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Self-avoiding walks in a slab: rigorous results

E J Janse van Rensburg[1], **E Orlandini**[2] **and S G Whittington**[3]

[1] Department of Mathematics and Statistics, York University, Toronto, Ontario M3J 1P3, Canada
[2] Dipartimento di Fisica e Sezione INFN, Università di Padova, Padova, Italy
[3] Department of Chemistry, University of Toronto, Toronto, Ontario M5S 3H6, Canada

E-mail: rensburg@yorku.ca

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Abstract
A polymer in the confined spaces between colloid particles loses entropy and exerts a repulsive entropic force on the confining particles. This situation can be modelled by a self-avoiding walk confined in a slab between two parallel planes in the lattice. In this paper, we prove the existence of a limiting free energy for the general case that the walk is interacting with the parallel bounding planes. We also prove that the limiting free energy is strictly increasing with the distance between the bounding planes in some regions of the phase diagram. These results demonstrate the presence of a non-zero repulsive entropic force in the model. Finally, we also examine the relation between the limiting free energy in this model and the limiting free energy in a model of walks adsorbing onto a single plane. We prove that these limiting free energies are equal in some regions of the phase diagram in the limit that the width of the slab between the parallel bounding planes is taken to infinity.

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1. Introduction

Polymers are often confined to narrow spaces in capillaries or in the interstitial spaces between particles. The consequent loss of entropy in the polymer results in a repulsive entropic force from the polymer on the confining particles or walls.

A case of particular interest is a colloidal dispersion stabilized by adsorbing polymers. If two colloidal particles approach one another, and a polymer is weakly adsorbed on one particle, then the polymer becomes confined to the space between the particles. The resulting loss of conformational entropy induces a repulsive force between the colloidal particles, preventing them from clustering in the solution. This is the phenomenon of steric stabilization of colloidal particles by a polymer.

On the other hand, it may be that the polymer is strongly adsorbed on colloidal particles. In this event it may bridge two colloidal particles, resulting in an attractive force between them which destabilizes the dispersion. This is the phenomenon of sensitized flocculation. See for example [2], and for a more recent review [18].

Steric stabilization and sensitized flocculation of colloidal particles have been modelled by bead-spring models of polymers interacting with spheres or walls [17]. Experimental work has also made the measurements of the effective interaction between colloidal particles and for a single particle near a wall possible [19, 22].

If the colloidal particles are large compared to the polymer, then the space between them can be approximated by the slab between two parallel planes. This gives a model of a polymer in a infinite slab geometry, and the monomers may interact with the bounding planes of the slab, which are models of the surface area of the confining colloidal particles.

Several models have been created to describe the configurational properties of the polymer molecules in confined spaces. In a classic paper, DiMarzio and Rubin [3] analysed a random walk model of a polymer between two parallel planes with a short-ranged attractive monomer-plane potential. They showed that there was a repulsive force between the planes at high temperatures where entropic terms dominate. They also showed that there is an attractive force at low temperatures corresponding to sensitized flocculation. The forces exerted by polymers in a two-dimensional strip were also examined by Stilck and Machado [21].

Brak *et al* [1] considered several directed walk models related to Dyck paths and generalized the model to the situation which includes different interactions with the two bounding planes. They found a rich phase diagram with three regimes characterized by a long-range repulsive force, a short-range repulsive force and a short-range attractive force between the planes.

In this paper, we examine a self-avoiding walk model of a polymer between two confining planes in the hypercubic lattice. Numerical simulations of this model were reported previously in [13], where the scaling properties of the entropic force were examined and where a phase diagram was conjectured based on numerical evidence. In this paper, we consider by rigorous means the limiting free energy in this model. We present some facts which we shall use about self-avoiding walks in section 2 and define our models in section 3. We prove existence of the limiting free energy in our model in section 4 and prove a pattern theorem in section 5. In section 6, we examine the properties of the free energy based on our results in sections 4 and 5. In figure 16, we present the phase diagram of the model and we discuss this in section 7. Figure 16 is consistent with the phase diagram conjectured in [13], and we are able to determine part of the phase diagram exactly and to give bounds and conjectures on the remaining part. We conclude the paper with a few final comments in section 8.

2. Self-avoiding walks

Let $\mathbb{Z}^d$ be the d-dimensional hypercubic lattice with coordinate axes $X, Y, \ldots, Z$. By default, X will always be the first coordinate, followed by Y, and so on. Z will be the dth coordinate axis. The coordinates of a lattice point $\mathbf{x}$ are $(X(\mathbf{x}), Y(\mathbf{x}), \ldots, Z(\mathbf{x}))$.

Representations of the lattice in figures will be with the X-axis in the horizontal direction and the Z-axis in the vertical direction. All other coordinates will be oriented normal to the page.

A self-avoiding walk from the origin is a sequence of unit length edges $\{e_i\}_{i=1}^n$ with endpoints in $\mathbb{Z}^d$, such that e_{i-1} and e_i are incident (share exactly one endpoint or vertex), and if $v_i = e_{i-1} \cap e_i$ is a vertex in the walk, then $v_i \neq v_j$ whenever $i \neq j$. Such a walk is oriented from the origin and has length n.

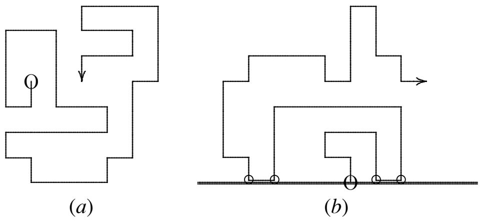

Figure 1. Self-avoiding walks in the hypercubic lattice: (a) a self-avoiding walk from the origin and (b) a self-avoiding walk from the origin in a half-space.

A self-avoiding walk from the origin is illustrated in figure 1(a). The most important quantity in this model is c_n, the number of self-avoiding walks of length n from the origin. c_n is a submultiplicative function [5]:

$$c_n c_m \geqslant c_{n+m}. \tag{1}$$

Since $c_n \geqslant d^n$ in d dimensions, this implies existence of the connective constant [5]

$$\lim_{n\to\infty} \frac{1}{n} \log c_n = \kappa \geqslant \log d. \tag{2}$$

2.1. Adsorbing self-avoiding walks

In this paper, a model of self-avoiding walks from the origin in the half-space $Z \geqslant 0$ is relevant (see figure 1(b)). These are *positive walks* and a *visit* in such a walk is a vertex, other than the origin, in the plane $Z = 0$.

We denote by $C_n^+(v)$ the number of positive walks from the origin of length n and making v visits to the *adsorbing plane* $Z = 0$. This is a model of an adsorbing polymer [6], and the partition function is defined in the usual way:

$$Z_n(a) = \sum_{v=0}^{n} C_n^+(v) a^v. \tag{3}$$

The existence of a limiting free energy

$$\mathcal{F}(a) = \lim_{n\to\infty} \frac{1}{n} \log Z_n(a) \tag{4}$$

is known and $\mathcal{F}(a)$ is also a convex function of $\log a$ [6]. The most interesting aspect of this model is that there exists a critical value a_c of a such that

$$\mathcal{F}(a) \quad \begin{cases} =\kappa, & \text{if } a \leqslant a_c; \\ >\kappa, & \text{if } a > a_c. \end{cases} \tag{5}$$

Thus $\mathcal{F}(a)$ is non-analytic at $a = a_c$, and this model exhibits a phase transition between a desorbed phase (where the walk wanders away from the adsorbing plane) and an adsorbed phase (where the walk remains in the vicinity of the adsorbing plane). It is also known that [11]

$$\log a_c \geqslant [\log(1 + \mathrm{e}^{-2\kappa})]/4 > 0. \tag{6}$$

In this paper, a variant of this model, where the walk is confined to a slab, rather than to a half-space, will be studied as a model of a polymer in a confined region.

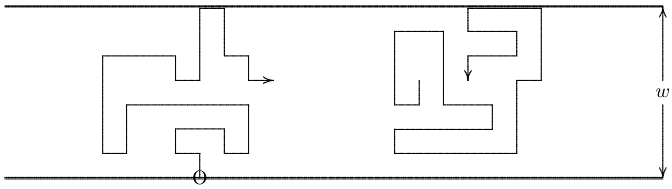

Figure 2. Walks in a slab $\mathbb{L}_w$ of width w. The walk on the left is rooted at the origin marked by an O, while the walk on the right is not rooted.

2.2. Walks in a slab

The sublattice

$$\mathbb{L}_w = \{\mathbf{x} \in \mathbb{Z}^d \mid 0 \leqslant Z(\mathbf{x}) \leqslant w\} \subset \mathbb{Z}^d \tag{7}$$

is the w-*slab* or the slab of width w. In two dimensions this is the w-slit, but we will abuse the terminology and refer to $\mathbb{L}_w$ as a slab in both two and higher dimensions.

There are several different models of self-avoiding walks in $\mathbb{L}_w$, and we refer to these generally as w-walks. Two models are illustrated in figure 2. The walk on the left starts at the origin, while the walk on the right is not rooted, but has a last vertex denoted by the arrow. Two rooted walks are equivalent if they become identical when their roots are identified. If walks are not rooted, then they are equivalent if they can be made identical by translation normal to the Z-axis. w-Walks are *distinct* if they are not equivalent.

The lexicographic first vertex in a w-walk is its *bottom vertex*, and the lexicographic last vertex will be its *top vertex*.

If a w-walk is rooted in one of its endpoints, then its edges will be oriented away from the root[4].

If the w-walk is not rooted, then its two endpoints are ordered lexicographically. The w-walk is then oriented from the lexicographic first endpoint to the lexicographic last endpoint.

Thus, the first and last vertices in any w-walk can be unambiguously defined, both in models where the walk is from the origin or in models where the walk is not rooted.

If the walk is rooted at a vertex other than one of its endpoints, then it is again oriented from the lexicographic first endpoint to the lexicographic last endpoint.

Let $C_n(w)$ be the number of self-avoiding walks from the origin in $\mathbb{L}_w$ of length n. The following properties of $C_n(w)$ are due to Hammersley and Whittington [8]:

(i) The connective constant $\lim_{n\to\infty} n^{-1} \log C_n(w) \equiv \kappa_w$ exists for all $w \geqslant 0$.
(ii) κ_w is strictly increasing with w: $\kappa_w < \kappa_{w+1}$ for all $w \geqslant 0$.
(iii) Finally, as $w \to \infty$, κ_w approaches the connective constant κ: $\lim_{w\to\infty} \kappa_w = \kappa$.

Very little is known rigorously when there are interactions of the walk with the two confining hyperplanes but the situation has been investigated numerically in [13]. Those results indicate that the phase diagram has the same qualitative form as for the directed walk model in [1].

3. Models of w-walks

The boundary of the slab $\mathbb{L}_w$ consists of two hyperplanes called the *bounding planes*. The plane $Z = 0$ is the *bottom bounding plane* of $\mathbb{L}_w$ and $Z = w$ is the *top bounding plane* of $\mathbb{L}_w$.

[4] That is, the edge incident with the root is oriented away from the root, and this induces a direction along the walk.

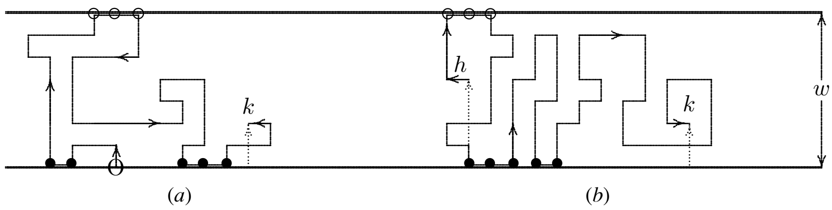

Figure 3. w-Walks in the slab $\mathbb{L}_w$. (*a*) A w-walk from the origin O. The walk is oriented by directing its first step away from the origin. The walk makes visits to the bottom bounding plane (marked by •) and to the top bounding plane (marked by ○). (*b*) A w-walk in the slab $\mathbb{L}_w$ with arbitrary endpoints. This walk is oriented from its lexicographic first endpoint to its lexicographic last endpoint. Walks such as these are equivalent under translations normal to the *Z*-direction. This walk makes visits to the bottom bounding plane (marked by •) and to the top bounding plane (marked by ○).

A vertex of a walk in the bottom bounding plane is a *bottom visit*. A vertex of a walk in the top bounding plane is a *top visit*. Such visits are illustrated in figure 3. Observe that a walk is oriented in the first instance (*a*) from its endpoint at the origin or secondly (*b*) from its lexicographic first endpoint.

We have defined $C_n(w)$ to be the number of self-avoiding walks from the origin in $\mathbb{L}_w$ of length n. Similarly, we define $c_n(w)$ to be the number of self-avoiding walks in $\mathbb{L}_w$, counted up to equivalency under translations parallel to the bottom bounding plane.

Next, define $c_n(w; h, k; v_b, v_t)$ to be the number of w-walks, counted up to equivalency under translations parallel to the bottom bounding plane, and with first (and lexicographic first) endpoint at height h above the bottom bounding plane (or with *Z*-coordinate equal to h) and with last endpoint at height k. These paths also have v_b bottom visits and v_t top visits. In figure 4(*a*), an example of a w-walk counted by $c_n(w; h, k; v_b, v_t)$ is given. In this example $v_b = 0$ and $v_t = 2$.

Similarly, define $C_n(w; k; v_b, v_t)$ to be the number of w-walks from the origin of length n, with last vertex at height k, and with v_b bottom visits and v_t top visits. An example of such a walk is given in figure 4(*b*). In this example $v_b = v_t = 2$.

In some cases, we will be interested in w-walks with endpoints at any heights above the bottom bounding plane. We define

$$\begin{aligned} c_n(w; v_b, v_t) &= \sum_{h,k} c_n(w; h, k; v_b, v_t), \\ C_n(w; v_b, v_t) &= \sum_{k} C_n(w; k; v_b, v_t), \end{aligned} \tag{8}$$

and observe that $c_n(w) = \sum_{v_b, v_t} c_n(w; v_b, v_t)$ and $C_n(w) = \sum_{v_b, v_t} C_n(w; v_b, v_t)$.

These models can be turned into a model of a w-walk interacting with the w-slab by introducing activities a and b and then by defining the partition function

$$g_n(w; h, k; a, b) = \sum_{v_b, v_t} c_n(w; h, k; v_b, v_t) a^{v_b} b^{v_t}. \tag{9}$$

The activity a is conjugate to bottom visits, while b is conjugate to top visits, and we generally assume that $a > 0$ and $b > 0$ in all our models, unless we explicitly choose one or the other to be zero. Similarly, one may define the partition function $g_n(w; a, b) = \sum_{v_b, v_t} c_n(w; v_b, v_t) a^{v_b} v^{v_t}$.

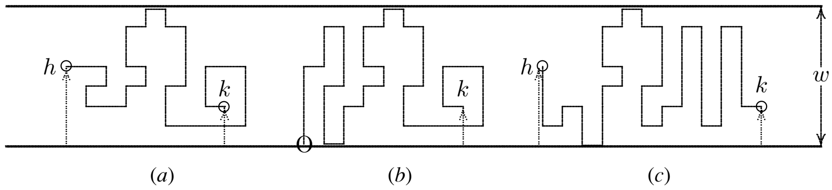

Figure 4. Walks with endpoints at heights h and k. (a) A walk in the slab. This walk is not rooted, and walks in this class are counted up to translations parallel to the bounding planes. (b) A walk from the origin in the bottom bounding plane with last vertex at height k. (c) An unfolded walk with endpoints at heights h and k.

For walks from the origin, the partition function

$$G_n(w; k; a, b) = \sum_{v_b, v_t} C_n(w; k; v_b, v_t) a^{v_b} b^{v_t} \tag{10}$$

can be defined, as well as $G_n(w; a, b) = \sum_{v_b, v_t} C_n(w; v_b, v_t) a^{v_b} b^{v_t}$.

There are also other models that could be considered, and we shall introduce and define them as they are needed in what follows.

3.1. Unfolded walks

A w-walk W with vertices $\{x_i\}_{i=0}^{n}$ is *unfolded* if $X(x_0) \leqslant X(x_i) < X(x_n)$ for $i = 1, 2, \ldots, n-1$. An example of an unfolded walk is given in figure 4(c).

Let $c_n^{\dagger}(w; h, k; v_b, v_t)$ to be the number of unfolded w-walks, counted up to equivalency under translations parallel to the bottom bounding plane, and with its first (lexicographic first) endpoint at height h above the bottom bounding plane (or with Z-coordinate equal to h) and with last endpoint at height k. These walks also have v_b bottom visits and v_t top visits. We will generally indicate the number of unfolded w-walks by using the superscript †.

Similarly, $C_n^{\dagger}(w; k; v_b, v_t)$ is the number of unfolded w-walks from the origin, with last vertex at height k above the bottom bounding plane, and with v_b bottom visits and v_t top visits.

We are in the first instance interested in $C_n(w)$ and also in $G_n(w; a, b)$. In particular, the existence of the *free energy* (this is equal to the connective constant if $a = b = 1$)

$$\kappa_w(a, b) = \lim_{n\to\infty} \frac{1}{n} \log G_n(w; a, b) \tag{11}$$

of the slab $\mathbb{L}_w$ is proven in section 4.1. The proof proceeds along the lines of arguments developed by Soteros and Whittington [20]. We also note in particular that $\kappa_w(a, b) \leqslant \kappa$ if $a, b \leqslant 1$ and that the pattern theorem for self-avoiding walks implies that $\kappa_w(1, 1) < \kappa$ for any finite w [14].

4. Existence of $\kappa_w(a, b)$

4.1. Unfolded w-walks

Let X_0 and X_1 be the X-coordinates of the bottom and top vertices of a w-walk W, respectively. W can be unfolded by the construction in figure 5. Recall that the number of unfolded walks of length n with endpoints of heights h and k, and with v_b and v_t bottom and top vertices, is $c_n^{\dagger}(w; h, k; v_b, v_t)$. The number of visits to the bottom or top bounding plane may change by

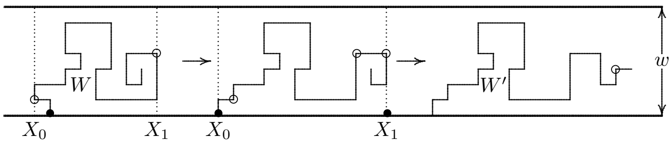

Figure 5. A w-walk can be unfolded by reflecting the parts of the path preceding and following its bottom and top vertices, respectively, through the planes $X = X_0$ and $X = X_1$ which pass through the top and bottom vertices. By repeatedly applying this construction, and by finally adding a single edge in the X-direction to the final vertex in the walk, an unfolded w-walk is obtained. Observe that this construction does not change the Z-coordinate of any of the vertices. The result of this construction is lemma 4.1, corollary 4.2 and lemma 4.3.

at most one when the last edge is appended to the walk. Further, the heights of the first and last vertices remain unchanged.

One may unfold walks [7] in the classes counted by $C_n(w; k; v_b, v_t)$ or $C_n(w)$. This construction leads to the following lemma (the methods of proof are identical to the techniques used in corollary 5.4 and theorem 5.5 in [12]).

Lemma 4.1. *For every slab $\mathbb{L}_w$ of fixed width w, there exists a constant $\gamma > 0$ and a finite N_γ such that for all positive integers $n > N_\gamma$,*

$$e^{-\gamma\sqrt{n}} C_n(w) \leqslant C^\dagger_{n+1}(w) \leqslant C_{n+1}(w).$$

In addition, if walks counted by $C_n(w; k; v_b, v_t)$ are unfolded, then

$$\begin{aligned} e^{-\gamma\sqrt{n}} C_n(w; k; v_b, v_t) &\leqslant C^\dagger_{n+1}(w; k; v_b, v_t) + C^\dagger_{n+1}(w; k; v_b + 1, v_t) + C^\dagger_{n+1}(w; k; v_b, v_t + 1) \\ &\leqslant C_{n+1}(w; k; v_b, v_t) + C_{n+1}(w; k; v_b + 1, v_t) + C_{n+1}(w; k; v_b, v_t + 1). \end{aligned}$$

One may also sum over k in this lemma to see that there exists a constant $\gamma > 0$ and a finite N_γ such that for all $n > N_\gamma$ it is the case that

$$\begin{aligned} e^{-\gamma\sqrt{n}} C_n(w; v_b, v_t) &\leqslant C^\dagger_{n+1}(w; v_b, v_t) + C^\dagger_{n+1}(w; v_b + 1, v_t) + C^\dagger_{n+1}(w; v_b, v_t + 1) \\ &\leqslant C_{n+1}(w; v_b, v_t) + C_{n+1}(w; v_b + 1, v_t) + C_{n+1}(w; v_b, v_t + 1). \end{aligned} \tag{12}$$

If $G^\dagger_n(w; a, b) = \sum_{v_b, v_t} C^\dagger_n(w; v_b, v_t) a^{v_b} b^{v_t}$ is the partition function, then the immediate corollary to lemma 4.1 is the following.

Corollary 4.2. *For every slab $\mathbb{L}_w$ of fixed width w, there exists a constant $\gamma > 0$ and a finite N_γ such that for all positive integers $n > N_\gamma$,*

$$e^{-\gamma\sqrt{n}} G_n(w; a, b) \leqslant (1 + 1/a + 1/b) G^\dagger_{n+1}(w; a, b) \leqslant (1 + 1/a + 1/b) G_{n+1}(w; a, b),$$

for all finite activities $a > 0$ and $b > 0$.

It is also necessary to unfold other classes of walks and, in particular, we will be unfolding walks in the classes counted by $c_n(w; h, k; v_b, v_t)$. The proof of lemma 4.3 is a standard construction; see for example [7, 15, 16]. The same arguments and techniques are also applied in corollary 5.4 and theorem 5.5 in [12].

Lemma 4.3. *For every fixed slab $\mathbb{L}_w$ of width w and for fixed integers h and $k \in [0, w]$, there exists a constant $\gamma > 0$ and a finite $N_\gamma > 0$ such that for all integers $n > N_\gamma$*

$$\begin{aligned} e^{-\gamma\sqrt{n}} c_n(w; h, k; v_b, v_t) &\leqslant c^\dagger_{n+1}(w; h, k; v_b, v_t) + c^\dagger_{n+1}(w; h, k; v_b + 1, v_t) \\ &\quad + c^\dagger_{n+1}(w; h, k; v_b, v_t + 1) \leqslant c_{n+1}(w; h, k; v_b, v_t) + c_{n+1}(w; h, k; v_b + 1, v_t) \\ &\quad + c_{n+1}(w; h, k; v_b, v_t + 1). \end{aligned}$$

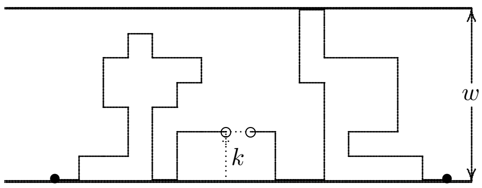

Figure 6. Two unfolded w-walks of length n starting at height zero and with height of their final vertices equal to k can be concatenated by reflecting one walk through the plane $X = 0$ and translating it so that its final vertex is adjacent to the final vertex of the other walk. By inserting an edge, a w-walk of length $(2n + 1)$ is obtained with final vertex of height 0.

By multiplying the inequalities in lemma 4.3 by $a^{v_b} b^{v_t}$ and summing over v_b and v_t, we obtain the following inequalities relating the partition functions of w-walks and unfolded w-walks.

Lemma 4.4. *For every fixed slab $\mathbb{L}_w$ of width w and for fixed integers h and $k \in [0, w]$, there exists a constant $\gamma > 0$ and a finite $N_\gamma > 0$ such that for all integers $n > N_\gamma$*

$$\begin{aligned} \mathrm{e}^{-\gamma\sqrt{n}} g_n(w; h, k; a, b) &\leqslant (1 + 1/a + 1/b) g^\dagger_{n+1}(w; h, k; a, b) \\ &\leqslant (1 + 1/a + 1/b) g_{n+1}(w; h, k; a, b), \end{aligned}$$

for all finite activities $a > 0$ and $b > 0$.

4.2. The limiting free energy of walks in a slab

Existence of the connective constant κ_w and the free energy $\kappa_w(a, b)$ follows from lemmas 4.3 and 4.4. Since $\kappa_w = \kappa_w(1, 1)$, we prove only the more general result. The existence of the free energy is first demonstrated for models of unfolded walks, before it is generalized to the general model.

Lemma 4.5. *If $a > 0$ and $b > 0$, then the limit*

$$\kappa_w(a, b) = \lim_{n\to\infty} \frac{1}{n} \log G^\dagger_n(w; a, b)$$

exists for $w \geqslant 0$. Moreover, in terms of the partition functions of unfolded w-walks,

$$\begin{aligned} \kappa_w(a, b) &= \lim_{n\to\infty} \frac{1}{n} \log g^\dagger_n(w; h, k; a, b) \\ &= \sup_{n\geqslant 2} \frac{1}{n} \log \left[a g^\dagger_{n-2}(w; 0, 0; a, b)\right], \end{aligned}$$

for any heights h and k in $[0, w]$. Lastly,

$$a g^\dagger_{n-2}(w; 0, 0; a, b) \leqslant \mathrm{e}^{n\kappa_w(a,b)}.$$

Proof. Let W_1 and W_2 be unfolded w-walks of lengths n and m and with leftmost endpoint at height $h = 0$ and last endpoint at height k. One such walk would be obtained if $h = 0$ in figure 4(c). Reflect W_2 through the plane $X = 0$, and then translate it so that its reflected final vertex is adjacent to the final vertex of W_1 in the X-direction. This gives the situation illustrated in figure 6.

The two walks may be concatenated by adding a single edge between the adjacent endpoints, and the new walk is a w-walk with final vertex of height 0. Observe that the number of bottom and top visits are not altered by this construction, since we concatenated the two walks in figure 6 by inserting an extra edge between them.

This construction maps pairs of unfolded w-walks of lengths n and m, and with heights of their final vertices equal to k to a w-walk of length $n+m+1$ and with final vertex of height 0. By deleting the $(n+1)$th edge in the walk resulting from the concatenation, the original unfolded w-walks can be recovered. By adding a single edge in the X-direction to the final vertex of the concatenated walk, an unfolded w-walk is obtained, with one more bottom visit than the sum of the bottom visits in the original walks. Thus, each pair of unfolded w-walks is mapped to a unique unfolded w-walk of length $n+m+2$ with final vertex of height 0.

Suppose that W_1 has $(v_b - w_b, v_t - w_t)$ bottom and top visits, and that W_2 has (w_b, w_t) bottom and top visits. Then this construction shows that

$$\sum_{w_b, w_t} c_n^{\dagger}(w; 0, k; v_b - w_b, v_t - w_t) c_m^{\dagger}(w; 0, k; w_b, w_t) \leqslant c_{n+m+2}^{\dagger}(w; 0, 0; v_b + 1, v_t).$$

Multiply this by $a^{v_b} b^{v_t}$, and sum over v_b and v_t. This gives

$$g_n^{\dagger}(w; 0, k; a, b) g_m^{\dagger}(w; 0, k; a, b) \leqslant (1/a) g_{n+m+2}^{\dagger}(w; 0, 0; a, b). \tag{13}$$

In particular, if $k = 0$ and n and m are replaced by $n-2$ and $m-2$, respectively, in equation (13), then one obtains the inequality

$$\left[a g_{n-2}^{\dagger}(w; 0, 0; a, b)\right]\left[a g_{m-2}^{\dagger}(w; 0, 0; a, b)\right] \leqslant \left[a g_{n+m-2}^{\dagger}(w; 0, 0; a, b)\right]. \tag{14}$$

In other words, the function $-\log\left[a g_{n-2}^{\dagger}(w; 0, 0; a, b)\right]$ is subadditive in n. Next, observe that

$$\begin{aligned} g_{n-2}^{\dagger}(w; 0, 0; a, b) &= \sum_{v_b, v_t} c_{n-2}^{\dagger}(w; 0, 0; v_b, v_t) a^{v_b} b^{v_t} \\ &\leqslant c_n^{\dagger} \sum_{v_b, v_t}^{n} a^{v_b} b^{v_t} \\ &\leqslant n^2 (2d)^n \max\{1, a^n, b^n, a^n b^n\}. \end{aligned} \tag{15}$$

Thus, $g_{n-2}^{\dagger}(w; 0, 0; a, b)$ is bounded by K^n, for some large finite value of K, for fixed values of a and b. Together with equation (14), a basic theorem on subadditive functions [10] implies that the limit

$$\begin{aligned} \kappa_w(a, b) &= \lim_{n\to\infty} \frac{1}{n}\left[a \log g_{n-2}^{\dagger}(w; 0, 0; a, b)\right] \\ &= \lim_{n\to\infty} \frac{1}{n} \log g_n^{\dagger}(w; 0, 0; a, b) \\ &= \sup_{n\geqslant 2} \frac{1}{n}\left[a \log g_{n-2}^{\dagger}(w; 0, 0; a, b)\right]. \end{aligned} \tag{16}$$

exists [4, 10, 23]. Moreover,

$$a g_{n-2}^{\dagger}(w; 0, 0; a, b) \leqslant \mathrm{e}^{n\kappa_w(a,b)} \tag{17}$$

for $n > 1$.

By adding $w+1$ edges on the last vertex of height k_1 of an unfolded w-walk, one can construct an unfolded w-walk with last vertex of arbitrary height k_2. If $k_2 = 0$ or $k_2 = w$, extra bottom or top visits may be created (add $|k_1 - k_2|$ edges first vertically to height k_2 and then add the remaining $w+1-|k_1-k_2|$ edges horizontally until exactly $w+1$ edges have been added). This shows that $c_n^{\dagger}(w; h, k_1; v_b, v_t) \leqslant c_{n+w+1}^{\dagger}\big(w; h, k_2; v_b + (w+2-k_1)\delta_{k_2,0}, v_t + (k_1+2)\delta_{k_2,w}\big)$.

Define $a_{\max} = \max\{1, a^{-1}\}$ and $b_{\max} = \max\{1, b^{-1}\}$. Multiply the last inequality by $a^{v_b} b^{v_t}$ and sum over v_b and v_t. This shows in terms of partition functions that

$$g_n^\dagger(w; h, k_1; a, b) \leqslant a_{\max}^{(w+2-k_1)\delta_{k_2,0}} b_{\max}^{(k_1+2)\delta_{k_2,w}} g_{n+w+1}^\dagger(w; h, k_2; a, b). \tag{18}$$

There is a most popular value of k, say k^*, such that $g_n^\dagger(w; 0, k; a, b) \leqslant g_n^\dagger(w; 0, k^*; a, b)$ for all k. In view of the last inequality (take $h = 0$ and $k_2 = 0$), this means for example that

$$g_{n-w-1}^\dagger(w; 0, 0; a, b) \leqslant g_{n-w-1}^\dagger(w; 0, k^*; a, b) \leqslant a_{\max}^{(w+2-k^*)} b_{\max}^{k^*+2} g_n^\dagger(w; 0, 0; a, b). \tag{19}$$

Take logarithms, divide by n and let $n \to \infty$ to see from equation (16) that

$$\kappa_w(a, b) = \lim_{n\to\infty} \frac{1}{n} \log g_n^\dagger(w; 0, k^*; a, b) \tag{20}$$

where k^* is the most popular value of k in $g_n^\dagger(w; 0, k; a, b)$. Similarly,

$$\kappa_w(a, b) = \lim_{n\to\infty} \frac{1}{n} \log g_n^\dagger(w; h^*, 0; a, b) \tag{21}$$

where h^* is the most popular value of h in $g_n^\dagger(w; h, 0)$. Since

$$g_n^\dagger(w; 0, k^*; a, b) \leqslant a_{\max}^{(w+2-k^*)\delta_{k,0}} b_{\max}^{(k^*+2)\delta_{k,w}} g_{n+w+1}^\dagger(w; 0, k; a, b),$$

by equation (18), and $g_n^\dagger(w; 0, k; a, b) \leqslant g_n^\dagger(w; 0, k^*; a, b)$, it follows that for every $k \in [0, w]$,

$$\kappa_w(a, b) = \lim_{n\to\infty} \frac{1}{n} \log g_n^\dagger(w; 0, k; a, b). \tag{22}$$

A similar argument shows that

$$\kappa_w(a, b) = \lim_{n\to\infty} \frac{1}{n} \log g_n^\dagger(w; h, k; a, b), \tag{23}$$

for any h and k in $[0, w]$.

Next, observe that by equation (18),

$$\begin{aligned} g_n^\dagger(w; h, k; a, b) &\leqslant \sum_k g_n^\dagger(w; h, k; a, b) \\ &\leqslant \sum_{h,k} g_n^\dagger(w; h, k; a, b) \\ &\leqslant (w+1)^2 g_n^\dagger(w; h^*, k^*; a, b) \\ &\leqslant (w+1)^2 a_{\max}^{(w+2-k)} g_{n+w+1}^\dagger(w; h^*, 0; a, b). \end{aligned} \tag{24}$$

Then by equation (21)

$$\begin{aligned} \kappa_w(a, b) &= \lim_{n\to\infty} \frac{1}{n} \log \sum_k g_n^\dagger(w; h, k; a, b) \\ &= \lim_{n\to\infty} \frac{1}{n} \log \sum_{h,k} g_n^\dagger(w; h, k; a, b). \end{aligned} \tag{25}$$

A similar argument (sum over h in the first inequality in equation (24) instead) shows that

$$\begin{aligned} \kappa_w(a, b) &= \lim_{n\to\infty} \frac{1}{n} \log \sum_h g_n^\dagger(w; h, k; a, b) \\ &= \lim_{n\to\infty} \frac{1}{n} \log \sum_{h,k} g_n^\dagger(w; h, k; a, b). \end{aligned} \tag{26}$$

Finally, since

$$\sum_k c_n^\dagger(w; 0, k; v_b, v_t) \leqslant C_n^\dagger(w; v_b, v_t) \leqslant 2\sum_k c_n^\dagger(w; 0, k; v_b, v_t), \tag{27}$$

it follows after multiplication by $a^{v_b} b^{v_t}$ and summation over v_b and v_t that

$$\kappa_w(a, b) = \lim_{n\to\infty} \frac{1}{n} \log G_n^\dagger(w; a, b). \tag{28}$$

This proves the lemma. □

A corollary to this lemma is as follows:

Corollary 4.6. *For $a > 0$ and $b > 0$, the limiting free energy of w-walks is defined by*

$$\begin{aligned}\kappa_w(a, b) &= \lim_{n\to\infty} \frac{1}{n} \log g_n^\dagger(w; h, k; a, b)\\ &= \lim_{n\to\infty} \frac{1}{n} \log \sum_k g_n^\dagger(w; h, k; a, b)\\ &= \lim_{n\to\infty} \frac{1}{n} \log \sum_{h,k} g_n^\dagger(w; h, k; a, b)\\ &= \lim_{n\to\infty} \frac{1}{n} \log G_n^\dagger(w; a, b)\end{aligned}$$

and these limits exist for all $w \geqslant 0$, and for any integer heights h and k in $[0, w]$.

The relationships between unfolded walks in $\mathbb{L}_w$ and walks in $\mathbb{L}_w$ are given in lemmas 4.3 and 4.4. Together with lemma 4.5, these results prove existence of $\kappa_w(a, b)$.

Corollary 4.7. *For $a > 0$ and $b > 0$, the limiting free energy of self-avoiding walks in $\mathbb{L}_w$ is defined by*

$$\kappa_w(a, b) = \lim_{n\to\infty} \frac{1}{n} \log G_n(w; a, b) \tag{29}$$

where $w \geqslant 0$ is the thickness of the slab, and where a is conjugate to the number of bottom visits and b is conjugate to the number of top visits of the walks in the bounding planes of the slab.

Furthermore, $\kappa_w(a, b)$ is also given by

$$\begin{aligned}\kappa_w(a, b) &= \lim_{n\to\infty} \frac{1}{n} \log g_n(w; h, k; a, b)\\ &= \lim_{n\to\infty} \frac{1}{n} \log \sum_k g_n(w; h, k; a, b)\\ &= \lim_{n\to\infty} \frac{1}{n} \log \sum_{h,k} g_n(w; h, k; a, b),\end{aligned}$$

and these limits exist for all $w \geqslant 0$, and for any integer heights h and k in $[0, w]$.

Lastly, if $w = 0$ and $d = 2$, then $\kappa_w(a, b) = \log(ab)$ (each visit is now weighted by ab). If $w > 0$ or $d > 2$, then $\kappa_w(a, b) > -\infty$.

Proof. Consider the first inequality in lemma 4.4. Take logarithms, divide by n and take the limsup of the left-hand side by taking $n \to \infty$. Since $\gamma > 0$ is a constant, it follows that

$$\limsup_{n\to\infty} \frac{1}{n} \log g_n(w; h, k; a, b) \leqslant \lim_{n\to\infty} \frac{1}{n} \log g_n^\dagger(w; h, k; a, b).$$

One may instead take the liminf of the second part of this inequality to obtain

$$\lim_{n\to\infty} \frac{1}{n} \log g_n^\dagger(w; h, k; a, b) \leqslant \liminf_{n\to\infty} \frac{1}{n} \log g_n(w; h, k; a, b).$$

Thus, the limit is shown to exist and is equal to $\kappa_w(a, b)$ as in lemma 4.5.

By considering the second and third inequalities in lemma 4.4, the limits

$$\lim_{n\to\infty} \frac{1}{n} \log \sum_k g_n(w; h, k; a, b) = \lim_{n\to\infty} \frac{1}{n} \log \sum_{h,k} g_n(w; h, k; a, b) = \kappa_w(a, b)$$

are similarly shown to exist.

Lastly, note that $g_n(w; 0, 0; a, b) \leqslant G_n(w; a, b) \leqslant 2 \sum_k g_n(w; 0, k; a, b)$. Thus,

$$\lim_{n\to\infty} \frac{1}{n} \log G_n(w; a, b) = \kappa_w(a, b)$$

by the squeeze theorem for limits.

Finally, if $w = 0$ and $d = 2$, then there are only two possible walks of length $n > 0$ from the origin. Since the slab has zero width, $G_n(0; a, b) = 2(ab)^n$, and so $\kappa_w(a, b) = \log(ab)$. On the other hand, if $w > 0$ and $d = 2$, then we obtain a lower bound on $G_n(w; a, b)$ by noting that a self-avoiding walk in a slab of width $w > 0$ can be constructed by stepping East on even numbered steps, and North or East, or South or East, alternating on odd numbered steps, starting from the origin. Thus, $G_n(1; a, b) \geqslant c^n 2^{\lfloor n/2 \rfloor}$, where $c = \min\{1, a, b\}$. This is also a lower bound if $w = 0$ and $d > 2$ if $c = ab$. Hence, $\kappa_w(a, b) > -\infty$, if $a > 0$ and $b > 0$.

This completes the proof. □

5. A pattern theorem for walks in a slab

In this section, we prove a pattern theorem for w-walks in a slab of width w. We use a method originally due to Hammersley [9] which relies on generating functions of various classes of w-walks. We assume that the activities a and b are both non-zero, and we are in particular interested in the generating function

$$G_w(t; a, b) = \sum_{n=0}^{\infty} G_n(w; a, b) t^n. \tag{30}$$

We first prove that the radius of convergence of this generating function is $e^{-\kappa_w(a,b)}$ and that $G_w(t; a, b)$ is divergent as $t \nearrow e^{-\kappa_w(a,b)}$.

5.1. Generating functions

Define the partition function of walks in a slab of width w by

$$U_n(w; a, b) = \sum_{h,k} g_n(w; h, k; a, b) \tag{31}$$

where $g_n(w; h, k; a, b) = \sum_{v_b, v_t} c_n(w; h, k; v_b, v_t) a^{v_b} b^{v_t}$.

Introduce the generating variable t of edges in the walks, and define the generating function

$$g_w(t; a, b) = \sum_{n=0}^{\infty} U_n(w; a, b) t^n. \tag{32}$$

Translate two walks in the slab of width w of lengths n and m so that the first vertex of the second walk is one lattice step away from the last vertex of the first walk in the X-direction.

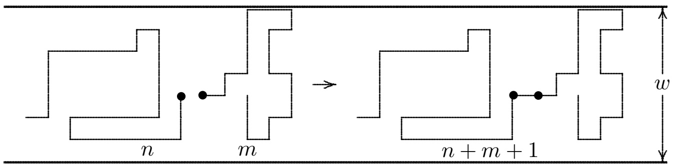

Figure 7. Concatenating two w-walks by the addition of a single edge. Every w-walk of length $n+m+1$ in the slab can be obtained by concatenating a w-walk of length n and a w-walk of length m. In some cases, the concatenation may not be possible. In that case the concatenation is not completed and the resulting object is not a w-walk. Observe that the numbers of bottom and top visits add under this construction.

These walks can be concatenated as illustrated in figure 7 by adding a single edge between the last vertex of the first walk and the first vertex of the second walk.

The resulting walk has length $n + m + 1$ and could be confined in the slab (or not). We note that every w-walk of length $n+m+1$ can be obtained in this way (to see this: consider a walk in a slab of length $n+m+1$ and cut it into two walks by deleting its $(n+1)$th edge—the resulting subwalks are self-avoiding walks in the slab of lengths n and m).

Since the paths counted by $\sum_{h,k} c_n(w; h, k; v_b, v_t)$ are oriented from their lexicographic first endpoint to their lexicographic last endpoint, this construction, which we illustrate in figure 7, shows that

$$\sum_{w_b,w_t}\left[\sum_{h,k} c_{n-1}(w; h, k; v_b - w_b, v_t - w_t)\sum_{h,k} c_{m-1}(w; h, k; w_b, w_t)\right]$$
$$\geqslant \sum_{h,k} c_{n+m-1}(w; h, k; v_b, v_t). \tag{33}$$

Observe that the numbers of bottom and top visits are additive in this construction, since none are created or destroyed by the addition of the new edge. Multiply this inequality by $a^{v_b}b^{v_t}$ and sum over v_b and v_t to see that

$$U_{n-1}(w; a, b)U_{m-1}(w; a, b) \geqslant U_{n+m-1}(w; a, b). \tag{34}$$

Define $W_n = U_{n-1}(w; a, b)$, then the last inequality may be expressed in terms of W_n as $W_n W_m \geqslant W_{n+m}$. In other words, $W_n = U_{n-1}(w; a, b)$ is a submultiplicative function on positive integers. By corollary 4.7, this gives the following lemma.

Lemma 5.1. *Suppose that* $a, b > 0$. *The limit*

$$\lim_{n\to\infty}[U_{n-1}(w; a, b)]^{1/n} = \mathrm{e}^{\kappa_w(a,b)} = \inf_{n>0}[U_{n-1}(w; a, b)]^{1/n}$$

exists and, moreover,

$$U_{n-1}(w; a, b) \geqslant \mathrm{e}^{n\kappa_w(a,b)} \qquad \textit{for} \quad n > 0.$$

Thus, by multiplying the last inequality by t^{n-1} *and summing* $n = 1, 2, 3, \ldots$, *one obtains*

$$g_w(t; a, b) \geqslant \frac{\mathrm{e}^{\kappa_w(a,b)}}{1 - t\,\mathrm{e}^{\kappa_w(a,b)}},$$

and $g_w(t; a, b) \to \infty$ *as* $t \to \mathrm{e}^{-\kappa_w(a,b)}$.

Proof. This lemma is an immediate result of the submultiplicative property of $W_n = U_{n-1}(w; a, b)$ in equation (34). The theorem then follows from a standard theorem on

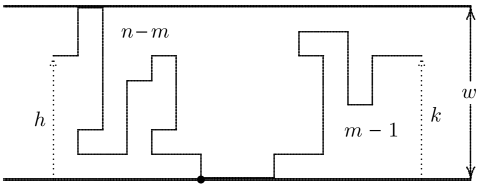

Figure 8. A w-walk with root at its lexicographic first bottom visit.

submultiplicative functions, see for example [10]. The radius of convergence of $g_w(t; a, b)$ is $e^{-\kappa_w(a,b)}$, and since $\kappa_w(a, b) > -\infty$ is finite (see corollary 4.7), we conclude that $g_w(t; a, b)$ is divergent at its radius of convergence. □

5.2. Divergent generating functions

We continue the discussion by considering walks in a w-slab with at least one visit in the bottom bounding plane and rooted at their lexicographic first visit in this plane (see figure 8). Define $c_n^\ddagger(w; h, k; v_b, v_t)$ to be the number of walks with (1) at least one vertex in the bottom bounding plane and (2) rooted at their lexicographic first bottom visit and (3) of length n and with endpoints at heights h and k, respectively. Define the partition function

$$V_n^\ddagger(w; a, b) = \sum_{v_b, v_t} \left[\sum_{h,k} c_n^\ddagger(w; h, k; v_b, v_t) \right] a^{v_b} b^{v_t}. \tag{35}$$

The generating function of this class of walks is

$$g_w^\ddagger(t; a, b) = \sum_{n=0}^{\infty} V_n^\ddagger(w; a, b) t^n. \tag{36}$$

The following lemma relates $g_w(t; a, b)$ and $g_w^\ddagger(t; a, b)$.

Lemma 5.2. *The radius of convergence of* $g_w^\ddagger(t; a, b)$ *is* $e^{-\kappa_w(a,b)}$, *and* $g_w^\ddagger(t; a, b) \to \infty$ *as* $t \to e^{-\kappa_w(a,b)}$ *for all* $a, b > 0$.

Proof. Suppose that $d = 2$. If $w = 0$, then $c_n^\ddagger(w; 0, 0; n-1, n) = 1$, and $g_w^\ddagger(t; a, b) = b/(1 - tab)$ so that $g_w^\ddagger(t; a, b)$ is divergent as $t \nearrow (ab)^{-1}$.

Consider $d > 2$ and $w = 0$ next. Clearly $c_n^\ddagger(w; 0, 0; n, n+1) = c_n(w; 0, 0; n, n+1)$ so that $g_w^\ddagger(t; a, b) = g_w(t; a, b)$, and by lemma 5.1, $g_w^\ddagger(t; a, b) \to \infty$ as $t \to e^{-\kappa_w(a,b)}$.

Finally, let $d \geqslant 2$ and $w > 0$. Then $c_n^\ddagger(w; h, k; v_b, v_t) \leqslant c_n(w; h, k; v_b, v_t)$. Thus, $V_n^\ddagger(w; a, b) \leqslant U_n(w; a, b)$, so that the inequality $g_w^\ddagger(t; a, b) \leqslant g_w(t; a, b)$ is immediate.

Next consider walks counted by $c_n(w; h, k; v_b, v_t)$. If $v_b > 0$, then these can be rooted at their lexicographic first bottom visit to obtain

$$c_n(w; h, k; v_b, v_t) \leqslant c_n^\ddagger(w; h, k; v_b, v_t) \qquad \text{if} \quad v_b > 0.$$

Otherwise, $v_b = 0$, and we continue as illustrated in figure 9. This shows that

$$c_n(w; h, k; 0, v_t) \leqslant w c_{n+2w}^\ddagger(w; h, k; 2, v_t),$$

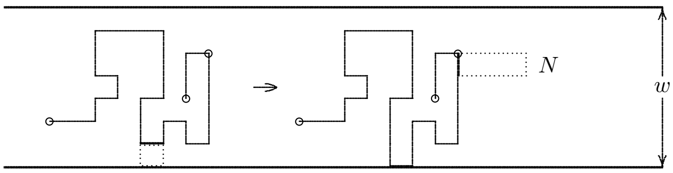

Figure 9. A w-walk which is not rooted in its bottom hyperplane can be rooted by finding the lexicographic first edge in the set of edges with minimum height. By adding at most $2w$ edges in a U-configuration to this edge, two visits are created in the bottom hyperplane. The lexicographic first visit in this hyperplane is fixed as the root and placed at the origin. To make sure that exactly $2w$ edges are added, more edges are added in the X-direction on the edge incident at the lexicographic last vertex (marked by a $\diamond$) in a U-shape. Alternatively, if possible, these edges may be added in the X-direction on the last vertex of the walk. We may arrange matters such that exactly $2w$ edges are added. If the walk had length n, then it has length $n+2w$ after the construction, and it is now rooted. This construction may turn at most w-walks into the same rooted w-walk.

so that the last two inequalities can be combined to obtain

$$\sum_{v_b,v_t} c_n(w;h,k;v_b,v_t)a^{v_b}b^{v_t} \leqslant \sum_{v_b,v_t} c_n^{\ddagger}(w;h,k;v_b,v_t)a^{v_b}b^{v_t} + \max\{1, wa^{-2}\} \sum_{v_b,v_t} c_{n+2w}^{\ddagger}(w;h,k;v_b,v_t)a^{v_b}b^{v_t}.$$

In other words, by summing over h and k as well,

$$V_n^{\ddagger}(w;a,b) \leqslant U_n(w;a,b) \leqslant V_n^{\ddagger}(w;a,b) + \max\{1, wa^{-2}\} V_{n+2w}^{\ddagger}(w;a,b).$$

Multiplying by t^n and summing over n then gives

$$g_w^{\ddagger}(t;a,b) \leqslant g_w(t;a,b) \leqslant g_w^{\ddagger}(t;a,b) + \max\{1, wa^{-2}\} t^{-2w} g_w^{\ddagger}(t;a,b).$$

Thus, by lemma 5.1 the radius of convergence of $g_w^{\ddagger}(t;a,b)$ is $\mathrm{e}^{-\kappa_w(a,b)}$, and since $g_w(t;a,b) \to \infty$ as $t \to \mathrm{e}^{-\kappa_w(a,b)}$, it follows that $g_w^{\ddagger}(t;a,b) \to \infty$ as $t \to \mathrm{e}^{-\kappa_w(a,b)}$. □

Next, we prove that the generating function $G_w(t;a,b)$ of w-walks from the origin also diverges as $t \to \mathrm{e}^{-\kappa_w(a,b)}$. There are $C_n(w;v_b,v_t)$ walks from the origin in $\mathbb{L}_w$ with v_b bottom visits and v_t top visits. We have defined the partition function

$$G_n(w;a,b) = \sum_{v_b,v_t} C_n(w;v_b,v_t)a^{v_b}b^{v_t}. \tag{37}$$

Let the generating function be

$$G_w(t;a,b) = \sum_{n=0}^{\infty} G_n(w;a,b)t^n. \tag{38}$$

By using the results of lemma 5.2, one may prove lemma 5.3.

Lemma 5.3. *The radius of convergence of $G_w(t;a,b)$ is $\mathrm{e}^{-\kappa_w(a,b)}$ and, moreover, $G_w(t;a,b) \to \infty$ as $t \to \mathrm{e}^{-\kappa_w(a,b)}$.*

Proof. Each w-walk counted by $c_n^{\ddagger}(w;h,k;v_b,v_t)$ is rooted at a visit in the bottom bounding plane. By cutting such w-walks in their roots into two subwalks, two w-walks from the origin are obtained, one of length (say) ℓ and the other of length $n-\ell$. This shows that

$$\sum_{h,k} c_n^{\ddagger}(w;h,k;v_b,v_t) \leqslant \sum_{\ell=0}^{n} \sum_{w_b,w_t} \left[\sum_{h,k} c_\ell(w;h,k;v_b-w_b,v_t-w_t) \right] \times \left[\sum_{h,k} c_{n-\ell}(w;h,k;w_b,w_t) \right].$$

Multiply this by $a^{v_b}b^{v_t}$ and sum over v_b and v_t to obtain

$$V_n^{\ddagger}(w;a,b) \leqslant \sum_{\ell=0}^{n} G_\ell(w;a,b)G_{n-\ell}(w;a,b).$$

Multiply this by t^n and sum over n to obtain

$$g_w^{\ddagger}(t;a,b) \leqslant [G_w(t;a,b)]^2. \tag{39}$$

On the other hand, each w-walk counted by $c_n(w;h,k;v_b,v_t)$ is also counted by $c_n^{\ddagger}(w;h,k;v_b,v_t)$; to see this, move the root from the first vertex of the walks counted by $c_n(w;h,k;v_b,v_t)$ at the origin to the lexicographic first visit of the w-walk in the bottom bounding plane. Thus, $aG_n(w;a,b) \leqslant V_n^{\ddagger}(w;a,b)$ (the extra factor of a compensates for the fact that the first vertex at the origin is not weighted by a in $G_n(t;a,b)$). Multiply now by t^n and sum over n to see that

$$aG_w(t;a,b) \leqslant g_w^{\ddagger}(t;a,b). \tag{40}$$

By lemma 5.2 the radius of convergence of $g_w^{\ddagger}(t;a,b)$ is $e^{-\kappa_w(a,b)}$, and $g_w^{\ddagger}(t;a,b) \to \infty$ as $t \to e^{-\kappa_w(a,b)}$. The inequalities in equation (39) and (40) complete the proof. □

Lemma 5.3 is a key ingredient in the proof of a pattern theorem for w-walks. It gives the radius of convergence of $G_w(t;a,b)$ in terms of $\kappa_w(a,b)$ and, more importantly, states that $G_w(t;a,b)$ is divergent at its radius of convergence.

5.3. l-Walks, fl-walks and more

In the previous sections we considered generating functions of various classes of w-walks. The radius of convergence of these models in every case is $e^{-\kappa_w(a,b)}$, and we showed in lemma 5.3 that the generating function $G_w(t;a,b)$ is divergent at $t = e^{-\kappa_w(a,b)}$. This result will be important in proving a pattern theorem for w-walks in a slab $\mathbb{L}_w$ interacting with the top and bottom bounding planes.

We proceed by dissecting w-walks into l and into fl-walks, and then by relating their generating functions with $G_w(t;a,b)$.

A w-walk in $\mathbb{L}_w$ is an l-walk if one endpoint is also its lexicographic last vertex (or *top vertex*). There are two kinds of l-walks. Firstly, there are l-walks which step from the origin (these are *fixed* l-walks). These walks form a subset amongst the walks counted by $\sum_k C_n(w;k;v_b,v_t)$. Secondly, there are l-walks which are not rooted in the bounding planes of the w-slab, but which are equivalent under translations parallel to the bounding planes. These are *unrooted* l-walks, and they form a subset in the walks counted by $\sum_{h,k} c_n(w;h,k;v_b,v_t)$. In figure 10 examples are given of fixed and unrooted l-walks.

An fl-walk in a w-slab is a walk whose endpoints are also its lexicographic first and last vertices. fl-Walks are equivalent under translations parallel to the bounding planes of the w-slab. In figure 11 examples of fl-walks are given. If the first vertex of an fl-walk has coordinates $(x_f, y_f, \ldots, z_f)$, and if its last vertex has coordinates $(x_l, y_l, \ldots, z_l)$, then the

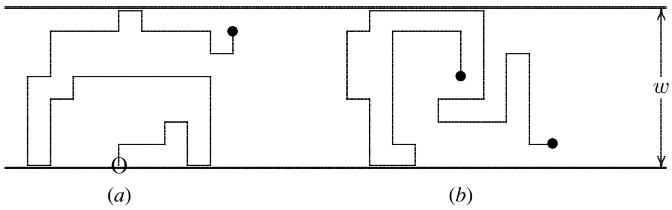

Figure 10. (*a*) A fixed *l*-walk from the origin and with final vertex also its lexicographic last vertex. (*b*) An unrooted *l*-walk. Unrooted *l*-walks are equivalent under translations parallel to the bounding planes of the w-slab.

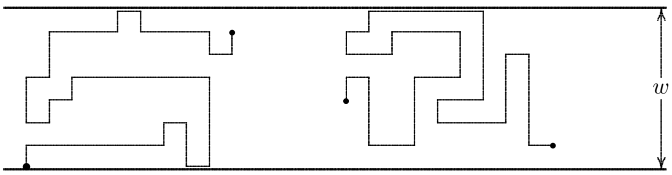

Figure 11. fl-Walks are walks in a w-slab with endpoints their lexicographic first and last vertices. These walks are equivalent under translations parallel to the bounding planes of the w-slab. If the first vertex of an fl-walk has coordinates $(x_f, y_f, \ldots, z_f)$, and if its last vertex has coordinates $(x_l, y_l, \ldots, z_l)$, then the *range* of the fl-walk is $(x_l - x_f, y_l - y_f, \ldots, z_l - z_f)$. fl-Walks can be partially ordered by the lexicographic increasing ordering of their ranges.

range of the fl-walk is the vector $(x_l - x_f, y_l - y_f, \ldots, z_l - z_f)$. fl-Walks can be ordered by the lexicographic increasing ordering of their ranges.

Suppose that the number of fixed *l*-walks of length n and with v_b bottom visits and v_t top visits in a w-slab is $\ell_n^w(v_b, v_t)$. Define the partition function

$$\ell_n^w(a, b) = \sum_{v_b, v_t} \ell_n^w(v_b, v_t) a^{v_b} b^{v_t}. \tag{41}$$

Similarly, define the number of unrooted *l*-walks in a w-slab by $u_n^w(v_b, v_t)$ and the number of fl-walks in a w-slab by $v_n^w(v_b, v_t)$. Define the corresponding partition functions

$$u_n^w(a, b) = \sum_{v_b, v_t} u_n^w(v_b, v_t) a^{v_b} b^{v_t}, \qquad v_n^w(a, b) = \sum_{v_b, v_t} v_n^w(v_b, v_t) a^{v_b} b^{v_t}. \tag{42}$$

Define the generating functions of these classes of walks:

$$L_w(t; a, b) = \sum_{n=0}^{\infty} \ell_n^w(a, b) t^n, \qquad U_w(t; a, b) = \sum_{n=0}^{\infty} u_n^w(a, b) t^n,$$

$$V_w(t; a, b) = \sum_{n=0}^{\infty} v_n^w(a, b) t^n.$$

A (fixed or unrooted) *l*-walk can be decomposed into a set of fl-walks of lexicographic decreasing ranges. The construction is illustrated in figure 12 for a fixed *l*-walk. In other words, given a set of fl-walks, one may order them with respect to lexicographic decreasing ranges, and then in alternating order identify their bottom and top vertices to create an *l*-walk. Every *l*-walk can be created in this way. In terms of generating functions,

$$L_w(t; a, b) \leqslant 1 + V_w(t; a, b) + \frac{1}{2!}[V_w(t; a, b)]^2 + \cdots + \frac{1}{N!}[V_w(t; a, b)]^N + \cdots = \mathrm{e}^{V_w(t;a,b)}, \tag{43}$$

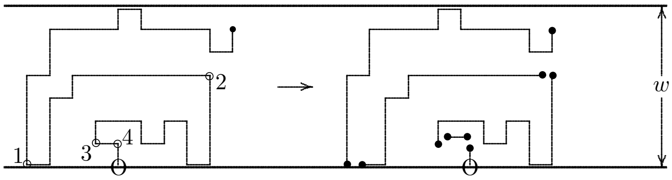

Figure 12. If an l-walk is cut at its lexicographic first vertex (marked by 1), then an fl-walk is peeled off. The remaining walk ends in its lexicographic first vertex, and it may be cut at its lexicographic last vertex (marked by 2) to peel off another fl-walk (now of lexicographic smaller range than the first), and to leave a l-walk. This process may be continued by repeated cutting of the remaining walk at its lexicographic first vertex (3) and the lexicographic last vertex (4), peeling off fl-walks of lexicographic decreasing ranges after each cut. This process ends when an fl-walk remains and the next cut would be in the endpoint of the walk.

where the factors $1/N!$ are inserted to account for the fact that only one ordering of the fl-walks in lexicographic decreasing ranges will produce an rooted l-walk. Similarly,

$$U_w(t; a, b) \leqslant \mathrm{e}^{V_w(t;a,b)}. \tag{44}$$

Lemma 5.4. *The radius of convergence of $V_w(t; a, b)$, $U_w(t; a, b)$ and $L_w(t; a, b)$ is $\mathrm{e}^{-\kappa_w(a,b)}$. Moreover, $V_w(t; a, b) \to \infty$, $U_w(t; a, b) \to \infty$ and $L_w(t; a, b) \to \infty$ as $t \to \mathrm{e}^{-\kappa_w(a,b)}$.*

Proof. Each w-walk from the origin can be cut at its top vertex into a fixed l-walk and an unrooted l-walk. Thus,

$$G_w(t; a, b) \leqslant L_w(t; a, b)U_w(t; a, b) \leqslant \mathrm{e}^{2V_w(t;a,b)}. \tag{45}$$

On the other hand, by adding at most w edges on the bottom vertex of each fl-walk, the walk can be rooted at the origin. Thus,

$$V_w(t; a, b) \leqslant (w + 1) \max\{a, t, t^2, \ldots, t^w\}G_w(t; a, b). \tag{46}$$

By equations (45) and (46), $V_w(t; a, b)$ has the same radius of convergence as $G_w(t; a, b)$, and $V_w(t; a, b) \to \infty$ as $t \to \mathrm{e}^{-\kappa_w(a,b)}$.

Finally, observe that $V_w(t; a, b) \leqslant U_w(t; a, b) \leqslant \mathrm{e}^{V_w(t;a,b)}$ and that $V_w(t; a, b) \leqslant L_w(t; a, b) \leqslant \mathrm{e}^{V_w(t;a,b)}$. Thus, $L_w(t; a, b)$ has the same radius of convergence as $V_w(t; a, b)$, and $L_w(t; a, b) \to \infty$ as $\to \mathrm{e}^{-\kappa_w(a,b)}$.

This proves the lemma. □

Any fl-walk can be turned into an unfolded walk by adding one edge to its lexicographic endpoint. In other words, if $G^\dagger_w(t; a, b) = \sum_{n=0}^{\infty} G^\dagger_n(w; a, b)$ is the generating function of unfolded w-walks from the origin, then $V_w(t; a, b) \leqslant [(1 + 1/a + 1/b)/t]G^\dagger_w(t; a, b)$. But every unfolded w-walk of length n is also an fl-walk. Thus, $G^\dagger_w(t; a, b) \leqslant V_w(t; a, b)$.

Thus, the corollary to lemma 5.4 is

Corollary 5.5. *The radius of convergence of $G^\dagger_w(t; a, b)$ is $\mathrm{e}^{-\kappa_w(a,b)}$. Moreover, $G^\dagger_w(t; a, b) \to \infty$ as $t \to \mathrm{e}^{-\kappa_w(a,b)}$.*

5.4. Patterns in w-walks

A *pattern* is any finite self-avoiding walk. A w-*pattern* is any finite w-walk. A w-pattern P *occurs* in a w-walk W if P can be translated parallel to the bounding planes of the slab to coincide with a subwalk of W.

A w-pattern is a *Kesten* w-pattern if it can occur three times independently in a w-walk (that is, if the three incidences of the pattern are disjoint). Kesten w-patterns have the property that there exist w-walks along which they can occur any number of times.

Theorem 5.6. *Any Kesten w-pattern can occur an arbitrary number of times along a w-walk.*

The proof of this theorem is virtually identical for the case of self-avoiding walks. See for example theorem 5.10 in [12], which has been adapted from [8]. The definition of Kesten w-patterns implies that any Kesten w-pattern can occur in an fl-walk.

Theorem 5.7. *Let P be a Kesten w-pattern. Then there is an fl-walk in which P occurs.*

Proof. Let P_1, P_2 and P_3 be three occurrences of a Kesten w-pattern in a w-walk. Let B be the smallest rectangular box containing P_2. Orient the walk and let ∂B be the boundary of B. There is a last vertex $v_1 \in \partial B$ before P_2 occurs in the w-walk, and a first vertex $v_2 \in \partial B$ after P_2 occurs in the walk. The part of the walk from v_1 to v_2 contains P_2 and has no vertices outside B. Since there were three occurrences of the pattern, deleting the parts of the w-walk preceding v_1 and following v_2 will destroy at most two copies of the pattern and will leave P_2 intact.

In three and more dimensions edges can be added to v_1 and v_2 outside B to create an fl-walk containing P_2.

In two dimensions, the situation is slightly more complicated. If the (vertical) height of B is less than w, then edges can be added as before to create an fl-walk. If the height of B is equal to w, then v_1 and v_2 are either on opposing sides of B or on the same side of B. If these vertices are on opposing sides, then edges can be added to create an fl-walk.

If v_1 and v_2 are on the same side, then one may suppose both are on the right-hand side of B. Since the height of B is equal to w, there is no path from either v_1 or v_2 to vertices to the left of B. Hence, P_1 and P_3 occur to the right of P_2. Since P_1 and P_3 are occurrences of the same pattern as P_2, it is possible to translate P_2 to coincide with P_1, and there is a self-avoiding path from v_1 or from v_2 to P_1. Let this path be from v_1. Since the height of P_1 is also w, this path enters the smallest box containing P_1 from the left. If there is a path from the smallest box containing P_1 on the right, then P_1 can be turned into an fl-walk containing the w-pattern. Otherwise, a path must exit the smallest box containing P_1 from the left. This implies that P_3 must be located between P_1 and P_2. But this is not possible, since the height of P_3 is w, and it will intersect any path from P_1 and P_2. $\square$

This corollary implies in particular that Kesten w-patterns can occur in unfolded w-walks with endpoints in the bottom bounding plane of the slab.

Corollary 5.8. *Let P be a Kesten w-pattern. Then there is an unfolded walk with both endpoints of height zero in which P occurs at least once.*

Proof. By theorem 5.7 there is an fl-walk containing P at least once. Add two edges on the endpoints of this walk in the X-direction and $-X$-direction, and then at most $2w$ edges in the $-Z$-direction to create a walk with endpoints in the bottom bounding plane of the slab. Add a last edge in the X-direction to turn this walk into an unfolded w-walk with endpoints in the bottom bounding plane. $\square$

This last corollary gives us the following definitions.

Definition 5.9. *A Kesten w-pattern is a fundamental pattern if it is an unfolded w-walk with endpoints in the bottom bounding plane.*

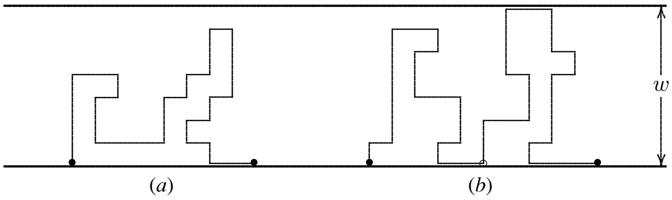

Figure 13. (a) A prime fundamental pattern. (b) A decomposable fundamental pattern which can be cut in ○ into two prime fundamental patterns.

Any Kesten w-pattern can occur as a subwalk in a fundamental pattern.

Definition 5.10. *A fundamental pattern is decomposable if it can be cut at a vertex in the bottom bounding plane into two fundamental patterns. A fundamental pattern is prime if it is not decomposable.*

Examples of fundamental patterns are given in figure 13.

The number of fundamental patterns of length n with v_b bottom visits and v_t top visits is $c_n^\dagger(w; 0, 0; v_b, v_t)$ (the number of unfolded walks with both endpoints of height zero). Let there be $p_n(w; v_b, v_t)$ prime fundamental patterns of length n and with v_b bottom visits and v_t top visits. Each fundamental pattern is prime or is composed of a prime fundamental pattern followed by a fundamental pattern. In other words, the number of fundamental patterns of length n satisfies the renewal equation

$$c_n^\dagger(w; 0, 0; v_b, v_t) = p_n(w; v_b, v_t) + \sum_{m=1}^{n-1} \sum_{u_b, u_t} p_m(w; u_b, u_t) c_{n-m}^\dagger(w; 0, 0, v_b - u_b, v_t - u_t). \tag{47}$$

In terms of partition functions (multiply by $a^{v_b} b^{v_t}$ and sum over v_b and v_t), this becomes

$$g_n^\dagger(w; 0, 0; a, b) = p_n(w; a, b) + \sum_{m=1}^{n-1} p_m(w; a, b) g_{n-m}^\dagger(w; 0, 0; a, b), \tag{48}$$

where $p_n(w; a, b) = \sum_{v_b, v_t} p_n(w; v_b, v_t) a^{v_b} b^{v_t}$. In terms of generating functions, this becomes

$$G_w^\star(t; a, b) = \frac{P_w(t; a, b)}{1 - P_w(t; a, b)}, \tag{49}$$

where $P_w(t; a, b) = \sum_{n=0}^{\infty} p_n(w; a, b) t^n$ is the generating function of prime fundamental patterns and $G_w^\star(t; a, b) = \sum_{n=0}^{\infty} g_n^\dagger(w; 0, 0; a, b) t^n$ is the generating function of fundamental patterns.

By lemma 4.5, corollary 5.5 and the last equation, we get the following theorem.

Theorem 5.11. *The radius of convergence of $G_w(t; a, b)$ and $G_w^\star(t; a, b)$ is $t = \mathrm{e}^{-\kappa_w(a,b)}$. In addition, $G_w(t; a, b)$ and $G_w^\star(t; a, b)$ are divergent as $t \to \mathrm{e}^{-\kappa_w(a,b)}$. Moreover, if $P_w(t; a, b)$ is the generating function of prime fundamental patterns, then $P(\mathrm{e}^{-\kappa_w(a,b)}; a, b) = 1$.*

Let P be any particular prime fundamental pattern, and consider models of w-walks in $\mathbb{L}_w$ in which P never occurs. Let $\sum_k C_n(w; k; v_b, v_t; \bar{P})$ be the number of such w-walks from the origin in $\mathbb{L}_w$ with v_b and v_t bottom and top vertices, and with endpoint at height k. Let $G_w(t; a, b; \bar{P})$ be the generating function of these paths. Similarly, we define $G_w^\star(t; a, b; \bar{P})$

to be the generating function of unfolded w-walks with both endpoints in the bottom bounding plane, and in which the fundamental pattern P never occurs. Observe that the existence of the limits

$$\begin{aligned} \lim_{n\to\infty} \frac{1}{n} \log \sum_k C_n(w; k; a, b; \bar{P}) &= \kappa_w(a, b; \bar{P}), \\ \lim_{n\to\infty} \frac{1}{n} \log \sum_k C_n^{\dagger}(w; k; a, b; \bar{P}) &= \kappa_w(a, b; \bar{P}), \end{aligned} \tag{50}$$

and other limits equal to $\kappa_w(a, b; \bar{P})$ may be demonstrated using virtually the same arguments as in section 4.1, as long as P is a prime fundamental pattern.

By examining this model as before, and by using the same set of arguments as above, one may similarly prove that an analogous theorem 5.11 also holds in this model.

Theorem 5.12. *The radius of convergence of $G_w(t; a, b; \bar{P})$ and $G_w^{\star}(t; a, b; \bar{P})$ is $t = \mathrm{e}^{-\kappa_w(a,b;\bar{P})}$. In addition, $G_w(t; a, b; \bar{P})$ and $G_w^{\star}(t; a, b; \bar{P})$ is divergent as $t \to \mathrm{e}^{-\kappa_w(a,b;\bar{P})}$. Moreover, if $P_w(t; a, b; \bar{P})$ is the generating function of the set of prime fundamental patterns excluding the prime pattern P, then $P_w(\mathrm{e}^{-\kappa_w(a,b;\bar{P})}, a, b) = 1$.*

But observe that $P_w(t; a, b; \bar{P}) < P_w(t; a, b)$ for all $0 < t \leqslant \mathrm{e}^{-\kappa_w(a,b)}$. In particular, $P_w(\mathrm{e}^{-\kappa_w(a,b)}; \bar{P}) < P_w(\mathrm{e}^{-\kappa_w(a,b)}) = 1$ at the radius of convergence of $G_w(t; a, b)$. But then theorem 5.12 implies that $G_w(\mathrm{e}^{-\kappa_w(a,b)}; a, b; \bar{P}) < \infty$, and since $G_w(t; a, b; \bar{P})$ is divergent at its radius of convergence, we conclude that $\kappa_w(a, b; \bar{P}) < \kappa_w(a, b)$. This gives the following theorem:

Theorem 5.13. *If P is a Kesten w-pattern, then $\kappa_w(a, b; \bar{P}) < \kappa_w(a, b)$.*

Proof. Since any Kesten w-pattern is a sub-walk of a fundamental pattern, eliminating walks containing P will also eliminate walks containing fundamental patterns which contain P. The theorem now follows from theorem 5.12. □

5.5. The pattern theorem

Let P be any prime fundamental pattern, and consider $\sum_{k,l} c_n(w; k, l; v_b, v_t; mP)$, the number of self-avoiding walks in $\mathbb{L}_w$ which contains exactly m occurrences of P. Define the partition function

$$g_n(w; a, b; mP) = \sum_{v_b, v_t} \sum_{k,l} C_n(w; k, l; v_b, v_t; mP) a^{v_b} b^{v_t}. \tag{51}$$

Let $\epsilon > 0$ be a small number. By again considering models of unfolded walks, one may prove existence of the limit

$$\lim_{n\to\infty} \frac{1}{n} \log g_n(w; a, b; \lfloor \epsilon n \rfloor P) = \kappa_w(a, b; \epsilon), \tag{52}$$

see for example theorem 3.4 in [12].

In addition, in terms of unfolded walks and in the notation above,

$$\begin{aligned} \kappa_w(a, b; \epsilon) &= \lim_{n\to\infty} \frac{1}{n} \log g_n^{\dagger}(w; h, k; a, b; \lfloor \epsilon n \rfloor P) \\ &= \lim_{n\to\infty} \frac{1}{n} \log \sum_{h,k} g_n^{\dagger}(w; h, k; a, b; \lfloor \epsilon n \rfloor P), \end{aligned} \tag{53}$$

for any fixed values of h and k in $[0, w]$, see corollary 4.7 for a proof.

Concatenation of walks counted by $c^{\dagger}_{n_1}(w; 0, 0; h, k; m_1 P)$ and $c^{\dagger}_{n_2}(w; 0, 0; h, k; m_2 P)$ as in figure 6 shows that in terms of generating functions,

$$g^{\dagger}_{n_1}(w; 0, 0; a, b; m_1 P) g^{\dagger}_{n_2}(w; 0, 0; a, b; m_2 P) \leqslant g^{\dagger}_{n_1+n_2+1}(w; 0, 0; a, b; (m_1 + m_2) P), \quad (54)$$

so that one may check that $g^{\dagger}_{n-1}(w; 0, 0; a, b; mP)$ satisfies assumptions 3.1 in [12]. This in particular implies that $\kappa_w(a, b; \epsilon)$ is a log-concave function of ϵ (theorem 3.5 in [12]). These considerations give the following version of the pattern theorem.

Theorem 5.14. *For every prime fundamental pattern P there exists an $\epsilon_P > 0$ such that for all $\epsilon \in (0, \epsilon_P)$,*

$$\kappa_w(a, b; \epsilon) < \kappa_w(a, b).$$

The proof of this theorem is identical to the proof of theorem 5.17 in [12]. The important corollary to theorem 5.14 is that almost all w-walks contain a positive density of the prime fundamental pattern P in the limit as $n \to \infty$. This may be stated as follows, and the proof is similar to that of corollary 5.18 in [12].

Corollary 5.15. *Let P be a prime fundamental pattern and let $\epsilon > 0$ be a small number. Suppose that $g^{\dagger}_n(w; 0, 0; a, b; \leqslant \lfloor \epsilon n \rfloor P)$ is the partition function of unfolded w-walks in which P occurs at most $\lfloor \epsilon n \rfloor$ times.*

Then, if ϵ is small enough, there exists a $k > 0$ and an $N_0 > 0$ such that

$$\begin{aligned} g^{\dagger}_n(w; 0, 0; a, b; > \lfloor \epsilon n \rfloor P) &= g^{\dagger}_n(w; 0, 0; a, b;) - g^{\dagger}_n(w; 0, 0; a, b; \leqslant \lfloor \epsilon n \rfloor P) \\ &\geqslant (1 - \mathrm{e}^{-kn}) g^{\dagger}_n(w; 0, 0; a, b), \end{aligned}$$

for all $n > N_0$.

This corollary shows in particular that for small enough $\epsilon > 0$ and for any prime fundamental prime pattern P,

$$\begin{aligned} \lim_{n\to\infty} \frac{1}{n} \log g^{\dagger}_n(w; 0, 0; a, b; > \lfloor \epsilon n \rfloor P) &= \lim_{n\to\infty} \frac{1}{n} \log \sum_{h,k} g^{\dagger}_n(w; h, k; a, b; > \lfloor \epsilon n \rfloor P) \\ &= \kappa_w(a, b). \end{aligned} \quad (55)$$

In other words, unfolded walks containing a positive density of the fundamental prime pattern P make an exponentially dominating contribution to the connective constant in this model. Since every Kesten w-pattern is a subpattern of a fundamental pattern, which is the union of prime fundamental patterns, corollary 5.15 is also true if P is a Kesten w-pattern.

6. Properties of $\kappa_w(a, b)$

6.1. $\kappa_w(1, 1)$

Consider first the case $a = b = 1$. Then the model is a self-avoiding walk from the origin in $\mathbb{L}_w$. We are particularly interested in the dependence of the free energy $\kappa_w(1, 1)$ on the width w of the slab $\mathbb{L}_w$. Since the free energy may be determined by considering unfolded walks (see, for example, lemma 4.5), we will approach this model by working with unfolded walks.

Consider unfolded w-walks of length n. In view of equations (16) and (55), we only have to consider unfolded walks with both endpoints in the bottom bounding plane. Thus, let W be an unfolded w-walk counted by $c^{\dagger}_n(w; 0, 0; > \lfloor \epsilon n \rfloor P)$, and where we choose P to be the fundamental prime pattern which is in the shaded areas in figure 14. Let $\epsilon > 0$ be a small number, and consider walks W in which P occurs at least $\lfloor \epsilon n \rfloor$ times.

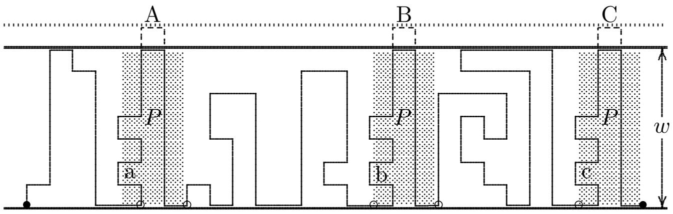

Figure 14. The pattern P occurs with positive density in all w-walks counted by $c_n^\dagger(w; 0, 0, > \lfloor\epsilon n\rfloor P)$. By replacing the squares by single edges at the locations marked by $a, b, c, \ldots$, and by placing two extra edges at the locations marked by $A, B, C, \ldots$, walks in a slab of width $w+1$ are formed. This construction shows that the inequality in equation (56) is valid.

Choose any m of these occurrences of P uniformly. Delete the small square part of the walk labelled by a small Roman letter $\{a, b, c, \ldots\}$ and replace it by the square walk in broken lines marked by a capital letters $\{A, B, C, \ldots\}$ on the top bounding plane. This gives an unfolded walk in a slab of width $w+1$.

There are $\sum_{v_b,v_t} c_n^\dagger(w; 0, 0; v_b, v_t; > \lfloor\epsilon n\rfloor P)$ choices of the unfolded walk W, and for each such walk, at least $\lfloor\epsilon n\rfloor$ choose m choices of the patterns where the small square walk is moved. Since the resulting walk is in a slab of width $w+1$, there are at most $\sum_{v_b,v_t} c_n^\dagger(w+1; 0, 0; v_b, v_t)$ distinct outcomes of the construction. We conclude that

$$\binom{\lfloor\epsilon n\rfloor}{m} \sum_{v_b,v_t} c_n^\dagger(w; 0, 0; v_b, v_t; > \lfloor\epsilon n\rfloor P) \leqslant \sum_{v_b,v_t} c_n^\dagger(w+1; 0, 0; v_b, v_t). \quad (56)$$

By corollary 5.15 we can choose an $\epsilon > 0$ small enough so that

$$\lim_{n\to\infty} \left[\log \sum_{v_b,v_t} c_n^\dagger(w; 0, 0; v_b, v_t; > \lfloor\epsilon n\rfloor P)\right] \Big/ n = \kappa_w(1, 1). \quad (57)$$

Let $\delta > 0$ be such that $\epsilon > \delta$, and put $m = \lfloor\delta n\rfloor$ in equation (56). Take the power $1/n$ on both sides, and let $n \to \infty$. The result is the following lemma.

Lemma 6.1. *For small enough $\epsilon > 0$ and $\epsilon > \delta > 0$, $\kappa_w(1, 1)$ and $\kappa_{w+1}(1, 1)$ are related by the inequality*

$$\left[\frac{\epsilon^\epsilon}{\delta^\delta(\epsilon-\delta)^{\epsilon-\delta}}\right] \mathrm{e}^{\kappa_w(1,1)} \leqslant \mathrm{e}^{\kappa_{w+1}(1,1)}.$$

In particular, if $\delta = \epsilon/2$, then

$$\kappa_w(1, 1) + \epsilon \log 2 \leqslant \kappa_{w+1}(1, 1).$$

In other words, since $\epsilon > 0$, it follows that $\kappa_w(1, 1) < \kappa_{w+1}(1, 1)$. Hence, $\kappa_w(1, 1)$ is a strictly increasing function of w.

The order of the limits in $\lim_{n\to\infty}[\lim_{w\to\infty} \frac{1}{n} \log g_n(w; 0, 0; 1, 1)]$ can be interchanged. This would be immediate if one could prove that $\kappa_w(1, 1)$ is a concave function of w, but such a result is lacking (and seems difficult). Instead, we give a direct proof (see also [8]).

Theorem 6.2

$$\lim_{w\to\infty} \kappa_w(1, 1) = \kappa.$$

Proof. Consider the number of unfolded walks

$$L_n^\dagger = \sum_w \sum_{v_b, v_t} c_n^\dagger(w; 0, 0; v_b, v_t)$$

in the half-space $Z \geqslant 0$ with endpoints fixed in the plane $Z = 0$. These walks are *unfolded loops* and it is known that [6, 8]

$$\lim_{n\to\infty} \frac{1}{n} \log L_n^\dagger = \kappa.$$

Given $\epsilon > 0$, there exists an $N > 0$ such that

$$\frac{1}{N} \log L_N^\dagger \geqslant \kappa - \epsilon.$$

For this value of N, all the loops counted by $L_N^\dagger$ would fit into a slab of width $w \geqslant \lceil N/2 \rceil = w_0(N)$.

Let $n = Np + r$ where $0 \leqslant r < N$. Since the loops are unfolded they can be concatenated as in figure 6, and if p loops are concatenated in sequence, then for any $w > w_0(N)$,

$$\sum_{v_b, v_t} c_n(w; 0, 0; v_b, v_t) \geqslant \left[L_N^\dagger\right]^p.$$

Take logarithms, divide by n, and let $p \to \infty$ with N fixed. Then $n \to \infty$, and

$$\kappa_w(1, 1) \geqslant \frac{1}{N} \log L_N^\dagger \geqslant \kappa - \epsilon.$$

Thus, for any $\epsilon > 0$ we can find a w such that $\kappa_w(1, 1) \geqslant \kappa - \epsilon$. □

Thus,

$$\lim_{n\to\infty} \left[\lim_{w\to\infty} \frac{1}{n} \log g_n(w; 0, 0; 1, 1)\right] = \lim_{w\to\infty} \left[\lim_{n\to\infty} \frac{1}{n} \log g_n(w; 0, 0; 1, 1)\right].$$

Observe that the collection of paths counted by the partition function $g_n^\dagger(w; 0, 0; 1, 1)$ is identical to the collection of paths counted by $g_n^\dagger(w + 1; 0, 0; 1, 0)$ where $a = 1$ and $b = 0$. In other words, by forbidding top visits, the walks are effectively limited to a slab of width less by one. The result is that $\kappa_w(1, 1) = \kappa_{w+1}(1, 0)$. In view of lemma 6.1, this means that for small enough $\epsilon > 0$, $\kappa_w(1, 0) + \epsilon \log 2 \leqslant \kappa_w(1, 1)$. In other words,

$$\kappa_w(1, 0) < \kappa_w(1, 1). \tag{58}$$

Alternatively, one may also note that $\kappa_w(1, 1) + \epsilon \log 2 \leqslant \kappa_{w+2}(1, 0)$ or that

$$\kappa_w(1, 1) < \kappa_{w+2}(1, 0). \tag{59}$$

One may continue this approach by noting that if $a = b = 0$, then $\kappa_{w+2}(0, 0) = \kappa_w(1, 1)$, and in view of the last equations this gives the strict inequalities

$$\kappa_w(0, 0) < \kappa_w(1, 0) < \kappa_w(1, 1) < \kappa_{w+2}(1, 0) < \kappa_{w+4}(0, 0). \tag{60}$$

6.2. $\kappa_w(a, 1)$

Next we consider the case that $b = 1$, while $a > 0$. The partition function in this model is

$$\sum_{v_b, v_t} \sum_k C_n(w; k; v_b, v_t) a^{v_b} \tag{61}$$

and we note that this is equal to $\sum_k G_n(w; k; a, 1)$. The results in corollaries 4.6 and 4.7 imply that

$$\kappa_w(a, 1) = \lim_{n\to\infty} \frac{1}{n} \log \sum_k G_n(w; k; a, 1) = \lim_{n\to\infty} \frac{1}{n} \log g_n^{\dagger}(w; h, k; a, 1) \tag{62}$$

so that we may only consider unfolded w-walks. Define $z_n^{\dagger}(w; v_b) = \sum_{v_t} c_n^{\dagger}(w; 0, 0; v_b, v_t)$ so that $g_n^{\dagger}(w; 0, 0; a, 1) = \sum_{v_b} z_n^{\dagger}(w; v_b)a^{v_b}$. Use the Cauchy–Schwarz inequality in the following:

$$\begin{aligned} g_n^{\dagger}(w; 0, 0; a_1, 1)g_n^{\dagger}(w; 0, 0; a_2, 1) &= \sum_{v_1} z_n^{\dagger}(w; v_1)a_1^{v_1} \sum_{v_2} z_n^{\dagger}(w; v_2)a_2^{v_2} \\ &\geqslant \left(\sum_v z_n^{\dagger}(w; v)[\sqrt{a_1 a_2}]^v \right)^2 \\ &= \left[g_n^{\dagger}(w; 0, 0; \sqrt{a_1 a_2}, 1)\right]^2. \end{aligned} \tag{63}$$

Take logarithms, divide by n and take $n \to \infty$ to obtain

$$\kappa_w(a_1, 1) + \kappa_w(a_2, 1) \geqslant 2\kappa_w(\sqrt{a_1 a_2}, 1). \tag{64}$$

In other words, $\kappa_w(a, 1)$ is a convex function of $\log a$. Since $\kappa_w(a, 1)$ is a finite real-valued function of $a > 0$, we get the following theorem.

Theorem 6.3. *$\kappa_w(a, 1)$ is a convex function of $\log a$, and so is continuous for $a > 0$. It is also differentiable almost everywhere in $a > 0$.*

The dependence of $\kappa_w(a, 1)$ on w is the next issue. To see that $\kappa_w(a, 1)$ is a strictly increasing function of w for any $a > 0$, consider again the construction in figure 14. Unlike the result in equation (56), we keep track of bottom and top visits here.

The number of bottom visits remains unchanged when completing the construction in figure 14, while the number of top visits changes. The result is the inequality

$$\binom{\lfloor \epsilon n \rfloor}{m} c_n^{\dagger}(w; 0, 0; v_b, v_t; > \lfloor \epsilon n \rfloor P) \leqslant c_n^{\dagger}(w + 1; 0, 0; v_b, 2m), \tag{65}$$

since the walks constructed have exactly $2m$ top visits. Observe now that by multiplying by a^{v_b} and by summing over all the values of both v_b and v_t for which the left-hand side is non-zero, the right-hand side can be bounded by

$$\sum_{v_b, v_t} c_n^{\dagger}(w + 1; 0, 0; v_b, 2m)a^{v_b} \leqslant \sum_{v_b, v_t} c_n^{\dagger}(w + 1; 0, 0; v_b, v_t)a^{v_b} = g_n^{\dagger}(w + 1; 0, 0; a, 1),$$

since the sum over v_b includes all walk with exactly $2m$ top visits. Thus, by multiplying equation (65) by a^{v_b} and summing over v_b and v_t, we get

$$\binom{\lfloor \epsilon n \rfloor}{m} g_n^{\dagger}(w; 0, 0; a, 1; > \lfloor \epsilon n \rfloor P) \leqslant g_n^{\dagger}(w + 1; 0, 0; a, 1). \tag{66}$$

By equation (55) there exists an $\epsilon > 0$ small enough so that $\lim_{n\to\infty}[\log g_n^{\dagger}(w; 0, 0; a, 1; > \lfloor \epsilon n \rfloor P)]/n = \kappa_w(a, 1)$. Fix $\epsilon > 0$ so that this is true.

Let $\delta > 0$ be such that $\epsilon > \delta$ and put $m = \lfloor \delta n \rfloor$ in equation (66). Take the power $1/n$ on both sides, and take $n \to \infty$. By equation (55) the result is the following lemma.

Lemma 6.4. *For any $a > 0$, $\kappa_w(a, 1)$ is a strictly increasing function of w. In particular, there exists small $\epsilon > 0$ and $\epsilon > \delta > 0$ such that*

$$\left[\frac{\epsilon^\epsilon}{\delta^\delta(\epsilon-\delta)^{\epsilon-\delta}}\right] \mathrm{e}^{\kappa_w(a,1)} \leqslant \mathrm{e}^{\kappa_{w+1}(a,1)}.$$

If $\delta = \epsilon/2$, then

$$\kappa_w(a, 1) + \epsilon \log 2 \leqslant \kappa_{w+1}(a, 1).$$

In other words, since $\epsilon > 0$, it follows that $\kappa_w(a, 1) < \kappa_{w+1}(a, 1)$.

Hence, $\kappa_w(a, 1)$ is an increasing bounded sequence in w. Thus, the limit $\lim_{w\to\infty} \kappa_w(a, 1)$ exists and is finite. In the case that $a = 1$ we proved in theorem 6.2 that the limit is equal to κ. In this case, we expect the limit to be equal to the limiting free energy $\mathcal{F}(a)$ of a self-avoiding walk in the half-plane $Z \geqslant 0$ and adsorbing in the $Z = 0$ plane, see equation (5).

Theorem 6.5. *Let $a > 0$, then $\lim_{w\to\infty} \kappa_w(a, 1) = \mathcal{F}(a)$, where $\mathcal{F}(a)$ is the limiting free energy of a self-avoiding walk in the half-space $X \geqslant 0$ adsorbing in the X-axis.*

Proof. Observe first that $\kappa_w(a, 1) < \mathcal{F}(a)$ and that $\{\kappa_w(a, 1)\}$ is an increasing sequence in w. Hence, the limit $\lim_{w\to\infty} \kappa_w(a, 1)$ exists.

A *loop* with vertices $\{x_j\}_{j=0}^n$ in the half-space $Z \geqslant 0$ is a self-avoiding walk such that $Z(x_n) \geqslant 0$ for all vertices in the loop, and with first and last vertices in the $Z = 0$ plane: $Z(x_0) = Z(x_n) = 0$. This loop is unfolded if $X(x_0) \leqslant X(x_j) < X(x_n)$ for $j = 0, 1, 2, \ldots, n-1$. Let the number of unfolded loops with v_b visits in the plane $Z = 0$ be $l_n^\dagger(v)$. Define the partition function of unfolded loops adsorbing in the bottom bounding plane by

$$L_n^\dagger(a) = \sum_v l_n^\dagger(v) a^v.$$

It is known that [6]

$$\mathcal{F}(a) = \lim_{n\to\infty} \frac{1}{n} \log L_n^\dagger(a).$$

For any $a > 0$ and given $\epsilon > 0$ there exists an $N > 0$ such that

$$\frac{1}{N} \log L_N^\dagger(a) \geqslant \mathcal{F}(a) - \epsilon.$$

For this value of N, all loops would fit into a slab of width at most $\lceil N/2 \rceil = w_o(N)$.

Choose $w > w_o(N)$, and let $n = Np + r$, where $p > 0$ is a fixed integer and $0 \leqslant r < N$. Since the loops are unfolded, they can be concatenated as in figure 6, and if p such loops are concatenated in sequence, then for any $w > w_o(N)$,

$$g_{Np+r}^\dagger(w; 0, 0; a, 1) \geqslant \left[g_N^\dagger(w; 0, 0; a, 1)\right]^p \geqslant \left[L_N^\dagger(a)\right]^p.$$

Take logarithms, divide by n and let $p \to \infty$ with N fixed. Then $n \to \infty$, and from the above,

$$\kappa_w(a, 1) \geqslant \mathcal{F}(a) - \epsilon, \qquad \forall w > w_0(N).$$

Thus, for any $\epsilon > 0$ we can find a w such that $\kappa_w(a, 1) \geqslant \mathcal{F}(a) - \epsilon$. This proves the theorem. $\square$

6.3. $\kappa_w(a, b)$

We next prove that $\kappa_w(a, b)$ is a convex function of $\log a$ and of $\log b$. This is an immediate result of the Cauchy–Schwarz inequality.

Lemma 6.6. *For any* $a_1 > 0, a_2 > 0, b_1 > 0$ *and* $b_2 > 0$,

$$2\kappa_w(\sqrt{a_1 a_2}, \sqrt{b_1 b_2}) \leqslant \kappa_w(a_1, b_1) + \kappa_w(a_2, b_2).$$

Thus, $\kappa_w(a, b)$ *is a convex function of* $\log a$ *and of* $\log b$. *Hence,* $\kappa_w(a, b)$ *is a continuous function, and it is differentiable almost everywhere in the ab-plane.*

Proof. Let $a_1 > 0, a_2 > 0, b_1 > 0$ and $b_2 > 0$ be fixed. Then by applying the Cauchy–Schwarz inequality twice,

$$\begin{aligned}
g_n(w; 0, 0; \sqrt{a_1 a_2}, \sqrt{b_1 b_2}) &= \sum_{u_b} \left(\sum_{u_a} c_n(w; 0, 0; u_a, u_b)[\sqrt{a_1 a_2}]^{u_a} \right) [\sqrt{b_1 b_2}]^{u_b} \\
&\leqslant \sum_{u_b} \left[\left(\sum_{v_a} c_n(w; 0, 0; v_a, u_b) a_1^{v_a} \right)^{1/2} \left(\sum_{w_a} c_n(w; 0, 0; w_a, u_b) a_2^{w_a} \right)^{1/2} \right] \\
&\quad \times [\sqrt{b_1 b_2}]^{u_b} \leqslant \left[\sum_{v_b} \sum_{v_a} c_n(w; 0, 0; v_a, v_b) a_1^{v_a} b_1^{v_b} \right]^{1/2} \\
&\quad \times \left[\sum_{w_b} \sum_{w_a} c_n(w; 0, 0; w_a, w_b) a_2^{w_a} b_2^{w_b} \right]^{1/2} \\
&= [g_n(w; 0, 0; a_1, b_1)]^{1/2} [g_n(w; 0, 0; a_2, b_2)]^{1/2}.
\end{aligned}$$

Take logarithms, divide by n and let $n \to \infty$ to see that

$$2\kappa_w(\sqrt{a_1 a_2}, \sqrt{b_1 b_2}) \leqslant \kappa_w(a_1, b_1) + \kappa_w(a_2, b_2).$$

In other words, $\kappa_w(a, b)$ is a convex function of $\log a$ and $\log b$. □

Thus, $\kappa_w(a, b)$ is a convex function of $\log a$ for fixed values of $b > 0$. Similarly, $\kappa_w(a, b)$ is a convex function of $\log b$ for fixed values of $a > 0$. Thus, $\kappa_w(a, b)$ is a continuous function and it is differentiable almost everywhere.

By concatenating two unfolded walks as illustrated in figure 15, one obtains the following inequality:

$$g_n^\dagger(w_1; 0, w_1; a, 1) g_n^\dagger(w_2; 0, w_2; 1, b) \leqslant g_{2n}^\dagger(w_1 + w_2; 0, w_1 + w_2; a, b). \tag{67}$$

Take logarithms of this, divide by n and take $n \to \infty$ to obtain

$$\kappa_{w_1}(a, 1) + \kappa_{w_2}(1, b) \leqslant 2\kappa_{w_1 + w_2}(a, b). \tag{68}$$

In the event that $w_1 = w_2$ this reduces to

$$\tfrac{1}{2}(\kappa_w(a, 1) + \kappa_w(1, b)) \leqslant \kappa_{2w}(a, b). \tag{69}$$

If $a = b$ and $w_1 = w_2 = w$, then this becomes

$$\kappa_w(a, 1) \leqslant \kappa_{2w}(a, a). \tag{70}$$

This gives the following theorem:

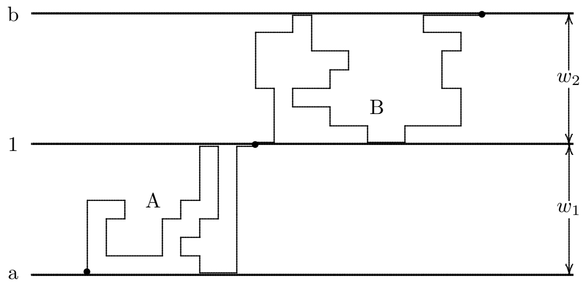

Figure 15. Stack two slabs of widths w_1 and w_2 and assign an activity a to the bottom bounding plane of the bottom slab and activity b to the top bounding plane of the top slab. Two unfolded walks, A in the bottom slab, and B in the top slab, may be concatenated to get an unfolded walk in a slab of width $w_1 + w_2$ and with visits in the bottom bounding plane weighed by a and in the top bounding plane weighed by b. The result is the inequality in equation (67).

Theorem 6.7. *It is the case that*

$$\liminf_{w\to\infty} \kappa_w(a,a) \geqslant \mathcal{F}(a)$$

and

$$\lim_{w\to\infty} \kappa_w(a,a) = \mathcal{F}(a) = \kappa$$

whenever $a \leqslant 1$.

Proof. By equation (70) and by theorem 6.5,

$$\lim_{w\to\infty} \kappa_w(a,1) = \mathcal{F}(a) \leqslant \liminf_{w\to\infty} \kappa_{2w}(a,a).$$

Observe next that $\kappa_{2w}(a,a) \leqslant \kappa_{2w}(a,1) \to \mathcal{F}(a)$ if $a \leqslant 1$, so that $\lim_{w\to\infty} \kappa_{2w}(a,a) \to \mathcal{F}(a) = \kappa$ if $a \leqslant 1$. If $a > 1$, then $\kappa_w(a,a) \geqslant \kappa_w(a,1) \to \mathcal{F}(a)$ proves that $\liminf_{w\to\infty} \kappa_w(a,a) \geqslant \mathcal{F}(a)$. □

In the case of $\kappa_w(a,b)$, we are able to prove the following:

Theorem 6.8. *If both* $a \geqslant 1$ *and* $b \geqslant 1$*, then*

$$\liminf_{w\to\infty} \kappa_w(a,b) \geqslant \max\{\mathcal{F}(a), \mathcal{F}(b)\}$$

Proof. If $a \geqslant 1$ and $b \geqslant 1$, then

$$\begin{aligned} G_n(w;a,b) &= \sum_{v_b,v_t} C_n(w;v_b,v_t) a^{v_b} b^{v_t} \\ &\geqslant \max\left\{\sum_{v_b,v_t} C_n(w;v_b,v_t) a^{v_b} 1^{v_t}, \sum_{v_b,v_t} C_n(w;v_b,v_t) 1^{v_b} b^{v_t}\right\} \\ &= \max\{G_n(w;a,1), G_n(w;1,b)\}. \end{aligned}$$

Take logs, divide by n and take $n \to \infty$ to prove the inequality. □

It is possible to bound $\kappa_w(a,b)$ in terms of $\kappa_w(a,1)$ if $0 \leqslant b \leqslant 1$. Observe for example that if $b \to 0^+$, then walks in a slab of width w are effectively confined to a slab of width $w-1$. This shows that $\kappa_w(a,0) = \kappa_{w-1}(a,1)$. The following lemma relates $\kappa_w(a,1)$ and $\kappa_w(a,b)$ for all $a > 0$ and $0 < b \leqslant 1$.

Lemma 6.9. *If $a > 0$, $0 < b \leqslant 1$ and $w \geqslant 1$, then*

$$\kappa_w(a, 1) \geqslant \kappa_w(a, b) > \kappa_w(a, 0) = \kappa_{w-1}(a, 1) \geqslant \kappa_{w-1}(a, b).$$

Proof. Since $0 < b \leqslant 1$, the first and last inequalities are immediate. The equality $\kappa_w(a, 0) = \kappa_{w-1}(a, 1)$ follows because there is a bijection between $(w-1)$-walks of length n in a slab of width $w-1$ and w-walks of length n in a slab of width w but with zero weight if they have top visits. This is true for all $a > 0$.

It remains to prove the strict inequality. Let P be a prime fundamental w-pattern in w-walks with both bottom and top visits. By theorem 5.13, we see that $\kappa_w(a, b) > \kappa_w(a, b; \overline{P})$.

Next, consider the w-walks from the origin in a $(w-1)$-slab. One may argue as follows: for any $0 < b \leqslant 1$,

$$\begin{aligned} G_n(w-1; a, 1) &= \sum_{v_b, v_t} C_n(w-1; v_b, v_t) a^{v_b} 1^{v_t} \\ &= \sum_{v_b} C_n(w; v_b, 0) a^{v_b} \\ &\leqslant \sum_{v_b, v_t} C_n(w; v_b, v_t; \overline{P}) a^{v_b} b^{v_t} \\ &= G_n(w; a, b; \overline{P}) \end{aligned}$$

where the second equality follows because every walk counted by $\sum_{v_t} C_n(w-1; v_b, v_t)$ is also counted by $C_n(w; v_b, 0)$, and these walks are weighted identically on their bottom visits. The inequality follows because

$$\sum_{v_b} C_n(w; v_b, 0) a^{v_b} = \sum_{v_b} C_n(w; v_b, 0; \overline{P}) a^{v_b},$$

where the right-hand side is the $v_t = 0$ term in $\sum_{v_b, v_t} C_n(w; v_b, v_t; \overline{P}) a^{v_b} b^{v_t}$.

By taking logarithms of the above, dividing by n, and taking $n \to \infty$, it follows that $\kappa_{w-1}(a, b) \leqslant \kappa_w(a, b; \overline{P})$. This, together with theorem 5.13, establishes the strict inequality. $\square$

We next consider the case that either $a \leqslant 1$ or $b \leqslant 1$ or both. In this event, we are able to prove the following theorem.

Theorem 6.10. *If either $0 < a \leqslant 1$ or $0 < b \leqslant 1$ or both, then*

$$\kappa(a, b) = \lim_{w \to \infty} \kappa_w(a, b) = \begin{cases} \mathcal{F}(a), & \text{if } b \leqslant 1; \\ \mathcal{F}(b), & \text{if } a \leqslant 1. \end{cases}$$

In other words, $\lim_{w \to \infty} \kappa_w(a, b)$ exists.

Moreover, if either $a \leqslant a_c$ and $b \leqslant 1$ or $a \leqslant 1$ and $b \leqslant b_c$, where $a_c = b_c$ is the smallest value such that $\mathcal{F}(a)$ is non-analytic (or $a_c = b_c$ is the critical activity for self-avoiding walks adsorbing in the plane), then

$$\lim_{w \to \infty} \kappa_w(a, b) = \kappa.$$

Proof. Suppose that $b \leqslant 1$ and assume that $w \geqslant 1$. Consider the sequence of inequalities in lemma 6.9. Take $w \to \infty$. By theorem 6.7 it follows by the squeeze theorem for limits that

$$\lim_{w \to \infty} \kappa_w(a, b) = \mathcal{F}(a).$$

Since $\kappa_w(a, b)$ is symmetric in (a, b), the result follows.

Next, suppose that $b \leqslant 1$ and assume that $a \leqslant a_c$, where a_c is the critical adsorption activity for self-avoiding walks adsorbing in a half-plane. We may assume without loss of generality that $a > b$. Then $\mathcal{F}(a) \geqslant \kappa$. In other words,

$$\lim_{w\to\infty} \kappa_w(a, b) \geqslant \kappa$$

for all non-negative (a, b).

But $\kappa_w(a, b) \leqslant \kappa_w(a, 1)$ since $b \leqslant 1$, and so $\kappa_w(a, b) \leqslant \mathcal{F}(a)$. Since $\mathcal{F}(a) = \kappa$ if $a \leqslant a_c$ (see for example [11]), this proves that $\lim_{w\to\infty} \kappa_w(a, b) = \kappa = \mathcal{F}(a)$ whenever both $b \leqslant 1$ and $a \leqslant a_c$. A similar argument shows that $\lim_{w\to\infty} \kappa_w(a, b) = \kappa$ if $b \leqslant b_c$ and $a \leqslant 1$. □

Theorem 6.10 shows that $\lim_{w\to\infty} \kappa_w(a, b) = \kappa$ if $a \leqslant a_c$ and $b \leqslant 1$ or if $a \leqslant 1$ and $b \leqslant a_c$. One may also prove that $\lim_{w\to\infty} \kappa_w(a, b) = \kappa$ at points outside this region by using the convexity of $\kappa_w(a, b)$ established in lemma 6.6.

Corollary 6.11. *If $ab \leqslant a_c$, and both $0 < a \leqslant a_c$ and $0 < b \leqslant a_c$, then*

$$\lim_{w\to\infty} \kappa_w(a, b) = \kappa.$$

Proof. Choose $a_1 = a_c = b_2$ and $a_2 = 1 = b_1$ in lemma 6.6. This shows that

$$2\kappa_w(\sqrt{a_c}, \sqrt{a_c}) \leqslant \kappa_w(a_c, 1) + \kappa_w(1, a_c).$$

Now take $w \to \infty$, then by theorem 6.10, it follows that

$$\limsup_{w\to\infty} \kappa_w(\sqrt{a_c}, \sqrt{a_c}) \leqslant \kappa.$$

Since $\liminf_{w\to\infty} \kappa_w(a, b) \geqslant \kappa$, it follows that $\lim_{w\to\infty} \kappa_w(\sqrt{a_c}, \sqrt{a_c}) = \kappa$. By repeated application of this construction, one may prove that $\lim_{w\to\infty} \kappa_w(a, b) = \kappa$ on a dense subsets of points on the curve $ab = a_c$, if $a \geqslant 1$ and $b \geqslant 1$. Since $\lim_{w\to\infty} \kappa_w(a, b)$ is convex in both its arguments, it must be equal to κ at every point on this curve.

Finally, since $\lim_{w\to\infty} \kappa_w(a, b)$ is a non-decreasing function of both its arguments, it follows that $\lim_{w\to\infty} \kappa_w(a, b) = \kappa$ for all points $ab \leqslant a_c$ if both $a \leqslant a_c$ and $b \leqslant a_c$. □

Theorem 6.10 and corollary 6.11 prove existence of the limit $\lim_{w\to\infty} \kappa_w(a, b)$ also at points outside the unit square in the ab-plane.

Since $\mathcal{F}(a) > \kappa$ if $a > a_c$ [11], another consequence of theorem 6.8 is corollary 6.12.

Corollary 6.12. *If both $a > a_c$ and $b > b_c$, where $a_c = b_c$ is the smallest values of a such that $\mathcal{F}(a)$ is non-analytic (or $a_c = b_c$ is the critical activity for self-avoiding walks adsorbing in the plane), then*

$$\liminf_{w\to\infty} \kappa_w(a, b) > \kappa.$$

In other words, if $\mathcal{C} = \{(a_t, b_t) \mid t \in [0, 1]\}$ is a simple curve with endpoints (a_0, b_0) and (a_1, b_1) such that either $a_0 < a_c$ and $b_0 < 1$, or $a_0 < 1$ and $b_0 < b_c$, and $a_1 > a_c$ and $b_1 > b_c$, then there is a smallest value of the parameter t, t_c, such that $\lim_{w\to\infty} \kappa_w(a_t, b_t) = \kappa$ if $t \leqslant t_c$, and there exists $\epsilon > 0$ such that $\liminf_{w\to\infty} \kappa_w(a_t, b_t) > \kappa$ if $t_c < t \leqslant t_c + \epsilon$.

This corollary proves the existence of a phase boundary in the $w \to \infty$ limit in this model between desorbed walks and walks adsorbed on either the top or bottom bounding planes.

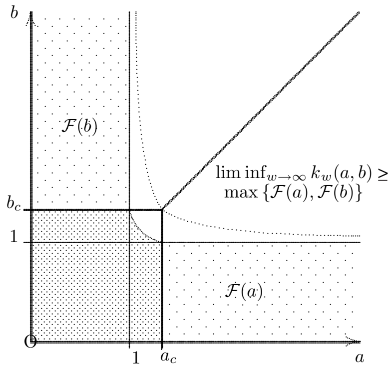

Figure 16. The phase diagram in the $w \to \infty$ limit. In the darker shaded region, $\kappa(a, b) = \kappa$, see theorem 6.10 and corollary 6.11, and in the lighter shaded regions, $\kappa(a, b) = \mathcal{F}(a)$ or $\kappa(a, b) = \mathcal{F}(b)$, respectively; see theorem 6.10 as well as equation (5). The boundary of the darker shaded regions runs along $b = b_c(=a_c)$ when $0 \leqslant a \leqslant 1$, then $ab = a_c$, and then $= a_c$ when $0 \leqslant b \leqslant 1$. We conjecture that $\kappa(a, b) = \kappa$ for all (a, b) such that $0 \leqslant a \leqslant a_c$ and $0 \leqslant b \leqslant a_c$. In the rest of the phase diagram $\liminf_{w\to\infty} \kappa(a, b) \geqslant \max\{\mathcal{F}(a), \mathcal{F}(b)\} > \kappa$. There are phase transitions along the lines $a = a_c$ and $0 \leqslant b \leqslant 1$ and $b = b_c$ and $0 \leqslant a \leqslant 1$ since $\mathcal{F}(a)$ is non-analytic at $a = a_c = b_c$. For any fixed value of $> a_c$, $\kappa(a, b)$ is independent of b for $0 \leqslant b \leqslant 1$. If the free energy becomes dependent on b if $b > 1$ and for fixed $a > a_c$, then there should be a further critical curve in this phase diagram. The only mechanism which would suggest such a critical curve is a changeover from adsorption on the bottom plane to adsorption on the top plane, and this should occur along the line $a = b > a_c$. Thus, we conjecture that the free energy is equal to $\mathcal{F}(a)$ for all $a > b > a_c$ and equal to $\mathcal{F}(b)$ for all $b > a > a_c$. In other words, the free energy is $\max\{\mathcal{F}(a), \mathcal{F}(b)\}$ for all $a > 0$ and $b > 0$. This conjecture implies that the transition along the line $a = b > a_c$ is a line of first-order phase transitions, since the gradient of the free energy is discontinuous when this line is crossed transversely. The limit of the zero force curves is indicated by a dotted line, and we conjecture that this curve passes through the point (a_c, a_c). This phase diagram can be compared to figure 6 in [13], and with the phase diagram for directed paths in a slit in [1]. The directed path in a slit model exhibits a similar region of a repulsive force compared to the above, as well as a regime where the forces are attractive for large values of a and b. The repulsive regime in the directed path model is long ranged when both a and b are small, but becomes short ranged when either a or b, but not both, is large.

7. The phase diagram and forces

Theorems 6.8 and 6.10 and corollary 6.12 suggest a phase diagram consistent with the diagram conjectured in [13]. This phase diagram is illustrated in figure 16 in the limit $w \to \infty$. Since there appears to be no other mechanism in this model for additional phases, we extend the results in theorems 6.8 and 6.10 as a conjecture:

Conjecture 7.1. *In the $w \to \infty$ limit, for all $a > 0$ and $b > 0$, we conjecture that the limiting free energy is given by*

$$\kappa(a, b) = \lim_{w\to\infty} \kappa_w(a, b) = \begin{cases} \mathcal{F}(a), & \text{if } b \leqslant a; \\ \mathcal{F}(b), & \text{if } b \geqslant a. \end{cases}$$

In other words, the free energy in the $w \to \infty$ limit decomposes into the free energy of an adsorbing self-avoiding walk in a half-space interacting with either the bottom or the top bounding planes. This is consistent with the results of the Dyck path model examined in [1].

This conjecture implies the presence of three phases in this model. If $a > a_c$ and $a > b$, then $\kappa(a, b) = \mathcal{F}(a)$ and the walk is adsorbed on the bottom bounding plane. If $b > b_c$

and $b > a$, on the other hand, then $\kappa(a, b) = \mathcal{F}(b)$ and the walk is adsorbed on the top bounding plane. These two phases meet along the line $a = b > a_c$ in a line of first-order phase transitions.

Conjecture 7.1 shows that there is a third desorbed phase which is the square $[0, a_c] \times [0, b_c]$. We have proven that this phase includes all the points in the darker shaded region in figure 16 and that the phase boundary separating this phase from the adsorbed phases runs along the lines $a = a_c, 0 \leqslant b \leqslant 1$ and $b = b_c, 0 \leqslant a \leqslant 1$. Consistent with the ideas of adsorbing walks, this phase boundary should correspond to second-order transitions in the $w \to \infty$ limit.

We can examine the forces the walk exerts on the bottom and top bounding planes by examining free energy differences. By lemma 6.9, for all values of $b < 1$,

$$\kappa_w(a, b) - \kappa_{w-1}(a, b) > \kappa_{w-1}(a, 1) - \kappa_{w-1}(a, 1) = 0 \tag{71}$$

and since the inequality is strict, there is a non-zero repulsive force between the bounding planes whenever $b < 1$. This argument is also valid for any $a < 1$ and arbitrary b. Thus, the darker and lighter shaded areas in figure 16 are regimes of a non-zero repulsive force between the bounding planes.

For $a > 1$ and $b > 1$, the walk is attracted to both bounding planes. Thus, if a and b are large enough, then the walk should bridge the gap between the planes and there should be an attractive force between the bounding planes. We were not able to prove the existence of this regime, but numerical results [13] and results from the study of directed versions of this model, strongly support this [1]. This attractive regime is separated from the repulsive regime by a curve of zero force. The presumed limit of this curve in the $w \to \infty$ limit is indicated by a dotted line in figure 16. We conjecture that this limiting curve passes through the point (a_c, a_c) and has asymptotes $a = 1$ and $b = 1$ in the $w \to \infty$ limit and that the three critical curves in this diagram also meet in this point.

In a Dyck path model of a polymer in a slab [1], the zero force curve is known to be independent of w for all $w \geqslant 1$. Is the zero force curve independent of w for all $w \geqslant 1$ in the self-avoiding walk model here? If this is true, then it must coincide with the zero force curve in figure 16.

For small values of (a, b) ($a < a_c$ and $b < a_c$) the walk is desorbed in the $w \to \infty$ limit from both walls of the slab, and we conjecture that for finite w the force will be long ranged and repulsive. For $a > a_c$ while b is below the line of zero force, or for $b > a_c$ while a is to the left of the line of zero force, the walk adsorbs in the $w \to \infty$ limit on either the bottom or top walls of the slab, and we conjecture that the net force for finite w will be short ranged and repulsive.

Finally, for values of (a, b) large enough to be in the adsorbed regime, we conjecture the force to be attractive and long ranged.

8. Conclusions

In this paper, we have examined models of self-avoiding walks confined in a slab and interacting with the bounding planes of the slab. We proved existence of the limiting free energy in this model in corollaries 4.6 and 4.7 in d dimensions.

We next proved a pattern theorem for walks in w-slabs. This was done using a generating function technique due to Hammersley [9], and the theorem is given in theorems 5.13 and in particular by theorem 5.14 and by corollary 5.15. We examined the properties of $\kappa_w(1, 1)$ in section 6.1, proving that $\kappa_w(1, 1) < \kappa_{w+1}(1, 1)$ and that $\lim_{w\to\infty} \kappa_w(1, 1) = \kappa$. These theorems generalize to the function $\kappa_w(a, 1)$: We proved that $\kappa_w(a, 1)$ is a convex function of $\log a$, that $\kappa_w(a, 1) < \kappa_{w+1}(a, 1)$ for all $a > 0$ and finally that $\lim_{w\to\infty} \kappa_w(a, 1) = \mathcal{F}(a)$, where $\mathcal{F}(a)$ is the limiting free energy of the walks in a half-space and adsorbing on the plane.

The function $\kappa_w(a, b)$ was also considered, and we showed that it is a convex function of both $\log a$ and of $\log b$. Along the diagonal, we found that $\liminf_{w\to\infty} \kappa_w(a, a) \geqslant \mathcal{F}(a)$ and this limit exists and the relation is an equality if $a \leqslant \sqrt{a_c}$ (see theorem 6.7, corollary 6.11 and figure 16). In addition, we proved that

$$\lim_{w\to\infty} \kappa_w(a, b) = \begin{cases} \mathcal{F}(a), & \text{if } b \leqslant 1; \\ \mathcal{F}(b), & \text{if } a \leqslant 1, \end{cases} \tag{72}$$

in theorem 6.10, but that $\liminf_{w\to\infty} \kappa_w(a, b) > \kappa$ if both $a > a_c$ and $b > a_c$, where a_c is the critical value of the activity in the adsorption problem (the adsorption transition of a adsorbing walk in a half-space with free energy $\mathcal{F}(a)$ is a_c).

These results are enough to make a firm conjecture about the nature of the phase diagram. We conjecture that the phase diagram in this model is given by figure 16 and by conjecture 7.1. There are three phases in the $w \to \infty$ limit. The first phase is a desorbed phase for small values of (a, b) (both less than $a_c = b_c$ in figure 16). In this phase, the walk exerts a repulsive force on the confining planes, and we prove that this force is non-zero in the shaded regions of figure 16, see equation (71).

For $a > a_c$ and $b < 1$ (or $a < 1$ and $b > b_c$), the walk adsorbs onto the bottom (or top) bounding plane. In this regime there is still a repulsive force, but because the walk tends to stay near one bounding plane, the force should be short ranged—this is suggested by the results for the directed path model in [1]. However, this force is still non-vanishing, as we see in equation (71).

Finally, for both $a > 1$ and $b > 1$ the walk is first attracted to both planes, and may be adsorbed onto the planes if $a > a_c$ and $b > b_c$, as we conjecture in conjecture 7.1. In this regime we expect the repulsive force to change over into a net attractive force along a curve of zero force, which we indicate by the broken curve in figure 16. This curve of zero force separates the regimes of steric stabilization from sensitized flocculation in our model.

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