons to centred polygons is weak enough so as to have no effect on the free energy.

Theorem 3. The free energy $\psi^S(a, y)$ exists for all $a, y \in \mathbb{R}^+$. Moreover,

$$\psi^S(a, y) = \psi^C(a, y).$$

(16)

We note here that the problem of adsorbing staircase polygons has been studied in the past by Janse van Rensburg [18] (see also [22, section 5.6]). One result obtained there is that the free energy for a certain subclass of staircase polygons (those with leftmost vertex at ordinate $y = 1$; one might call them ‘semi-grafted’), the free energy $\kappa^{SG}(a)$ is given by

$$\kappa^{SG}(a) = \frac{1}{2} \log 2 + \frac{1}{2} \kappa^P(a)$$

(17)

$$= \begin{cases} \log 2 & a \leq 2 \\ \frac{1}{2} \log 2 + \frac{1}{2} \log a - \frac{1}{4} \log(a - 1) & a > 2. \end{cases}$$

(18)

Observe then that for $y \leq 1$,

$$\psi^G(a, y) = \psi^C(a, y) = \psi^S(a, y) = \kappa^{SG}(a).$$
In the next section we will employ some of the ideas used in [18, 22] in order to generalise
to the adsorbing and pulled case.

3. Pairs of paths

A key tool in computing the partition functions and free energies defined in the previous
section will be a formulation of staircase polygons—with given length, height and number of
visits—in terms of pairs of nonintersecting lattice paths. Such a technique is well known—see
for example [22, section 5.6]. Indeed, we will take as our starting point a result from [22].

Let $P$ be a configuration of two nonintersecting binomial paths of length $n$ in $\mathbb{L}^+$, with
the lower path starting at $(0, j_0 - l_0)$ and finishing at $(n, j_0 - l_0 + 2)$, and the upper path starting at
$(0, j_0 + l_0 + 2)$ and finishing at $(n, j_0 + l_0 + 2)$. Furthermore, suppose the lower path accumu-
lates a weight $a$ for every vertex in the boundary $y = 0$. See figure 4. Let $r_n(j_0, l_0; j, l)$ be the
total weight of all such configurations.

We denote by $\text{CT}_S[X]$ the constant term of the Laurent series $X$, with respect to the set of
variables $S$. Also let $x = 1/x$.

**Lemma 4 ([22, equation (5.168)]).** The partition function $r_n(j_0, l_0; j, l)$ is given by

$$r_n(j_0, l_0; j, l) = \text{CT}_S(\zeta_1, \zeta_2) \left[ \Lambda^n \zeta_1 \zeta_2 \left( \zeta_1 \zeta_2^{j_0 + l_0} + \zeta_1 \zeta_2^{j_0 + l_0 + 2} - \zeta_1 \zeta_2^{j_0 + l_0 + 2} \right) \right],$$

where

$$\Lambda = \zeta_1 + \zeta_2 + \zeta_3,$$

$$\mathcal{I}_1 = -\frac{\Lambda - a (\zeta_1 + \zeta_2)}{\Lambda - a (\zeta_1 + \zeta_2)} \quad \text{and} \quad \mathcal{I}_2 = -\frac{\Lambda - a (\zeta_1 + \zeta_2)}{\Lambda - a (\zeta_1 + \zeta_2)}.$$

This result is obtained by finding a recurrence relation satisfied by $r_n$. This is straightforward: one can construct pairs of paths of length $n$ by appending steps to pairs of paths of
length $n - 1$, taking care to make sure that the two paths do not intersect and that the bottom
path does not step below the surface, as well as accounting for the weight $a$ when the bottom
path touches the surface. This recurrence can then be solved with a general Bethe ansatz,
where Cauchy’s integral formula allows one to write a contour integral as the constant term of a Laurent series.

The most obvious way to obtain a staircase polygon from a pair of binomial paths is to take \( l_0 = l = 0 \), so that the two paths start and end as near to each other as possible. The addition of two edges on the left and two edges on the right then joins the paths up to form a polygon. This would correctly account for the \( a \) weight in the partition function; however, it gives us no information about the height of the resulting polygon.

We will thus use a different strategy; taking two pairs of paths of length \( n \), both with \( l_0 = 0 \) and with matching values of \( j \) and \( l \), then reflecting one of the pairs through the vertical axis, gluing the two pairs together, and finally adding two edges at the left and right to close up the whole thing into a polygon. The number of visits for the resulting polygon is the sum of the numbers of visits of the two pairs (unless \( j = l \), in which case one visit has been counted twice), while the height of the resulting polygon is \( j + l + 2 \).

We thus set \( l_0 = 0 \) in (19). Following [22], we perform the change of variables \( \zeta_1 = \eta_1 \eta_2 \) and \( \zeta_2 = \eta_1 \tau_2 \). Then \( \Lambda = (\eta_1 + \eta_2)(\tau_2 + \tau_3) \), and if we define

\[
\mathcal{H}(\eta) = -\eta^2 - (a - 1) \eta^2
\]

then \( \mathcal{S}_1 = \mathcal{H}(\eta_1) \) and \( \mathcal{S}_2 = \mathcal{H}(\eta_2) \). (Note that this corrects [22, equation (5.170)].) We will write \( \mathcal{H}_1 = \mathcal{H}(\eta_1) \) and \( \mathcal{H}_2 = \mathcal{H}(\eta_2) \) for short. Then

\[
r_n(j_0, 0; j, l) = \text{CT}_{\{\eta, \tau\}} \left[ \Lambda^n \eta_1^{j+1} \eta_2^{l-1} \left( \eta_1^{h_0} \tau_2^{h_1} \mathcal{H}_2 \tau_2^{h_2} - \eta_1^{l_0} \tau_2^{l_1} - \eta_1^{l_2} \tau_2^{l_3} - \mathcal{H}_1 \eta_1^{l_2} \tau_2^{l_3} \right) \right].
\]

(20)

3.1. Grafted polygons via pairs of paths

Let \( s_a(k, m) = r_a \left( 0, 0; \frac{k+m}{2}, \frac{k-m}{2} \right) \), with the specialisation \( s_a(k, m) = s_a(k, m) \big|_{a=1} \). This can be extracted directly from (20); it is [22, equation (5.172)]

\[
s_a(k, m) = \text{CT}_{\{\eta, \tau\}} \left[ (\eta_1 + \eta_2)^n (\tau_2 + \tau_3)^n \eta_1^2 \tau_2^2 (1 - \eta_1^2)^n (1 - \eta_2^2)^n \right]
\]

\[
= \frac{(k+3)(m+1)(k-m+2)(k+m+4)}{4(n+1)(n+2)(n+3)^2} \left( \frac{n+3}{\frac{1}{2}(n+6)} \right) \left( \frac{n+3}{\frac{1}{2}(n+m+4)} \right).
\]

(21)

The general \( a \) case is then obtained by expanding \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) in (20) as power series; we have [22, equation (5.173)]

\[
s_a(k, m) = a \sum_{w=0}^{n} \sum_{p=0}^{w} (a-1)^w s_a^2(k+2p, m+2w-2p).
\]

(22)

Note that \( s_a(k, m) \) should only be nonzero when \( 0 \leq m \leq k \leq n \) and \( k \equiv m \equiv n \) (mod 2); in other words, the binomial coefficients should be taken to be zero if either argument is not a natural number.

The arguments outlined above give the following lemma.

**Lemma 5.** For even \( n \), the partition function \( P_{2n}^a(a, y) \) is given by

\[
P_{2n}^a(a, y) = \frac{1}{a} \sum_{k=0}^{\frac{n}{2}} \left( s_{a+1}(k, 0) \right)^2 y^{k+2} + \sum_{k=0}^{\frac{n}{2}} \sum_{m=1}^{\frac{k}{2}} \left( s_{a+2}(k, m) \right)^2 y^{k+2}.
\]

(23)
Proof. \( s_{n+2} (k, m) \) is the total weight of pairs of paths of length \( n+2 \), starting at \((0, 0)\) and \((0, 2)\) and ending at \((\frac{n+2}{2}, m)\) and \((\frac{n+2}{2}, k + 2)\). For given \( k \) and \( m \), we can take two such pairs, reflect one of them through the vertical line \( x = \frac{n+2}{2} \), and take the whole thing to be one large pair of paths, the lower going from \((0, 0)\) to \((n - \frac{2}{2}, 0)\) and the upper going from \((0, 2)\) to \((n - \frac{2}{2}, 2)\). The surface weight of this new pair of paths (that is, \(a\) raised the power of the total number of visits) will be equal to the product of the weights of the original two pairs, unless \( m = 0 \), in which case it will be off by a factor of \(a\). The height of the upper ‘middle’ vertex will be \(k + 2\). Since each of the original paths had length \(\frac{n+2}{2}\), the total length of this new pair is \(2n - 4\), adding two edges at the left and right to close things up gives total length of \(2n\).

To deal with the odd \(n\) case, define \( \hat{s}_n(k, m) = r_n \left(1, 0; \frac{k+m}{2}, \frac{k-m}{2}\right) \), with the specialisation \( \hat{s}_n^1(k, m) = \hat{s}_n(k, m)|_{a=1} \). This time we have

\[
\hat{s}_n^1(k, m) = \frac{CT_{\{\eta_1, \eta_2\}} \left[ (\eta_1 + \eta_2)^n (\eta_1 + \eta_2)^n \eta_1^{k-1} \eta_2^{n-1} (1 - \eta_1^2) (1 - \eta_2^2) (\eta_1^2 - \eta_2^2) (\eta_1^2 - \eta_2^2) \right]}{(k+3)(m+1)(k-m+2)(k+m+4) \left( \frac{n+4}{4(n+2)(n+3)(n+4)^2} \right) \left( \frac{n+4}{2(n+k-1)} \right) \left( \frac{n+4}{2(n+m+5)} \right)},
\]

(24)

Then \( \hat{s}_n(k, m) \) expands in the same way as (22):

\[
\hat{s}_n(k, m) = \sum_{w=0}^{n} (a-1)^w \sum_{p=0}^{w} \hat{s}_n^1(k+2p, m+2w-2p).
\]

(25)

This time \( \hat{s}_n(k, m) \neq 0 \) only if \(0 \leq m \leq k \leq n+1\) and \(k \equiv m \equiv n+1 \pmod{2}\). The following can be proved in the same way as lemma 5.

Lemma 6. For odd \(n\), the partition function \( P_{2n}^G(a, y) \) is given by

\[
P_{2n}^G(a, y) = 1 \hat{s}_{n-1} (k, 0) \hat{s}_{n-1} (k, 0) y^{k+2} + \sum_{k=0}^{n} \sum_{m=1}^{k} \hat{s}_{n-1} (k, m) \hat{s}_{n-1} (k, m) y^{k+2}.
\]

(26)

3.2. Centred polygons via pairs of paths

The methods of section 3.1 can be repeated to give an explicit formula for the partition function \( P_{2n}^G(a, y) \). It requires taking \( j = l \) in (20) and then computing the constant term as a function of \( n, j_0 \) and \( l \). However, the significant cancellations which led to the nice formulations of (21) and (24) cannot be applied here, and as a result the final formula is much more complicated.

This would not be so bad if it were still possible to work with said formula (or, more precisely, for Mathematica to do so). However, we have not been able to successfully carry out all the calculations outlined in section 4 for centred polygons. For this reason we will not go into any details regarding the exact formula for \( P_{2n}^G(a, y) \).

4. Exact asymptotics for grafted polygons

In this section we will compute the asymptotic behaviour of \( P_{2n}^G(a, y) \) as \(n \to \infty\) for all \(a\) and \(y\), in the process providing a proof of theorem 1. There are nine different \((a, y)\) regimes which each give different asymptotics. For brevity we will not go through all nine, and will instead provide details for three different cases only. We will also focus only on even \(n\), as the
procedure for odd \( n \) is virtually identical. Similar techniques for computing asymptotics have been used previously—see for example [22, chapter 5].

4.1. The multicritical point: \((a, y) = (2, 1)\)

The partition function \( P_{2n}^{G_1}(a, y) \) is (as per lemma 5) given by a triple sum (over \( k, w, p \)) plus a quadruple sum (over \( k, m, w, p \)), which we write as

\[
P_{2n}^{G_1}(a, y) = \frac{1}{a} P_{2n}^{G_1}(a, y) + P_{2n}^{G_2}(a, y).
\]  

(27)

We first focus on \( P_{2n}^{G_1}(a, y) \). Note that this is nonzero only if \( n \equiv 2 \pmod{4} \), so we assume this to be the case.

We begin by observing that the dominant contributions to \( P_{2n}^{G_1}(2, 1) \) come from values of \( k, w \) and \( p \) which are all \( O(\sqrt{n}) \). (This is easily seen with numerical data, or by analytically maximising the summands.) To avoid fractional powers of \( n \), we thus set \( n = \tilde{n}^2 \), and then rescale the other parameters as \( k = \kappa \tilde{n}, w = \omega \tilde{n} \) and \( p = \rho \tilde{n} \).

Next, take \( s_n^1(k+2p,2w−2p) = s_n^1(\kappa \tilde{n} + 2\rho \tilde{n}, 2\omega \tilde{n} − 2\rho \tilde{n}) \) and apply Stirling’s approximation

\[
x! \sim \sqrt{2\pi x} \left(\frac{x}{e}\right)^x.
\]  

(28)

As \( \tilde{n} \to \infty \) one finds

\[
s_n^1(\kappa \tilde{n} + 2\rho \tilde{n}, 2\omega \tilde{n} − 2\rho \tilde{n}) = \frac{4\tilde{n}^2}{n} \times \frac{64(\kappa + 2\rho)(\kappa + 2\omega)(\omega − \rho)(\kappa + 4\rho − 2\omega)e^{\frac{\tilde{n}^2}{\pi} - \frac{1}{2} \omega - \frac{4}{\pi} \omega^2 + \frac{1}{\pi} \omega^2}}{\pi}
\]  

(29)

We will now compute the asymptotics of \( P_{2n}^{G_2}(2, 1) \) by replacing the triple sum with a triple integral. Multiply the dominant term of (29) by \( \tilde{n} \) to account for the change of variables \( \frac{dp}{d\rho} = \tilde{n} \), and integrate the result in \( \rho \) over \((0, \omega)\) (corresponding to the inner sum in (22)). This leaves

\[
\frac{4\tilde{n}^2}{n^2} \times \frac{64e^{-\frac{1}{2}(\kappa + 2\omega)}(\kappa + 2\omega)(e^{2\kappa\omega}(2\kappa\omega − 1) + 1)}{\pi}
\]  

(30)

Again multiply by \( \tilde{n} \), and then integrate in \( \omega \) over \((0, \infty)\). Then multiply by \( \alpha = 2 \) (from the front of (22)), to get

\[
s_n^2(\kappa \tilde{n}, 0) \big|_{\alpha=2} \sim \frac{4\tilde{n}^2}{n^2} \times \frac{16e^{-\frac{1}{2} \kappa^2}}{\pi n^4}.
\]  

(31)

We will next square the above, multiply by \( \tilde{n} \) and integrate in \( \kappa \) over \((0, \infty)\) in lieu of summing over \( k \). Before doing so, however, recall that \( s_n^2(k, 0) \) is nonzero only if \( k \equiv n \pmod{2} \). To account for this in the integral over \( \kappa \), we should also divide by 2, so as to include the contributions from every second value of \( k \) only. Performing these operations gives

\[
\frac{16\tilde{n}^2}{n^2} \times \frac{48}{\pi^{3/2}}.
\]  

(32)

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Finally adjusting $n^2 \mapsto n \mapsto n^2$ we find
\[
P^{G_1}_{2n}(2,1) \sim \frac{24\sqrt{2}}{\pi^{3/2}} \times \frac{4^n}{n^{7/2}}, \quad n \equiv 2 \mod{4}.
\] (33)

For $P^{G_2}_{2n}(2,1)$, the dominant contribution to the summands is when all of $k, m, w$ and $p$ are $O(\sqrt{n})$. We follow the same procedure as above, with the additional substitution $m = \mu n$ and integral in $\mu$ over $(0, \kappa)$. This time we must account for not only including every second value of $k$, but also every second value of $m$, as we only want terms with $k \equiv m \equiv n \mod{2}$. We must thus divide by 2 twice. We arrive at
\[
P^{G_2}_{2n}(2,1) \sim \frac{4}{\pi} \times \frac{4^n}{n^3}, \quad n \text{ even.}
\] (34)

Note that $P^{G_2}_{2n}(2,1)$ is of strictly greater order than $P^{G_1}_{2n}(2,1)$.

4.2. Weakly attractive or repulsive surface and no force: $a < 2$ and $y = 1$

When $a < 2$ the energetic gain from a surface visit is less than the entropic loss. As a result, the dominant contribution to $P^{G_1}_{2n}(a,1)$ is now from terms with $w$ and $p$ in $O(1)$, with $k$ still $O(\sqrt{n})$. We start with $s_n^k(k,0)$ as before, and again set $n = \tilde{n}^2$ and $k = \kappa \tilde{n}$, but leave $w$ and $p$ as constants (with respect to $\tilde{n}$). The dominant behaviour as $\tilde{n} \to \infty$ is found to be
\[
s_n^k(\kappa \tilde{n} + 2p, 2w - 2p) = \frac{2^{11} 32 \pi^2 \kappa (a - 1)^w (2w - 2p + 1)}{\pi} \left( 1 + O \left( \frac{1}{\tilde{n}} \right) \right).
\] (35)

The leading term is then summed over $p = 0, 1, \ldots, w$ and $w = 0, 1, \ldots$. We then square this, integrate in $\kappa$ over $(0, \infty)$, and divide by 2 (for the same reason as above). Finally, we convert from $\tilde{n}$ back to $n$, and adjust $n \mapsto n^{\frac{3}{2}}$. This gives
\[
P^{G_1}_{2n}(a,1) \sim \frac{1920 \sqrt{2} a^4}{\pi^{1/2} (a - 2)^6} \times \frac{4^n}{n^{3/2}}, \quad n \equiv 2 \mod{4}, a < 2.
\] (36)

The calculation for $P^{G_2}_{2n}(a,1)$ is analogous:
\[
P^{G_2}_{2n}(a,1) \sim \frac{48 a^2}{\pi (a - 2)^4} \times \frac{4^n}{n^3}, \quad n \text{ even, } a < 2.
\] (37)

4.3. Strongly attractive surface with pulling force: $a > 2$ and $y > 1$

In this regime, polygons with a large number of visits and a large height will dominate the partition function. For grafted polygons, there is no conflict here, because the pulling force is only ‘felt’ by the upper walk and the visits are only ‘felt’ by the lower walk.

For $P^{G_1}_{2n}(a,y)$, we first think of $(s_n(k,0))^2 y^{k+2}$ as $\left( s_n(k,0) y^{\frac{4k+2}{4}} \right)^2$, and thus consider a pair of paths with a weight $a$ associated with surface visits and a weight $\sqrt{2}$ associated with the height of the upper path’s endpoint. We can check (numerically or otherwise) that the dominant contribution comes from summations with $k$ and $w$ of $O(n)$ and $p$ of $O(1)$. If we set $k = \gamma n$ and $w = \delta n$, then we need to find the values of $\gamma$ and $\delta$ which maximise the asymptotic expression for the summations.
To do this, we take \( s_0^2(k + 2p, 2w - 2p)(a - 1)^{y + \frac{y^2}{2}} \), apply Stirling’s approximation, make the above substitutions for \( k \) and \( w \), and keep the dominant term as \( n \to \infty \). Then take the logarithm, divide by \( n \), separately take a derivative with respect to \( \gamma \) and with respect to \( \delta \), and finally send \( n \to \infty \) in each. This results in

\[
\frac{1}{2} \log \left( \frac{y(1 - \gamma)}{1 + \gamma} \right) \quad \text{and} \quad \log \left( \frac{(a - 1)(1 - 2\delta)}{1 + 2\delta} \right).
\]

The values of \( \gamma \) and \( \delta \) which set these two quantities to 0, and thus maximise the asymptotic growth rate, are \( \frac{\gamma^{-1}}{3} \) and \( \frac{y + \frac{y^2}{2}}{2} \) respectively. Furthermore, it can be verified that the peak in the asymptotic growth rate, as a function of \( k \) or of \( w \), is of width \( O(\sqrt{n}) \).

We then repeat the procedure of sections 4.1 and 4.2, this time with \( \gamma = \gamma_0 \) and \( \delta = \delta_0 \). (Note that for all regions with \( a > 2 \) and/or \( y < 1 \), the amplitude depends on the value of \( n \) (mod 4) (as in section 4.3), but the growth rate and exponent are independent of this.)

By taking logs, dividing by \( 2n \) and taking \( n \to \infty \), we exactly obtain theorem 1.

The regions \( G_0, G_1, G_{10} \) and \( G_{11} \) correspond to the four different phases for grafted polygons: free, adsorbed, ballistic, and mixed (adsorbed and ballistic) respectively. See figure 6.
5. Lower bounds for centred polygons

In section 4 we found the exact dominant asymptotics for $P_{2n}^C(a, y)$, thus verifying theorem 1 directly. For centred polygons, things are not so straightforward. The partition function $P_{2n}^C(a, y)$ can be computed exactly as per section 3, but the final form is sufficiently complicated so that we have not been able to obtain exact asymptotics. Instead, we will use several techniques to find upper and lower bounds for $P_{2n}^C(a, y)$, and whose asymptotics will be found to be sharp. In this section we focus on lower bounds.

5.1. Grafted and centred polygons

A slight modification to the calculations of section 4 will give a sharp lower bound in regions $G_1$, $G_{II}$ and $G_{IV}$.

We will say that a polygon $\pi \in P_{2n}^S$ is grafted and centred if

- the vertex $\pi \left\lceil \frac{n}{2} \right\rceil$ has $y$-coordinate 0, and
- if $n \equiv 0 \pmod{4}$, the leftmost and rightmost vertices of $\pi$ have $y$-coordinate 2,
- if $n \equiv 1 \pmod{4}$, the leftmost (resp. rightmost) vertex of $\pi$ has $y$-coordinate 2 (resp. 1),
- if $n \equiv 2 \pmod{4}$, the leftmost and rightmost vertices of $\pi$ have $y$-coordinate 1, or
- if $n \equiv 3 \pmod{4}$, the leftmost (resp. rightmost) vertex of $\pi$ has $y$-coordinate 1 (resp. 2).

That is, $\pi$ is grafted and centred if it is centred and if its leftmost and rightmost vertices have the smallest possible $y$-coordinates. Let $P_{2n}^{GC}$ be the set of grafted and centred polygons of length $2n$, with associated partition function $P_{2n}^{GC}(a, y)$.

**Lemma 7.** The free energy

$$\psi^{GC}(a, y) = \lim_{n \to \infty} \frac{1}{2n} \log P_{2n}^{GC}(a, y)$$

exists and is equal to $\psi^G(a, y)$. Furthermore,

$$\psi^G(a, y) = \psi^{GC}(a, y) \leq \liminf_{n \to \infty} \frac{1}{2n} \log P_{2n}^S(a, y).$$

**Proof (sketch).** Since grafted and centred polygons are a subset of centred polygons, we have $P_{2n}^{GC}(a, y) \leq P_{2n}^C(a, y)$ for all $a, y$. The inequality in (43) immediately follows.

For the first part of the proof, observe that $P_{2n}^{GC}(a, y)$ can be computed exactly using the quantities defined in section 3. Namely,

$$P_{2n}^{GC}(a, y) = \left\{ \begin{array}{ll}
    \frac{1}{2} \sum_{k=0}^{\frac{n-1}{2}} \left( \hat{s}_{n-k}^2(k, 0) \right)^2 y^{k+2} & n \equiv 0 \pmod{4} \\
    \frac{1}{2} \sum_{k=0}^{\frac{n-1}{2}} \hat{s}_{n-k}^2(k, 0) y^{k+2} & n \equiv 1 \pmod{4} \\
    \frac{1}{2} \sum_{k=0}^{\frac{n-1}{2}} \left( \hat{s}_{n-k}^2(k, 0) \right)^2 y^{k+2} & n \equiv 2 \pmod{4} \\
    \frac{1}{2} \sum_{k=0}^{\frac{n-1}{2}} \hat{s}_{n-k}^2(k, 0) y^{k+2} & n \equiv 3 \pmod{4}. 
\end{array} \right.$$

The asymptotics can then be computed in the same way as in section 4 (in fact, things are simpler, since there is no $m$ to sum over). We omit details. In some regions the critical exponent differs from those given in table 1, but the exponential growth rate does not change, and hence $\psi^{GC}(a, y) = \psi^G(a, y)$. \[\Box\]
5.2. Binomial bridges

The lower bound (43) is valid in region $G_{III}$ but is not sharp there. To obtain a sharp lower bound on the free energy of centred polygons in region $G_{III}$, we will use a different construction. We define a binomial bridge (or just bridge) of length $n$ and height $h$ to be a binomial path $(\omega_0, \omega_1, \ldots, \omega_n)$ satisfying

$$0 = y(\omega_0) < y(\omega_i) \leq y(\omega_n) = h$$

for $i = 1, \ldots, n - 1$.

That is, it is a binomial path which starts at $y = 0$ and ends at $y = h$, with all non-terminal vertices having $y$-coordinate between 1 and $h$. Let $b_{n,h}$ be the number of bridges of length $n$ and height $h$, and define the partition function

$$B_n(y) = \sum_{h=1}^{n} b_{n,h} y^h.$$

**Lemma 8.** For $y > 1$,

$$\lim_{n \to \infty} \frac{1}{n} \log B_n(y) = \lambda^P(y) = \log (y^2 + 1) - \log y. \quad (45)$$

This statement is proved in the appendix.

**Lemma 8** will allow us to prove the following.

**Lemma 9.** For $y > 1$,

$$\liminf_{n \to \infty} \frac{1}{2n} \log \mathcal{C}_{2n}(a, y) \geq \lambda^P(\sqrt{y}) = \log(y + 1) - \frac{1}{2} \log y. \quad (46)$$

**Proof.** For given $n$ and $y > 1$, define $h^* \equiv h^*(n, y)$ to be the value of $h$ between 1 and $n$ which maximises $b_{n,h^*} y^{h^*}$ (the so-called ‘most popular’ $h'$). Then

$$b_{n,h^*} y^{h^*} \leq B_n(y) \leq nb_{n,h^*} y^{h^*}, \quad (47)$$

so that

$$\lim_{n \to \infty} \frac{1}{n} \log \left( b_{n,h^*} y^{h^*} \right) = \lambda^P(y). \quad (48)$$

Now we can construct a centred polygon of length $4n$ and height $2h$ by reflecting, translating and joining together four bridges of length $n$ and height $h$, as per figure 5 (left). In particular, given $y > 1$, this can be done with $h = h^*$. Then

| $y > 1$ | $a < 2$ | $a = 2$ | $a > 2$ |
|---------|---------|---------|---------|
| $n^{-2} \times \left( \frac{2(y+1)}{\sqrt{y}} \right)^n$ | $n^{-1} \times \left( \frac{2(y+1)}{\sqrt{y}} \right)^n$ | $n^{-1/2} \times \left( \frac{a(y+1)}{\sqrt{(a-1)y}} \right)^n$ |
| $n^{-5} \times 4^n$ | $n^{-3} \times 4^n$ | $n^{-3/2} \times \left( \frac{2a}{\sqrt{a-1}} \right)^n$ |
| $n^{-10} \times 4^n$ | $n^{-6} \times 4^n$ | $n^{-3} \times \left( \frac{2a}{\sqrt{a-1}} \right)^n$ |

Table 1. The dominant asymptotic behaviour of $\mathcal{C}_{2n}(a, y)$ for all values of $a, y > 0$, with amplitudes omitted.
where the factor of $a$ appears because the constructed polygon would have a single surface visit.

Centred polygons of length $4n + 2$ can be constructed in a similar way, with the addition of two extra edges, as per figure 5 (right). This gives

$$a \left( b_{4n+2} h^* \right)^4 \leq P_{4n+2}^C (a, y^2),$$

(50)

Taking logs, dividing by $4n$ and sending $n \to \infty$ in (49) and (50), we obtain

$$\liminf_{n \to \infty} \frac{1}{2n} \log P_{2n}^C (a, y^2) \geq \lambda P(y),$$

(51)

and (46) follows.

By examining the lower bounds given by lemmas 7 and 9, it can be seen that the RHS of (15) is a lower bound for

$$\lim_{n \to \infty} \{ \log P_{2n}^C (a, y) \}.$$ 

6. Upper bounds via noninteracting pairs of paths

6.1. Upper bounds for centred polygons

To obtain a tight upper bound on the free energy of centred polygons, we will again consider configurations of pairs of paths. This time, however, we will relax the nonintersecting constraint. This simplifies matters, as the number of pairs of paths with no nonintersecting constraint is just the square of the number of single paths. We must still account for surface interactions, however.

Let $B_n$ be the set of binomial paths of length $n$ in $\mathbb{L}^+$ which have leftmost vertex in the line $x = 0$. We then define $t_n(i, k)$ to be the total weight of all paths in $B_n$ which start at height $y = i$ and end at height $y = k$, and associate a weight $a$ for each vertex in the surface $y = 0$. Also define the specialisation $t_n(i, k) = t_n(i, k)|_{a=1}$. (Note that $t_n(i, k)$ is nonzero only if $i - k \equiv n \pmod{2}$.) As with pairs of nonintersecting paths, the quantity $t_n(i, k)$ can be computed using a constant term method. The result is given in [22], to which we direct the reader for details.
Table 2. The values of \(w, i\) and \(k\) which give the greatest contributions to \(T_{4n}(a, y)\), as per (54). Here \(\gamma = \frac{1 - \sqrt{1 - 4\Delta}}{2}\), \(\Delta = \frac{y - a}{y + a}\), and \(g(y)\) is the phase boundary given by \(g(y) = 2\) if \(y \leq 1\) and \(g(y) = y + 1\) if \(y > 2\). For the \(y > 1\), \(a = g(y)\) case, \(\epsilon_n\) can be any quantity between 0 and 1 (not necessarily a constant), and the growth rate will be independent of \(\epsilon_n\). For \(T_{4n+2}(a, y)\) as per (55), \(i_1\) and \(i_2\) take the same values as \(i\) given here.

| \(a < g(y)\) | \(a = g(y)\) | \(a > g(y)\) |
|----------------|----------------|----------------|
| \(y > 1\) \(w = O(1), i \sim \gamma, k \sim 2\gamma\) \(w \sim \frac{(1 + \epsilon_n)^2}{n}, i \sim \epsilon_n \gamma n,\) \(k \sim (1 + \epsilon_n) \gamma n, 0 \leq \epsilon_n \leq 1\) | \(w = \delta n, i = O(1), k = \gamma n\) | \(w = \delta n, i = O(1), k = O(1)\) |
| \(y = 1\) \(w = O(1), i \sim O(\sqrt{n}), k = O(\sqrt{n})\) | \(w = O(\sqrt{n}), i = O(\sqrt{n}), k = O(\sqrt{n})\) | \(w = O(\sqrt{n}), i = O(\sqrt{n}), k = O(1)\) |
| \(y < 1\) \(w = O(1), i = O(\sqrt{n}), k = O(1)\) | \(w = O(\sqrt{n}), i = O(\sqrt{n}), k = O(1)\) | \(w = \delta n, i = O(1), k = O(1)\) |

Lemma 10 ([22, equation (5.33)]).

\[
t_n(i, k) = \left(\frac{n}{2}(n - i + k)\right) - \left(\frac{n}{2}(n + i + k)\right) + a \sum_{w=0}^{\frac{1}{2}(n-i-k)} \left[\left(\frac{n}{2}(n + i + k) + w\right) - \left(\frac{n}{2}(n + i + k) + w + 1\right)\right] (a - 1)^w.
\]

(52)

In particular,

\[
t_n^i(i, k) = \left(\frac{n}{2}(n - i + k)\right) - \left(\frac{n}{2}(n + i + k) + 1\right).
\]

(53)

We now define

\[
T_{2n}(a, y) = \frac{1}{a} \sum_{k=0}^{2n} \sum_{i_1, i_2=0}^{n} t_n^i(i, k)t_n(i_1, 0)t_n(i_2, 0)y^k = \frac{1}{a} \sum_{k=0}^{2n} \left(\sum_{i_1=0}^{n} t_n^i(i, k)t_n(i, 0)\right)^2 y^k.
\]

(54)

Observe that the summands count configurations of four (not necessarily nonintersecting) binomial paths: from \((0, i_1)\) to \((n, k)\) (without \(a\) weights), from \((0, i_1)\) to \((n, 0)\) (with \(a\) weights), from \((n, k)\) to \((2n, i_2)\) (without \(a\) weights), and from \((n, 0)\) to \((2n, i_2)\) (with \(a\) weights).

We likewise define

\[
T_{4n+2}(a, y) = \frac{1}{a} \sum_{k=0}^{2n} \left(\sum_{i_1=0}^{n} t_n^i(i, k)t_n(i, 0)\right) \left(\sum_{i_{12}=0}^{n+1} t_{n+1}^i(k, i_2)t_{n+1}(i_{12}, 0)\right) y^k.
\]

(55)

This is the same as (54), except the final point is \((2n + 2, i_2)\) instead of \((2n, i_2)\).

Note that the objects counted by \(T_{2n}(a, y)\) include all centred polygons of length \(2n\): these are simply the configurations where the paths do not intersect. We thus have

\[
T_{2n}(a, y) \geq P_{2n}^a(a, y)
\]

(56)

for all \(a, y > 0\).

Since (56) is a fairly crude upper bound, we are not interested in the detailed asymptotic behaviour of \(T_{2n}(a, y)\). Instead, only the exponential growth rate is of interest. To determine this it is only necessary to find the values of \(w, k\) and \(i\) (or \(i_1\) and \(i_2\)) which give the greatest contributions to (54) and (55). These can be found using the same methods as in section 4. (The subsequent summations and integrals used in section 4 were only necessary for determining the critical exponents, not the growth rates.) We summarise the results in table 2.
Once the dominant values of \( w, k \) and \( i \) (or \( i_1 \) and \( i_2 \)) have been found, finding the exponential growth rate of \( T_{2n}(a, y) \) is simply a matter of applying Stirling’s approximation to the summands of (54) and (55), substituting the values from table 2, taking logs, dividing by 4\( n \) and taking \( n \to \infty \). We omit details. The resulting growth rate is exactly given by the RHS of (15).

**Proof of theorem 2.** By the results of section 5, the RHS of (15) has been shown to be a lower bound for \( \lim \inf_{n \to \infty} \frac{1}{2n} \log P_{2n}^c(a, y) \). By the results of this section, the RHS of (15) is also the growth rate of \( T_{2n}(a, y) \). Then by (56), this is an upper bound for \( \lim \sup_{n \to \infty} \frac{1}{2n} \log P_{2n}^c(a, y) \). The theorem immediately follows. \( \square \)

Similarly to grafted polygons, the regions \( C_I, C_{II}, C_{III} \) and \( C_{IV} \) correspond to the four different phases for centred polygons: free, adsorbed, ballistic, and mixed (adsorbed and ballistic) respectively. See figure 6.

**6.2. Upper bounds for all half-space polygons**

By slightly generalising the arguments of the previous section, we can obtain in a similar way a sharp upper bound for \( \psi^S(a, y) \), the free energy of all half-space polygons. Fix \( q \) between 0 and \( 2n \), and consider a pair of binomial paths, both starting at \((0, i_1)\) and finishing at \((2n, i_2)\) (but not necessarily nonintersecting). Designate one path as the ‘lower path’, and only consider cases where the lower path has at least one vertex in the surface \( y = 0 \). Furthermore, consider only cases where the leftmost vertex of the lower path which is in the surface occurs at \((q, 0)\). Let the lower path gain a weight \( a \) for each vertex in the surface, and associate a weight \( y \) with the height of the middle vertex of the upper path, as usual. Let \( S_{2n,q}(a, y) \) be the total weight of all such configurations (i.e. sum over all \( i_1 \) and \( i_2 \)).

Using \( t_n(i, k) \) and \( t_n^1(i, k) \) as defined in the previous section, it is not difficult to see that if \( q > 1 \) we have

\[
S_{2n,q}(a, y) = \sum_{k=0}^{\min\{n+q,3n-q\}} a^{2n-q} \sum_{i_1=1}^{q} \sum_{i_2=0}^{i_1} t_n^1(i_1, k) t_n^{i_1-1}(i_1-1, 0) t_n^1(k, i_2) t_{2n-q}(0, i_2) y^k,
\]

Figure 6. (a) The phase diagram for grafted staircase polygons, as implied by theorem 1. (b) The phase diagram for centred staircase polygons, and thus all staircase polygons, as implied by theorems 2 and 3. Solid lines indicate second-order phase transitions, while dashed lines indicate first-order transitions.

Once the dominant values of \( w, k \) and \( i \) (or \( i_1 \) and \( i_2 \)) have been found, finding the exponential growth rate of \( T_{2n}(a, y) \) is simply a matter of applying Stirling’s approximation to the summands of (54) and (55), substituting the values from table 2, taking logs, dividing by 4\( n \) and taking \( n \to \infty \). We omit details. The resulting growth rate is exactly given by the RHS of (15).
The value of $q$ which gives the greatest contribution to $S_{4n}(a,y)$, as per (57)-(59). For the $y > 1$, $a = g(y)$ case, $\epsilon_n$ is as per table 2. For the four cases with $*$, the growth rate is entirely independent of $q$. The results are the same for $S_{4n+1}(a,y)$.

| $a < g(y)$ | $a = g(y)$ | $a > g(y)$ |
|------------|------------|------------|
| $y > 1$    | $q \sim n$ | $q \sim \epsilon_n$, $0 \leq \epsilon_n \leq 1$ | $q = O(1)$ |
| $y = 1$    | $*$        | $*$        | $q = O(1)$ |
| $y < 1$    | $*$        | $*$        | $q = O(1)$ |

while for $q = 0$

$$S_{4n,0}(a,y) = \sum_{k=0}^{n} \sum_{i_2=0}^{2n} t^4_n(0,k)t^4_n(k,i_2)t_{2n}(0,i_2)y^i.$$ (58)

Similar expressions can be found for $S_{4n+2,q}(a,y)$.

Then define

$$S_{4n}(a,y) = \sum_{q=0}^{2n} S_{4n,q}(a,y)$$ (59)

and similarly for $S_{4n+2}(a,y)$. The relationship between $S_{2n}(a,y)$ and $P^S_{2n}(a,y)$ is the same as that of $T_{2n}(a,y)$ and $P^S_{2n}(a,y)$: the polygons are exactly the configurations where the upper and lower paths do not intersect. We thus have

$$S_{2n}(a,y) \geq P^S_{2n}(a,y)$$ (60)

for all $a,y > 0$.

We then proceed as in the previous section. We are interested only in the asymptotic growth rate of $S_{2n}(a,y)$, and thus in the values of $w, k, i_1, i_2$ and $q$ which contribute the most to $S_{2n}(a,y)$. The relevant values of $w, k, i_1$ and $i_2$ are as given in table 2. For $q$, a similar analysis can be performed, with the dominant values given in table 3. Note that in some cases the growth rate is entirely independent of $q$.

With the relevant values of $q$ in hand, the asymptotics of $S_{2n}(a,y)$ can be found in the same way as for $T_{2n}(a,y)$: apply Stirling’s approximation to the summands of (57), substitute the relevant values of $w, i_1, i_2, k$ and $q$, take logs, divide by $2n$ and send $n \to \infty$. We omit details. The resulting growth rate is found to be equal to the RHS of (15).

Proof of theorem 3. The proof is analogous to that of theorem 2. We have

$$P^C_{2n}(a,y) \leq P^S_{2n}(a,y) \leq S_{2n}(a,y).$$ (61)

Take logs, divide by $2n$ and send $n \to \infty$. The LHS and RHS both go to the RHS of (15), and the result follows.

7. Conclusion

We have defined several models of staircase polygons which interact with an impenetrable surface and have a pulling or pushing force applied at a fixed vertex. These are greatly simplified versions of two-dimensional self-avoiding polygons, which nevertheless allow for both exact solvability and a range of different physical behaviours.
The phase diagrams for the models solved here are given in figure 6. The locations and natures of the phase transitions follow immediately from the free energies given in theorems 1 and 2.

There are still open questions regarding the more general SAP model. Perhaps the most important question is whether two-dimensional SAPs exhibit a ‘mixed’ phase, as staircase polygons do in region $G_{IV}$. (It is known [12] that such behaviour does not occur for SAPs in three or more dimensions.) If SAPs do have a mixed phase then another question arises: is the phase boundary between the adsorbed and mixed phases a horizontal line at $y = 1$ (as it is for staircase polygons), or does it increase with $a$? For staircase polygons the horizontal boundary is inevitable (because we cannot move from the mixed phase to the adsorbed phase by increasing $a$), but for a more general model this is not clear.

There are other ‘intermediate’ models which are still simpler than SAPs but may display more complex asymptotic behaviour, the most obvious being column-convex polygons on the square lattice. Exact solutions for such models may not be easy to come by, however. Another alternative is to consider staircase polygons with a force applied at the highest vertex, rather than the middle vertex. As discussed in [12], one would expect the free energy to be the same in all regions of the phase diagram, but when $y < 1$ the sub-dominant asymptotic behaviour of the partition functions will likely involve more complex ‘stretched exponential’ terms (see [6, 10]).

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Appendix. Binomial bridges

This section is dedicated to a proof of lemma 8. Binomial bridges (sometimes called directed bridges) have been studied in the past—see for example [7, 8]. However, we have been unable to find in the literature the exact result that we require, and thus we present a brief proof here.

First, recall the generating function $C(t; a, y)$ for half-plane binomial paths from section 2.1. We will not need surface visits here, so we set $a = 1$. We will then similarly define the generating function for bridges as

$$B(t; y) = \sum_{n,h} b_{n,h} t^n y^h.$$  

Now there is a standard method for decomposing a half-plane walk (of the type counted by $C(t; 1, y)$) into an alternating sequence of bridges and reflected bridges. We refer the reader to [17, chapter 3] for details (the focus there is on self-avoiding walks, but the same principles apply). In particular, the equivalent form of [17, equation (3.1.13)] here is

$$tC(t; 1, 1) \leq \exp \left( B(t; 1) \right).$$  \hspace{1cm} (A.1)

To incorporate the weight $y$, we use the fact that appending a bridge to a walk will increase the height of its endpoint, while attaching a reflected bridge will decrease the height. The inequality (A.1) becomes

$$tyC(t; 1, y) \leq \exp \left( B(t; y) + B(t; 1/y) \right).$$  \hspace{1cm} (A.2)
Proof of lemma 8. Since the exponential function is entire, the radius of convergence of the RHS of (A.2) (considered as a power series in \( t \)) is equal to the radius of convergence of 
\[ B(t; y) + B(t; 1/y) \] 
For \( y > 1 \), we have \( B_n(y) > B_n(1/y) \), and so that radius of convergence is really that of \( B(t; y) \).

Meanwhile, by inclusion we clearly have \( B(t; y) \leq tyC(t; 1, y) \). Combining these ideas, it follows that for \( y > 1 \) the radius of convergence of \( tyC(t; 1, y) \) (and hence that of \( C(t; y) \)) is equal to that of \( B(t; y) \). So the growth rate of \( C_n(1, y) \) is equal to that of \( B_n(y) \), and then by (5), the result follows.

\[ \square \]

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References

[1] Atapour M, Soteros C E and Whittington S G 2009 Stretched polygons in a lattice tube J. Phys. A: Math. Theor. 42 322002
[2] Beaton N R 2015 The critical pulling force for self-avoiding walks J. Phys. A: Math. Theor. 48 16FT03
[3] Beaton N R, Eng J W and Soteros C E 2016 Polygons in restricted geometries subjected to infinite forces J. Phys. A: Math. Theor. 49 424002
[4] Beaton N R, Guttmann A J and Jensen I 2012 Two-dimensional self-avoiding walks and polymer adsorption: critical fugacity estimates J. Phys. A: Math. Theor. 45 055208
[5] Beaton N R, Bousquet-Mélou M, de Gier J, Duminil-Copin H and Guttmann A J 2014 The critical fugacity for surface adsorption of self-avoiding walks on the honeycomb lattice is \( 1 + \sqrt{2} \)
Commun. Math. Phys. 326 727–54
[6] Beaton N R, Guttmann A J, Jensen I and Lawler G F 2015 Compressed self-avoiding walks, bridges and polygons J. Phys. A: Math. Theor. 48 454001
[7] Brak R, Essam J W and Owczarek A L 1999 Exact solution of \( n \) directed non-intersecting walks interacting with one or two boundaries J. Phys. A: Math. Gen. 32 2921–9
[8] Brak R, Owczarek A L, Rechnitzer A and Whittington S G 2005 A directed walk model of a long chain polymer in a slit with attractive walls J. Phys. A: Math. Gen. 38 4309–25
[9] Flajolet P and Sedgewick R 2009 Analytic Combinatorics (Cambridge: Cambridge University Press)
[10] Guttmann A J 2015 Analysis of series expansions for non-algebraic singularities J. Phys. A: Math. Theor. 48 045209
[11] Guttmann A J, Jensen I and Whittington S G 2014 Pulling adsorbed self-avoiding walks from a surface J. Phys. A: Math. Theor. 47 015004
[12] Guttmann A J, Jensen I and Whittington S G 2017 Polygons pulled from an adsorbing surface J. Phys. A: Math. Theor. (arXiv:1702.06564) submitted
[13] Hammersley J M, Torrie G M and Whittington S G 1982 Self-avoiding walks interacting with a surface J. Phys. A: Math. Gen. 15 539–71
[14] Haupt B J, Ennis J and Sevick E M 1999 The detachment of a polymer chain from a weakly adsorbing surface using an AFM tip Langmuir 15 3886–92
[15] Krawczyk J, Owczarek A L, Prellberg T and Rechnitzer A 2005 Pulling adsorbing and collapsing polymers from a surface J. Stat. Mech. P05008
[16] Luo M-B 2008 The critical adsorption point of self-avoiding walks: a finite-size scaling approach J. Chem. Phys. 128 044912
[17] Madras N and Slade G 2013 The Self-Avoiding Walk. Modern Birkhäuser Classics (New York: Birkhäuser) (reprint of the 1996 original)
[18] Janse van Rensburg E J 1999 Adsorbing staircase walks and staircase polygons Ann. Combin. 3 451–73
[19] Janse van Rensburg E J 1999 Collapsing and adsorbing polygons J. Phys. A: Math. Gen. 31 8295–306
[20] Janse van Rensburg E J 2002 Knotting in adsorbing lattice polygons Physical Knots: Knotting, Linking, and Folding Geometric Objects in $\mathbb{R}^3$ (Las Vegas, NV, 2001) (Contemporary Mathematics vol 304) (Providence, RI: American Mathematical Society) pp 137–51

[21] Janse van Rensburg E J 2003 Statistical mechanics of directed models of polymers in the square lattice J. Phys. A: Math. Gen. 36 R11–R61

[22] Janse van Rensburg E J 2015 The Statistical Mechanics of Interacting Walks, Polygons, Animals, and Vesicles 2nd edn (Oxford: Oxford University Press)

[23] Janse van Rensburg E J and Rechnitzer A 2004 Multiple Markov chain Monte Carlo study of adsorbing self-avoiding walks in two and in three dimensions J. Phys. A: Math. Gen. 37 6875–98

[24] Janse van Rensburg E J and Whittington S G 2017 Self-avoiding walks adsorbed at a surface and pulled at their mid-point J. Phys. A: Math. Theor. 50 p 055001

[25] Janse van Rensburg E J, Orlandini E, Tesi M C and Whittington S G 2008 Knotting in stretched polygons J. Phys. A: Math. Theor. 41 015003

[26] Soteros C E 1992 Adsorption of uniform lattice animals with specified topology J. Phys. A: Math. Gen. 25 3153–73