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Directed paths in a layered environment

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Abstract

A polymer in a layered environment is modeled as a directed path in a layered square lattice composed of alternating A-layers of width w_a and B-layers of width w_b. In this paper we consider general cases of this model, where edges in the path interact with the layers, and vertices in the path interact with interfaces between adjacent layers. The phase diagram exhibits different regimes. In particular, we found that the path may be localized to one layer, be adsorbed on an interface between two layers or be delocalized across layers. We examine special aspects of the model in detail: the asymptotic regimes of the models are examined, and entropic forces on the interfaces are determined. We focus on several different cases, including models with layers of equal or similar width. More general models of layers with different but finite widths, or with one layer of infinite width, are also examined in detail. Several of these models exhibit phase behavior which relate to well-studied polymer phase behavior such as adsorption at an impenetrable wall, pinning at an interface between two immiscible solvents, steric stabilization of colloidal particles and sensitized flocculation of colloidal particles by polymers.

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1. Introduction

A path in a layered lattice may serve as a model of a homopolymer in a layered fluid, say of oil and water. If the monomers in the polymer are hydrophilic, then the polymer will favor conformations with most of its monomers in the water layer. In this case the polymer is ‘localized’ in the water layer. Similarly, if the monomers in the polymer are hydrophobic, then the polymer will favor conformations with most of its monomers in the oil layer and the polymer is ‘localized’ in the oil layer. If the monomers dissolve in both the oil and the water layers, then the polymer will explore conformations with monomers in both layers and the

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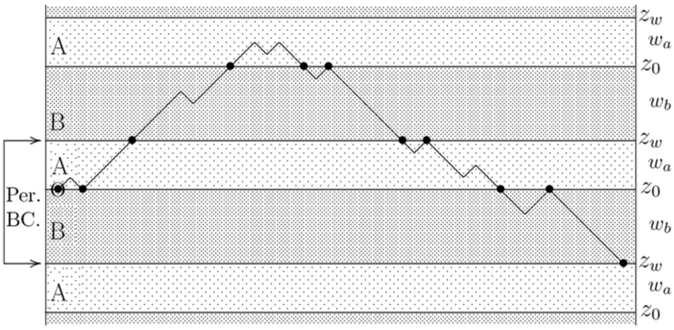

Figure 1. A directed path in a layered environment composed of alternating A-layers of width w_a and B-layers of width w_b. The path starts at the origin and ends at an interface between the two layers. By imposing periodic boundary conditions on the interfaces as indicated by the arrows on the left, this model is equivalent to a path on a tube with circumference $w_a + w_b$. The BA-interfaces in the lattice are the lines $Y = N(w_a + w_b)$ for $N \in \mathbb{Z}$ where the B-layers are below the A-layers at the interface, while the AB-interfaces are the lines $Y = w_a + N(w_a + w_b)$ for $N \in \mathbb{Z}$ where the A-layers are below the B-layers.

polymer is in an 'expanded' or 'delocalized' phase. If the monomers are repelled strongly by both the oil and the water molecules, then the polymer may localize at an interface between the two layers and we say that the polymer is 'adsorbed' or 'pinned' at the interface.

The basic model is illustrated in figure 1. A directed path giving NE- and SE-steps from the origin in the square lattice is the basic object in our model. The square lattice is layered into alternating layers of two types (A-layers of width w_a and B-layers of width w_b) in the Y-direction. A directed path starts at the origin in the layered lattice and ends at an interface between two layers[4]. Each edge in the path which is in an A-layer is weighted by a Boltzmann factor a, while each edge in the path which is in a B-layer is weighted by a Boltzmann factor b. Vertices in the path are assumed to interact with the interfaces between the layers: vertices in the interface with the B-layer below and the A-layer above (this is the BA-interface) are weighted by a Boltzmann factor z_0. Vertices in the interfaces where the A-layer is below and the B-layer is above the interface (this is the AB-interface) are weighted by a Boltzmann factor z_w. Generally, BA-interfaces are given by the lines $Y = N(w_a + w_b)$ for $N \in \mathbb{Z}$, while the AB-interfaces are the lines $Y = w_a + N(w_a + w_b)$ for $N \in \mathbb{Z}$.

In this paper we examine the combinatorics and statistical mechanics of the model of paths in figure 1. We are particularly concerned with the limiting free energy of the model and with the thermodynamic forces which the path exerts on the interfaces between two layers. If these forces are repulsive, then they will tend to widen the layers, while attractive forces will tend to shrink the layers.

Polymers in a lipid–water system have been modeled by self-avoiding walks, random walks and directed path models. Normally, a polymer (such as a protein) is considered to be near a cell-membrane and modeled as a walk or path in a layered environment, see for example references [18, 20, 21]. In these models, there are several phases, including an adsorbed or pinned phase where the polymer is adsorbed onto the interface between the layers, or desorbed phases but localized phases of the polymer in either the lipid or the water layer, and finally a delocalized phase of the polymer over both layers and their interfaces.

[4] This condition is a convenient one—one may relax it, but with an increase in the complexity of the solutions. The phase diagram will not be affected by this.

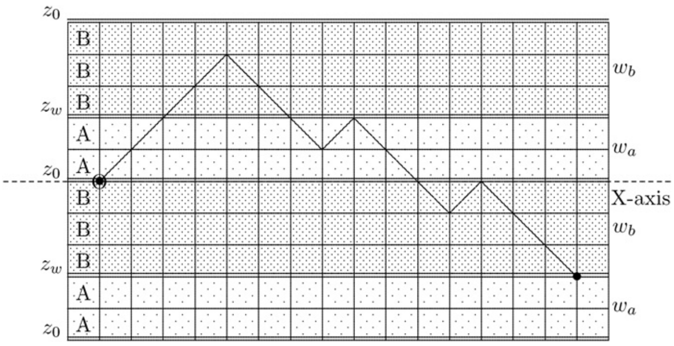

Figure 2. A path in a layered environment with $w_a = 2$ and $w_b = 3$. This path starts in the X-axis and ends at an a AB-interface. It is counted by the generating function g_0. The X-axis is a BA-interface, and the line $Y = w_a$ is an AB-interface. These paths can be turned into a model of paths winding around a tube by introducing periodic boundary conditions which identifies the line $Y = w_a$ with the line $Y = -w_b$.

Studies of a polymer confined to a slit or slab have been carried in [3, 19, 23, 25–28]. These are special cases of the model in figure 1, and are generalized in this paper. Generally, studies of paths or walks confined to slits or slabs are carried out as models of a polymer confined between colloidal particles [19], both as directed models [3, 23] with a focus on the entropic forces in the polymer (see also [22]), and as a self-avoiding walk model from both a theoretical and a numerical point of view [12–14]. In addition, directed path models of a heteropolymer in a layered environment have been examined in [5, 6, 9, 15, 16], while heteropolymers undergoing pinning or localization at an interface between immiscible fluids were considered in [8, 10, 24].

In figure 2, a directed path in a layered lattice of A-layers of width w_a and B-layers of width w_b is illustrated. Edges in the path in the A-layer are weighted by a, and in the B-layer are weighted by b, while visits to the interfaces are weighted by z_0 and z_w as indicated. These paths reduce to several different models in the cases $w_a = w_b = \infty$, $z_0 = z_w$ or $z_0 = z_w = 1$, or $a = 1$ with $b = 0$ or $b = 1$. These models have received considerable attention in the literature [2, 4, 7, 11, 22], and are illustrated in figure 3.

In the case $w_a = w_b = \infty$ and $a = 1$ with $b = 0$ or $b = 1$ several different limiting models are obtained. Putting $z_0 = z$ and $b = 0$ gives a model of a directed path in the half-space $Y \geqslant 0$. If the path has a free endpoint, then it is illustrated in figure 3(a). The generating function is given by

$$g = \frac{z(1 - 2t + \sqrt{1 - 4t^2})}{(1 - 2t)(2 - z(1 - \sqrt{1 - 4t^2})}. \tag{1}$$

If the final vertex of the path is in the X-axis, then this becomes a model of *adsorbing Dyck Paths*. This is a directed model of a polymer adsorbing on a hard wall, and its generating function is given by

$$g = \frac{2z}{2 - z(1 - \sqrt{1 - 4t^2})}. \tag{2}$$

This model is illustrated in figure 3(b). Both these models exhibit critical behavior when $z = z_c = 2$, where the free energy $\mathcal{F}_z$ is non-analytic and for $z > z_c$ becomes dominated by paths with a positive density of visits in the X-axis. This is the adsorbed phase. For $z < 2$, the free energy is dominated by paths with a zero density of visits to the X-axis. See [11].

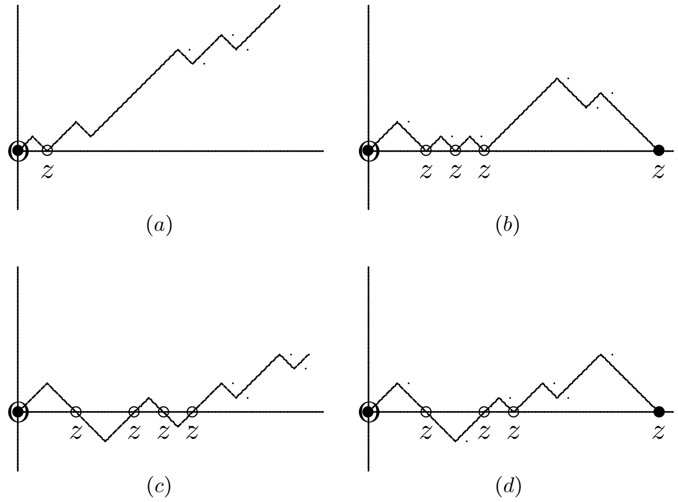

Figure 3. (*a*) A path from the origin in a half-space with the generating function given by equation (1). (*b*) A Dyck path from the origin with the generating function given by equation (2). (*c*) A directed path from the origin with the generating function given by equation (3). (*d*) A Dyck path from the origin with the generating function given by equation (4). Visits of these paths to the *X*-axis are weighted by z.

In the case $w_a = w_b = \infty$ and $a = b = 1$ the paths interact with a defect line (the *X*-axis), but are otherwise unconstrained. The simplest such model is a path from the origin with visits in the *X*-axis weighted by z. The generating function in this case is given by

$$g = \frac{z(1-4t^2+\sqrt{1-4t^2})}{(1-2t)(1-4zt^2+\sqrt{1-4t^2})}. \tag{3}$$

This model is illustrated in figure 3(*c*). If the final vertex in this model is constrained to lie in the *X*-axis, then this simplifies to

$$g = \frac{z}{1-z(1-\sqrt{1-4t^2})}. \tag{4}$$

This model is illustrated in figure 3(*d*). Both these models exhibit critical behavior when $z = z_c = 1$, where the free energy $\mathcal{F}_z$ is non-analytic and for $z > z_c$ becomes dominated by paths with a positive density of visits in the *X*-axis. This is the adsorbed phase. For $z < 1$, the free energy is dominated by paths with a zero density of visits to the *X*-axis. See [11].

In the case $w_a = w_b = w$ and $z_0 = z_w = z$ in figures 1 or 2 we obtain the *diagonal model*. In section 2 we give the recurrences for the generating functions of the diagonal model and solve these explicitly in some simple cases for small values of $w \leqslant 3$ to demonstrate the small width properties of the model. In addition, we determine free energies in these cases, and examine forces of the path on the AB- and BA-interfaces in the model.

In section 3 we consider the general diagonal model. We give a complete solution of the recurrences first introduced in section 2. For finite, but asymptotic values of the width w, we consider several cases of this model. In particular, the model with $b = 0$ is a model of a path in a slit of width w with hard walls. The vertices in the path adsorb onto the walls of the slit with activity z. We recover asymptotic expansions for the free energy and forces in this model in section 3.1, consistent with the solution given in [3]. These results show that the forces can be attractive or repulsive and either short ranged or long ranged. We consider the diagonal model with $a = b$ in section 3.2, and determine as a function of z the free energy and forces in this model.

The interpretations of these results in a model of polymer in a layered environment are as follows: for small values of z the polymer exerts a steric repulsive force on the interfaces between the layers. This will tend to swell the layers. For large z the forces are attractive, and will tend to shrink the width of the layers.

In section 3.3 the case $z = 1$ is considered. We give approximate solutions in two cases, namely when $a \approx b, a \gg b$ or $a \ll b$. We note that this walk is delocalized over the layers in this model, but that there is crossover between a regime where the walk explores conformations delocalized over the A-layers when $a \gg b$, and over the B-layers when $a \ll b$. There is a crossover regime when $a \approx b$, and in the $w \to \infty$ limit the crossover is a phase transition where the path is confined to either the A-layer if $a > b$ or the B-layer of $a < b$, and delocalized over both layers if $a = b$. There is first-order phase transition at $a = b$.

In section 3.4, the case $w \to \infty$ in the diagonal model is examined briefly for arbitrary values of z. We determine the location of a critical adsorption transition as a function of a and b. If $z > 1$, then the path adsorbs or is pinned on the AB-interface in the limit that $w \to \infty$.

In section 4 we consider the general model. We give recurrences and determine the generating function. The general model appears not to have simple solutions. However, the model has many interesting aspects, and we examine several cases. In section 4.1 we examine the case $b = 0$. In this version the model reduces to a directed path in a slit with hard walls. This model was examined in [1, 3]. We examine the correspondences between the generating functions of the layered model and the generating functions of bridges and loops derived in [3].

In section 4.2 we put $z_w = 0$ and $a = b$ with $w_a = w_b = w$ to obtain a path in a slab of width $2w$ with a centered defect line onto which it may absorb. We determine the free energy and show that in the $w_a \to \infty$ limit the model has a pinning transition at $z_0 = 1$. The nature of the entropic forces changes at this point: we determine asymptotic expressions for the free energy and entropic forces. These forces are only repulsive, namely, short-ranged repulsive when $z_0 > 1$ and long-ranged repulsive when $z_0 < 1$.

In section 4.3 we consider a slit-model with an off-centered defect line by putting $w_a = w$ and $w_b = w + m$ with $m \ll w$. This is a model with a defect line near the center of the slit. We determine asymptotic expressions for the free energy and show that in this case there is also a pinning transition as $w_a \to \infty$ at $z_0 = 1$. Coincident with this are a changeover in the force regimes: for small $z_0 < 1$ there is a long-ranged repulsive force, while for large z_0 the walk is pinned on the defect line and the forces on the walls of the slit are short ranged.

A similar result is obtained in section 4.4 where a defect line is close to one of the hard walls of the slit by putting $w_a = w$ and $w_b = wm$ with $m \ll w$. We determine asymptotic expressions for the free energy and for the repulsive net forces on the walls of the slit. In the $w \to \infty$ limit the path is also pinned to the defect plane if $z_0 > 1$. Similar to the case in section 4.3 there are two force regimes: for small $z_0 < 1$ there is a long-ranged repulsive force, while for large z_0 the walk is pinned on the defect line and the forces on the walls of the slit are short ranged.

In section 4.5 we consider the model with $w_b = \infty$. This is a model of the path close to a defect slit of width w_a. For large values of a the path should stay close or in the (finite width) A-layer, while for large b it will be expelled from the A-layer into the (infinite width) B-layer. We determine general expressions for the asymptotic solutions of this model and then consider the asymptotics explicitly for several special cases, namely (1) $z_0 = z_w = 1$ in section 4.5.1, (2) $z_0 = 1$ and $z_w = 0$ in section 4.5.2, (3) $a = b$ in section 4.5.3 and (4) $b = 0$ in

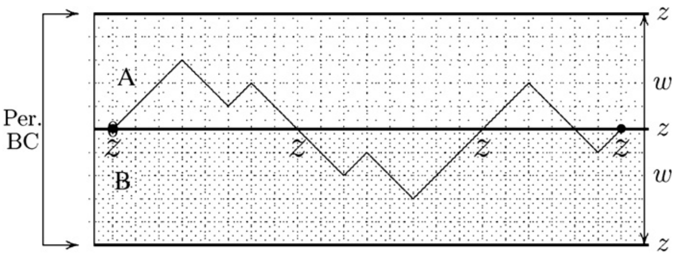

Figure 4. The diagonal model. In this case $w_a = w_b = w$ and $z_0 = z_w = z$ in a layered environment which extends to infinity in the *Y*-direction. This is equivalent to a bilayered model with periodic boundary condition as indicated.

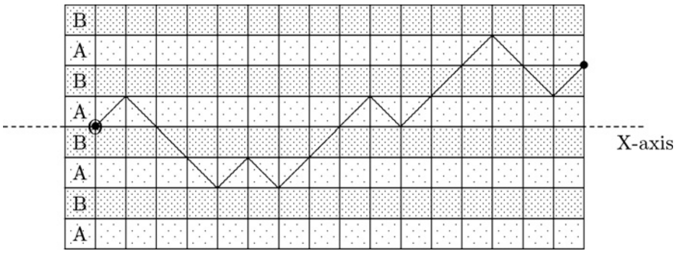

Figure 5. A directed path in a layered environment of thickness $w = 1$. The final vertex has height Nw (where N is an integer).

section 4.5.4. In each model asymptotic expressions for the free energy and forces are determined. The walk is shown to localize to the A-layer for large values of a, and to delocalize to the B-layer for large values of b. In addition, there are pinning transitions of the model at the interfaces for large values of z_0 and z_w. We determine the phase diagram in these cases, and show that there are attractive, repulsive and short-ranged and long-ranged force regimes in this model.

We conclude this paper with some final comments in section 5.

2. The diagonal model

In this section we consider a special case of the model in figure 1, the case where both widths are the same, that is $w_a = w_b = w$, and where both interface interaction strengths are the same, that is $z_0 = z_w = z$ (see figure 4).

In this model, edges whose midpoints have *Y*-coordinates in the intervals $(2Nw, (2N+1)w)$, for $N \in \mathbb{Z}$, are said to be in the A-layer, and each of these edges is weighted by a factor a. On the other hand, edges whose midpoints have *Y*-coordinates in the intervals $((2N-1)w, 2Nw)$, for $N \in \mathbb{Z}$, are said to be in the B-layer, and each one of these edges is weighted by a factor b. For example, if $w = 1$ (see figure 5) then the edges in the A-layers are all edges whose midpoints have *Y*-coordinates in the intervals $(2N, 2N+1)$, while the edges in the B-layers are all edges whose midpoints have *Y*-coordinates in the intervals $(2N-1, 2N)$.

The value of the *Y*-coordinate of a vertex in the path is the *height* of the *vertex*. In this model, all vertices at an interface between two layers are weighted by a factor z. These vertices have heights Nw, for $N \in \mathbb{Z}$.

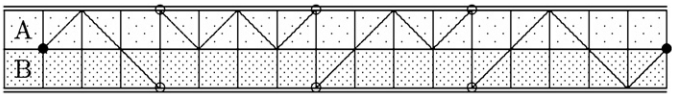

Figure 6. The directed path in figure 5 in a bilayered environment of thickness $2w = 2$ with periodic boundary conditions at the top and bottom boundaries. The path starts at the origin, and the mapping of paths in a layered environment with layers of thickness w to a periodic bilayered slit of width $2w$ is a bijection. An alternative way to consider this model is to imagine the slit to be rolled into a tube of circular cross section with perimeter length $2w$, and with the path winding around the tube, but constrained to end at a vertex in an interface between the two layers.

In general, the diagonal model can be mapped to a model of a directed path in a bilayered slit of width $2w$ with periodic boundary conditions. For example, the path in figure 5 becomes the path in figure 6 in a bilayered slit of width 2 with periodic boundary conditions. Solving for the generating function of paths in this periodic bilayered slit is the equivalent to solving for the generating function of paths in the layered diagonal model. This mapping of the layered lattice to a periodic bilayered slit is also applicable to the general model of figure 2.

The force exerted by the path on the interfaces between layers can be obtained as the derivative of the free energy with respect to the width of the layers, that is

$$f_w = \frac{\mathrm{d}\mathcal{F}_w}{\mathrm{d}w}. \tag{5}$$

The width w is a discrete parameter, therefore one may approximate the force by taking free energy differences. This gives a finite-difference definition of the force $f_w = \mathcal{F}_{w+1} - \mathcal{F}_w$. In what follows, we shall use the former definition, rather than considering finite differences, unless indicated otherwise.

2.1. Recurrences for the generating function of paths in the diagonal model

In order to determine the generating function of paths in the diagonal model we consider paths in the equivalent periodic bilayered slit. The X-axis is chosen at a BA-interface, that is, an interface where the A-layer is above and the B-layer is below.

The paths we are interested in start at the origin and end at an interface, but by reversing directions, we can instead count paths that start at an interface and end at the origin. More precisely, we will determine g_0, the generating function of paths starting at an interface on the Y-axis, and ending on the X-axis.

Defining the following generating functions of paths in the periodic bilayered slit, all of which start at an interface on the Y-axis:

g_0 = paths ending on the X-axis;

g_w = paths ending at an AB-interface (heights $\pm w$);

h_j = paths ending at height j, $j = 1, 2, \ldots, w-1$;

k_j = paths ending at height $-j$, $j = 1, 2, \ldots, w-1$;

where we designate $h_w \equiv k_w \equiv g_w$ and $h_0 \equiv k_0 \equiv g_0$, in what follows.

The generating functions above satisfy the following set of linear recurrence relations:

$$\begin{aligned}
g_0 &= z + zah_1 + zbk_1, & h_1 &= ag_0 + ah_2, & k_1 &= bg_0 + bk_2;\\
g_w &= z + zah_{w-1} + zbk_{w-1}, & h_2 &= ah_1 + ah_3, & k_2 &= bk_1 + bk_3;\\
& & \ldots &= \ldots, & \ldots &= \ldots;\\
& & h_{w-1} &= ah_{w-2} + ag_w, & k_{w-1} &= bk_{w-2} + bg_w.
\end{aligned} \tag{6}$$

Since the paths have last vertices at an interface and so are weighted by an overall factor of z, both g_0 and g_w have the starting term z in the above recurrences.

Generally, the generating function g_0 has leading terms $z(1 + O(a + b))$. If $z \to 0$, then $g_0 \to 0$, since each path carries at least one factor of z. By considering g_0/z instead, the weight of the first vertex in the paths are changed to 1, and $g_0/z \not\to 0$ as $z \to 0$.

2.2. Simple cases

Consider simple cases of the diagonal model for small values of w.

2.2.1. The case $w = 1$. In the case $w = 1$ the recurrences for the generating functions (6) reduce to

$$g_0 = z + zag_w + zbg_w \qquad \text{and} \qquad g_w = z + zag_0 + zbg_0, \tag{7}$$

which can be solved exactly as

$$g_0 = g_w = \frac{z}{1 - z(a + b)}. \tag{8}$$

We introduce the edge generating variable t by substituting $a \to at$ and $b \to bt$ and consider the generating function

$$G_1 = \frac{g_0}{z} = \frac{1}{1 - z(a + b)t}. \tag{9}$$

Putting $a = b = 1$ and expanding G_1 in powers of t yields

$$G_1 = 1 + 2zt + 4z^2t^2 + 8z^3t^3 + 16z^4t^4 + \cdots \tag{10}$$

which corresponds to the number of directed paths from the origin with no restriction on their endpoints. This is to be expected because each path generated by G_1 starts at an interface and ends on the X-axis, so that by reversing the direction of the path and noticing that in this case every vertex is at an interface, we get the desired one-to-one correspondence.

The free energy can be determined from the singularities in G_1, which in this case consist of a simple pole at $t = t_c = 1/(za + zb)$. Hence, the free energy is given by

$$\mathcal{F}_1 = -\log t_c = \log(a + b) + \log z. \tag{11}$$

Setting $z = 1$ gives $G_1 = 1/(1 - (a + b)t)$ and $\mathcal{F}_1 = \log(a + b)$. The free energy is that of a path stepping on edges with weights either a or b. If, in addition we set $a = b = 1$, then $\mathcal{F}_1 = \log 2$ and the number of paths of length n grows as 2^n, as we have already observed.

Finally, setting $b = 0$ yields $G_1 = 1/(1 - zat)$ and $\mathcal{F}_1 = \log a + \log z$. G_1 is the generating function of a directed path confined to a slit of width 1 with hard walls and with steps alternating in the NE- and SE-directions.

2.2.2. The case $w = 2$. In the case $w = 2$ one can solve for the generating functions from the linear system in equation (6): the solutions are given by

$$g_0 = \frac{z}{1 - 2z(a^2 + b^2)t^2}; \qquad g_2 = \frac{z}{1 - 2z(a^2 + b^2)t^2};$$

$$h_1 = \frac{2az}{1 - 2z(a^2 + b^2)t^2}; \qquad k_1 = \frac{2bz}{1 - 2z(a^2 + b^2)t^2}.$$

The generating function of paths starting at the origin and ending at an interface, with the first vertex weighted by $z = 1$ is given by

$$G_2 = \frac{g_0}{z} = \frac{1}{1 - 2z(a^2 + b^2)t^2}, \tag{12}$$

which generates paths of even length from the origin constrained to end at an even height.

The free energy is determined by examining the two simple poles in G_2 to find its radius of convergence. It is given by

$$\mathcal{F}_2 = -\log t_c = \log \sqrt{a^2 + b^2} + \log \sqrt{2z}. \tag{13}$$

Observe that $\mathcal{F}_2$ does not have singular points, so that this model does not have a phase transition which pins the path to an interface: since every step of the path is incident (on one endpoint) with an interface, the z dependence in the free energy per vertex is linear in $\log z$ for all values of z. That is, each path of length n has $\lfloor n/2 \rfloor$ visits to an interface, and by changing z the free energy changes proportional to $\log z$. Thus, there is no adsorption transition in this case.

For fixed values of z the free energy smoothly depends on a and b. While the path does explore more of the A-layer if $a > b$, and vice versa, the crossover from one regime to the other is smooth, and no phase transition localizes the path in the A-layer for a large compared to b.

Setting $a = b = z = 1$ yields $G_2 = 1/(1-4t^2)$ and $\mathcal{F}_2 = \log 2$. G_2 counts paths starting at the origin and ending at an even height. These paths have length $2n$ and the number of such paths grows as 2^{2n}.

Finally, setting $b = 0$ gives $G_2 = 1/(1 - 2za^2t^2)$ and $\mathcal{F}_2 = \log a + \log \sqrt{2z}$. This case corresponds to directed paths in a slit of width 2 with hard walls and with edges weighted by a. The number of such paths grows as $O(2^{n/2})$.

2.2.3. The case $w = 3$. In the case $w = 3$, the solution to the linear system (6) is given by

$$g_0 = g_3 = \frac{(1-at)(1-bt)z}{(1-at)(1-bt) - za^2(1-bt)t^2 - zb^2(1-at)t^2};$$
$$h_1 = h_2 = \frac{zat(1-bt)}{(1-at)(1-bt) - za^2(1-bt)t^2 - zb^2(1-at)t^2};$$
$$k_1 = k_2 = \frac{zbt(1-at)}{(1-at)(1-bt) - za^2(1-bt)t^2 - zb^2(1-at)t^2}.$$

The generating function of paths starting at the origin and ending at an interface, with the first vertex weighted by $z = 1$, is given by

$$G_3 = \frac{g_0}{z} = \frac{(1-at)(1-bt)}{(1-at)(1-bt) - za^2(1-bt)t^2 - zb^2(1-at)t^2}. \tag{14}$$

Taking $z \to 0$ shows that $G_3 \to 1$. This is because the end-vertex of each path generated by G_3 is weighted by z. However, one can factor this last vertex out, in which case $z \to 0$ restricts the paths to slits of width 1 with hard walls (stepping between two lines in each A and B layer, without being able to visit an interface or crossing it). In this context we note that

$$\lim_{z\to 0}\left[\frac{G_3 - 1}{z}\right] = \frac{a^2t}{1-at} + \frac{b^2t}{1-bt}. \tag{15}$$

This is the generating function of paths in two slits of widths 1 with edges weighted by a in one slit and by b in the other slit, as expected.

More generally the free energy is determined by simple poles in G_3, which are the solutions of the cubic polynomial in t given by

$$(1-at)(1-bt) - za^2(1-bt)t^2 - zb^2(1-at)t^2 = 0, \tag{16}$$

for given values of z. In the event that $z \to 0$, this reduces to the roots of $(1-at)(1-bt) = 0$, which shows that the radius of convergence of $\lim_{z\to 0}[(G_3 - 1)/z]$ in this case is given by $t_c = \min\{1/a, 1/b\}$. Therefore, the free energy in this special case is

$$\lim_{z\to 0} \mathcal{F}_3^{\dagger} = \max\{\log a, \log b\}. \tag{17}$$

This is the first model which shows a phase transition. In the AB-plane there is a critical line $a = b$ of first-order transitions separating a phase of paths localized in the A-layer from a phase of paths localized in the B-layer. When $a = b$, the path is localized over both layers, but observe that since $z = 0$ it cannot cross an interface.

More generally the roots of equation (16) are complicated algebraic expressions. If $a = b$, then equation (16) reduces to $(1-at)^2 - 2za^2t^2(1-at)$, whose solutions are given by

$$t = \frac{-1 \pm \sqrt{1+8z}}{4za} \qquad \text{and} \qquad t = \frac{1}{a}. \tag{18}$$

Note that $(\sqrt{1+8z}-1)/(4z) < 1$ if $z \in (0,\infty)$ and $\lim_{z\to 0^+}(\sqrt{1+8z}-1)/(4z) = 1$. Thus, for all values of $z \in [0,\infty)$ the radius of convergence is determined by $t_c = (\sqrt{1+8z}-1)/(4za)$.

The free energy can be determined to be

$$\mathcal{F}_3 = \log\left(\frac{4za}{\sqrt{1+8z}-1}\right), \qquad \text{if} \quad a = b. \tag{19}$$

There is no non-analiticity in $\mathcal{F}_3|_{a=b}$ with increasing a for any value of $z \in [0,\infty)$ along the line $a = b$.

On the other hand, if one fixes z at a non-zero value, and assume that $at < 1$ and $bt < 1$, then equation (16) can be rewritten as

$$1 - \frac{za^2t^2}{1-at} - \frac{zb^2t^2}{1-bt} = 0. \tag{20}$$

By the intermediate value theorem, there is a solution for $t \in (0, 1/a)$ if $a > b$ and for $t \in (0, 1/b)$ if $a < b$. This shows that

$$\mathcal{F}_3 \geqslant \max\{\log a, \log b\}, \qquad \text{if} \quad a \neq b. \tag{21}$$

Furthermore, as $z \to 0^+$, $\mathcal{F}_3$ approaches $\mathcal{F}_3^{\dagger}$ in equation (19) from above.

Taking $b = 0$ reduces equation (16) to

$$(1-at) - za^2t^2 = 0 \tag{22}$$

with solutions $t_c = (\pm\sqrt{1+4z}-1)/2za$. This shows that the free energy is

$$\mathcal{F}_3 = \log\left(\frac{2za}{\sqrt{1+4z}-1)}\right), \qquad \text{if} \quad b = 0. \tag{23}$$

There is no non-analiticity in $\mathcal{F}_3|_{b=0}$ with increasing a for any value of $z \in (0,\infty)$ along the line $b = 0$. However, taking $z \to 0^+$ gives the free energy in equation (14).

2.2.4. Forces for small values of w. For small values of width w, entropic forces can be computed by using the finite-difference definition $f_w = \mathcal{F}_w - \mathcal{F}_{w-1}$. For example, if $b = 0$ then the forces on the walls of a slit of widths $w = 2$ and $w = 3$ are given by

$$\begin{aligned} f_2 &= (\mathcal{F}_2 - \mathcal{F}_1)_{b=0} = \log\sqrt{2/z}, \\ f_3 &= (\mathcal{F}_3 - \mathcal{F}_2)_{b=0} = \log\left(\frac{\sqrt{2z}}{\sqrt{1+4z}-1}\right). \end{aligned} \tag{24}$$

In particular, for $0 \leqslant z < 2$ the forces are repulsive (positive), but become attractive (negative) when $z > 2$. There is no net force when $z = 2$.

More generally, one may compute free energy differences for non-zero values of b. In this case the path steps across many layers, and a positive free energy difference will indicate a force to 'stretch' the layers, while a negative difference shows a force which will 'contract' the layers. In the simplest case above (for $w = 2$) we see that

$$f_2 = \mathcal{F}_2 - \mathcal{F}_1 = \log\left(\frac{\sqrt{a^2+b^2}}{a+b}\right) + \log\sqrt{2/z}. \tag{25}$$

In this case there is a critical value of z given by $z_c = 2(a^2+b^2)/(a+b)^2$. For values of $z < z_c$, the force tends to stretch the layers, and for $z > z_c$ the force tends to contract the layers.

3. The general solution of the diagonal model

In this section we consider the solution of the generating function for general values of w in the diagonal model. The presentation is simplified by making use of the following transformations:

$$a \to at = \frac{p}{1+p^2} \qquad \text{and} \qquad b \to bt = \frac{q}{1+q^2} \tag{26}$$

where once again t generates edges (steps) in the paths, weighted by a in the A-layer and by b in the B-layer. Solving for p and q in the transformations (26) gives

$$p = \frac{1 \pm \sqrt{1-4a^2t^2}}{2at} \qquad \text{and} \qquad q = \frac{1 \pm \sqrt{1-4b^2t^2}}{2bt}. \tag{27}$$

The selection of the minus signs in these solutions yields power series with non-negative coefficients for p and q, and we call these the 'physical solutions'. These solutions generate Dyck paths with vertices weighted by at or by bt respectively.

Using the transformations (26) one can solve the linear system (6) in terms of p and q. The solution is given by the following theorem:

Theorem 3.1. *The solution to the system of equations (6) is given by*

$$g_0 = g_w = \frac{z}{1 - \frac{z(p^2+p^w)}{(1+p^2)(1+p^w)} - \frac{z(q^2+q^w)}{(1+q^2)(1+q^w)}}$$

$$h_i = \frac{z(p^{-i}(1-p^w) - p^i(1-p^{-w}))}{1 - \frac{z(p^2+p^w)(p^{-w}-p^w)}{(1+p^2)(1+p^w)} - \frac{z(q^2+q^w)(p^{-w}-p^w)}{(1+q^2)(1+q^w)}} \qquad i = 1, \ldots, w-1$$

$$k_i = \frac{z(q^{-i}(1-q^w) - q^i(1-q^{-w}))}{1 - \frac{z(p^2+p^w)(q^{-w}-q^w)}{(1+p^2)(1+p^w)} - \frac{z(q^2+q^w)(q^{-w}-q^w)}{(1+q^2)(1+q^w)}} \qquad i = 1, \ldots, w-1.$$

Proof. The solutions are verified by direct substitution and simplification of the generating functions in the recurrences. □

For $w \leqslant 3$ these solutions reduce to the cases given in section 2.2. For finite values of w, the generating function of interest is g_0 given by

$$g_0 = \frac{1}{1 - \frac{z(p^2+p^w)}{(1+p^2)(1+p^w)} - \frac{z(q^2+q^w)}{(1+q^2)(1+q^w)}}. \tag{28}$$

It is interesting to note the high degree of symmetry in this solution. Not only are there the obvious symmetries such as $(p, q) \leftrightarrow (q, p)$, but there also are symmetries of the form

$$\frac{p^2+p^w}{(1+p^2)(1+p^w)} =$$

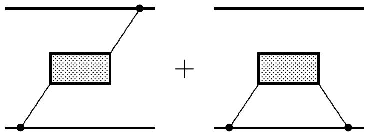

Figure 7. The term $(p^2+p^w)/(1+p^2)(1+p^w)$ in the denominator of equation (28) generates paths in a slit of width w which start at the bottom bounding line of the slit and end the first time they reach either one of the two bounding lines of the slit.

$(p^2 \leftrightarrow p^w)$ and $(q^2 \leftrightarrow q^w)$, as well as $(p \leftrightarrow 1/p)$ and $(q \leftrightarrow 1/q)$. Note also the separation of the p and q terms in the denominator of equation (28).

Consider the term $(p^2+p^w)/(1+p^2)(1+p^w)$. By setting $a = 1$, so that $p = (1-\sqrt{1-4t^2})/2t$, one can verify that this term generates paths in a slit of width w starting at the bottom bounding line of the slit, and ending on the first vertex that visits either bounding line of the slit. For example,

$$\frac{p^2+p^w}{(1+p^2)(1+p^w)} = \begin{cases} t & \text{if} \quad w=1, \\ 2t^2 & \text{if} \quad w=2, \\ \frac{t^2}{1-t} & \text{if} \quad w=3, \\ \frac{t^2}{1-2t^2} & \text{if} \quad w=4, \\ \frac{t^2(1-t)}{1-t-t^2} & \text{if} \quad w=5, \end{cases}$$

and so on. If $w = 1$ then there is only one path starting in the bottom bounding line and ending the first time it reaches either one of the two bounding lines: it is the path of length one with a NE-step to the top bounding line. If $w = 2$, then there are two paths (both of length 2) starting in the bottom bounding line and ending the first time they reach either one of the two bounding lines: a path with two consecutive NE-steps (it ends at the top bounding line), and a path with a NE-step followed by a SE-step (it ends at the bottom bounding line).

One may similarly examine the other expressions above. These observations explain the structure of the generating functions obtained in theorem 3.1 and equation (28). We illustrate this in figure 7.

Selecting the negative signs in the transformations (27) and substituting these into g_0, as given by (28), give a generating function which becomes singular when $t \to 1/2a$ or $t \to 1/2b$, because these are branch points in p and q. The radius of convergence of g_0 is determined either by these branch points, or by the curve of simple poles in the pq-plane given implicitly by solutions of

$$\begin{aligned}(1+p^2)&(1+p^w)(1+q^2)(1+q^w) \\ &= z(p^2+p^w)(1+q^2)(1+q^w) + z(q^2+q^w)(1+p^2)(1+p^w), \end{aligned} \tag{29}$$

for given values of z. This equation is obtained by equating the denominator of g_0 to zero and rearranging terms. Determining the exact solutions of this equation is generally not possible, even in simplified models. Therefore we shall consider mostly some special cases and asymptotic solutions.

3.1. The case $b = 0$.

In the case $b = 0$ we have $q = 0$ as well, and we obtain the model in figure 8. This corresponds to a model of paths in a slit of width w [3], adsorbing onto the hard walls with activity z, and

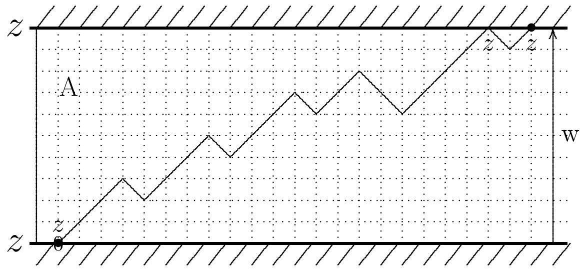

Figure 8. A path in a slit of width w with hard walls. This model is obtained by setting $b = 0$ in equation (29). This in turn sets $q = 0$, and the roots of equation (30) give the critical values of t.

with edges weighted by a. Equation (29) reduces to

$$(1 + p^2)(1 + p^w) = z(p^2 + p^w). \tag{30}$$

For $1 \leqslant w \leqslant 3$ this reproduces the cases examined in section 2.2. Exact solutions can also be obtained for $w = 4, 5, 6, 8, 10, 12$ using Maple 10 [17].

For finite values of w asymptotic expressions for the free energy have been obtained in [3]. These are

$$\mathcal{F}_w = -\log t_c$$
$$\simeq \begin{cases} \log\left(\dfrac{za}{\sqrt{z-1}}\right) + \dfrac{(z-2)^2}{2(z-1)\sqrt{(z-1)^w}} + O(w(z-1)^{-w}), & \text{if} \quad z \geqslant 2; \\ \log(2a) - \dfrac{\pi^2}{2w^2} + \dfrac{2\pi^2 z}{(2-z)w^3} + O(w^{-4}), & \text{if} \quad z < 2. \end{cases} \tag{31}$$

If $w \to \infty$ this reduces to the free energy of an adsorbing Dyck path on the X-axis (see, for example, equation (2):

$$\mathcal{F}_\infty = \begin{cases} \log\left(\dfrac{az}{\sqrt{z-1}}\right), & \text{if} \quad z \geqslant 2; \\ \log(2a), & \text{if} \quad z < 2. \end{cases} \tag{32}$$

Setting $a = 1$ reduces this case to the model in figure 3(a) of an adsorbing directed path in a half-space. There is an adsorption transition at $z_c = 2$, and for $z > z_c$ density of the visits to the hard walls is positive, while for $z < z_c$ it is zero. For finite values of w there is a crossover between an expanded regime for small z to a regime where the path is close to one of the hard walls. This is not a phase transition, but it has effects on the entropic force exerted by the path on the walls of the slit.

The entropic forces can be determined by taking the derivative of $\mathcal{F}_w$ with respect to w:

$$f_w \simeq \begin{cases} -\dfrac{(z-2)^2 \log(z-1)}{4(z-1)\sqrt{(z-1)^w}} + O((z-1)^{-w}), & \text{if} \quad z \geqslant 2; \\ \dfrac{\pi^2}{w^3} - \dfrac{6\pi^2 z}{(2-z)w^4} + O(w^{-5}), & \text{if} \quad z < 2. \end{cases} \tag{33}$$

For small values of $z < 2$, the force is positive (repulsive) and it decays as an inverse power with increasing w—this is a long-ranged repulsive force. For large values of $z > 2$ the force is negative (a net attraction between the walls of the slit) and it decays exponentially with increasing w—this is a short-ranged attractive force.

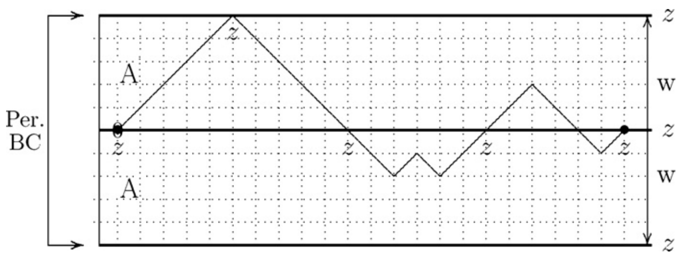

Figure 9. A path in a slit of width $2w$ with periodic boundary conditions (as denoted by the arrows on the left) and with two evenly spaced defect lines. The path can terminate at either one of the defect lines. This model is obtained by setting $b = a$ in equation (29). This results in $q = p$, and the roots of equation (34) give the critical values of t.

3.2. The case $b = a$

If we set $b = a$, and hence $q = p$, we obtain the model in figure 9. In this case, the denominator of g_0, given in equation (29), reduces to

$$(1 + p^2)(1 + p^w) = 2z(p^2 + p^w). \tag{34}$$

If one substitutes $z \to z/2$, then this becomes identical to equation (30). In other words, the same remarks apply here as in section 3.1, but with z replaced by $2z$. The free energy in this model is

$$\mathcal{F}_w = -\log t_c$$
$$\simeq \begin{cases} \log\left(\dfrac{2za}{\sqrt{2z-1}}\right) + \dfrac{2(z-1)^2}{(2z-1)\sqrt{(2z-1)^w}} + O(w(2z-1)^{-w}), & \text{if} \quad z \geqslant 1 \\ \log(2a) - \dfrac{\pi^2}{2w^2} + \dfrac{2\pi^2 z}{(1-z)w^3} + O(w^{-4}), & \text{if} \quad z < 1, \end{cases} \tag{35}$$

and if $w \to \infty$ this reduces to the free energy of a directed path interacting with a defect line in the lattice (see, for example, [11]). This is a model of a polymer being pinned at the interface between two fluids. There is a pinning transition at $z_c = 1$. If $z < 1$, then the path is expanded over the layers, but for $z > 1$ the path has a positive density of visits to the defect lines and is pinned to it.

For finite values of w there is no phase transition between the expanded and pinned phases, but there are two regimes as suggested by the asymptotic expressions for the free energy above. The path exerts an entropic force on the interfaces between layers, and for large values of z this is an attractive force, bringing together the BA- and AB-interfaces, while for small values of z it will be a repulsive force. Asymptotic expressions for these forces can be determined by taking the derivative of $\mathcal{F}_w$ with respect to w:

$$f_w \simeq \begin{cases} -\dfrac{(z-1)^2 \log(2z-1)}{2(2z-1)\sqrt{(2z-1)^w}} + O((2z-1)^{-w}), & \text{if} \quad z \geqslant 1; \\ \dfrac{\pi^2}{w^3} - \dfrac{6\pi^2 z}{(1-z)w^4} + O(w^{-5}), & \text{if} \quad z < 1. \end{cases} \tag{36}$$

Similarly to the case when $b = 0$, for small values of $z < 1$, the force is positive (repulsive) and long ranged because it decays as an inverse power of w with increasing w. This repulsive force vanishes to order $O(w^{-5})$ when $z = z_* = w/(w + 6)$, and we call z_* the zero force

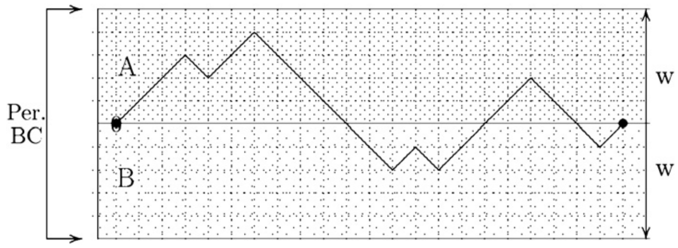

Figure 10. A path in a bilayered slit with periodic boundary conditions of width $2w$, and with two layers of equal width w. This model is obtained by setting $z = 1$. Then $q = p$ and the critical values of t are obtained by examining the roots of equation (38).

point. For $z < z_*$ the force is repulsive and long ranged, but for z in the range $(z_*, 1)$ is an attractive long-ranged force.

For large values of $z > 1$ the force is negative (inducing a net attraction between the interfaces of the layers) and short ranged because it decays exponentially in w with increasing w.

Hence, this model exhibits three force regimes: for small values of $z < z_*$ there is a repulsive short-ranged force which becomes attractive short ranged for $z_* < z < 1$ and which in turn becomes an attractive long-range force when $z > 1$. With increasing values of w the regime of attractive short range forces narrows and disappears in the $w \to \infty$ limit.

3.3. The case $z = 1$

If we set $z = 1$ this becomes a model of a path in a bilayered environment with alternating A-layers and B-layers of equal thickness w, as illustrated in figure 10. The generating function is given by

$$g_0|_{z=1} = \frac{(1+p^2)(1+q^2)(1+p^w)(1+q^w)}{(1+p^{w+2})(1+q^{w+2}) - (p^2+p^w)(q^2+q^w)}, \tag{37}$$

which generates directed paths in A- and B-layers of width w, starting at the origin and terminating at an interface between the two layers. Roots in the denominator of the generating function are given by solutions of

$$(1+p^{w+2})(1+q^{w+2}) = (p^2+p^w)(q^2+q^w). \tag{38}$$

Consider first the case $b > a$ (the case $a > b$ can be obtained by interchanging a and b in the solution). To determine an approximate solution for p, we proceed by solving for q in terms of p:

$$q(p) = \frac{a(1+p^2)\left(1 - \sqrt{1 - \frac{4b^2p^2}{a^2(1+p^2)^2}}\right)}{2bp}. \tag{39}$$

We write the denominator in equation (38) as

$$q - \left(\frac{p^w(q^2-p^2) + q^2p^2 - 1}{p^w(p^2q^2-1) + q^2 - p^2}\right)^{\frac{1}{w}} = 0 \tag{40}$$

and note that asymptotic solutions can be obtained by expanding this as

$$q - 1 - \frac{1}{w}\log\left(\frac{p^2q^2-1}{q^2-p^2}\right) - \frac{1}{2w^2}\left[\log\left(\frac{p^2q^2-1}{q^2-p^2}\right)\right]^2 - \cdots = 0 \tag{41}$$

asymptotically in w.

Substitute the expression for q in equation (39) into this and assume that asymptotically in w,

$$p = \mathrm{e}^{\frac{\mathrm{i}\pi}{2w}}\left(c_0 + \frac{c_1}{w} + \frac{c_2}{w^2} + \frac{c_3}{w^3} + \frac{c_4}{w^4} + O(w^{-5})\right). \tag{42}$$

Substituting this ansatz for p into the denominator, and again expanding asymptotically in w allows one to determine the c_i term-by-term in the expansion. The results are

$$c_0 = \frac{b - \sqrt{b^2 - a^2}}{a}, \tag{43}$$

and

$$c_1 = -\frac{\mathrm{i}\pi c_0}{2}, \qquad c_2 = -\frac{\pi^2 c_0}{8}, \qquad c_3 = \frac{\mathrm{i}\pi^3 c_0}{48}, \qquad \text{and} \qquad c_4 = \frac{\pi^4 c_0}{384}. \tag{44}$$

The asymptotic expression of the critical value of t is obtained from $at_c = p/(1+p^2)$. The result is

$$at_c \simeq \frac{a}{2b}. \tag{45}$$

The physical root is given by the positive sign. A similar argument gives the asymptotic behavior of t_c in the case $a > b$.

This result shows that if $b \gg a$, then the path steps mostly in the B-layers, and only a vanishing fraction of its edges will be in the A-layer, which it must cross to move between B-layers. Since the path is delocalized over the lattice, there is no residual dependence on w.

If $a \approx b$, then it follows from equation (39) that $aq \approx bp$. Substituting $q = bp/a$ into the denominator gives a polynomial in p of degree $2w+4$:

$$(p^{w+2}+1)((pb/a)^{w+2}+1) - (p^w + p^2)((bp/a)^w + (bp/a)^2) = 0. \tag{46}$$

The roots of this polynomial is evidently given by roots of unity, or roots of unity multiplied by the factor $\sqrt{a/b}$. Thus, assume that p is approximated by equation (42) and substitute and expand the result asymptotically in w to determine the c_i term-by-term. The results are

$$\begin{aligned} c_0 &= \sqrt{\frac{a}{b}}, \qquad c_1 = -\frac{\mathrm{i}\pi c_0}{2}, \qquad c_2 = -\frac{\pi^2 c_0}{8}, \\ c_3 &= \frac{\mathrm{i}\pi^3 c_0}{48}, \qquad \text{and} \qquad c_4 = \frac{\pi^4 c_0}{384}, \end{aligned} \tag{47}$$

and with this selection the denominator of g_0 is equal to $2w(a-b)^2/b^2 + O((a-b)^3$ so that it vanishes up to terms of order $O(w(a-b)^2)$. In other words, this solution is good when $w(a-b)^2 = o(1)$. In other words, with increasing w, the crossover regime between $a \gg b$ and $a \ll b$ will shrink proportional to $1/\sqrt{w}$.

From this one can determine the critical value of a by examining $at = p/(1+p^2)$. The result is that

$$at_c \simeq \frac{\sqrt{ab}}{a+b} = \frac{1}{2} - \frac{(a-b)^2}{16a^2} + \cdots. \tag{48}$$

This result shows that if $a \approx b$, then the path is delocalized over the lattice stepping freely in both layers. Since this is a delocalized regime, there is no residual dependence on w. A similar result is obtained if one examines this model by approximating q instead, with b and a interchanged in the results.

The free energy of the model can be determined from these approximations of t_c:

$$\mathcal{F}_w \simeq \begin{cases} \log 2a, & \text{if} \quad \text{a} \gg \text{b}; \\ \log a - \log\left(\dfrac{\sqrt{ab}}{a+b}\right), & \text{if} \quad \text{a} \gtrapprox \text{b}; \\ \log b - \log\left(\dfrac{\sqrt{ab}}{a+b}\right), & \text{if} \quad \text{b} \gtrapprox \text{a}; \\ \log 2b, & \text{if} \quad \text{b} \gg \text{a}. \end{cases} \tag{49}$$

Thus, for large $a \gg b$, then path steps in A-layers, with only a vanishing number of steps in B-layers, while when a approaches b the path will delocalize over both layers. Thus, both regimes in this model are delocalized.

3.4. The case $w \to \infty$

Assume that $p < 1$ and $q < 1$ and consider the model in the limit $w \to \infty$. Then, the generating function g_0 becomes

$$\begin{aligned} g_\infty = \lim_{w\to\infty} g_0 &= \frac{z}{1 - \frac{zp^2}{1+p^2} - \frac{zq^2}{1+q^2}} \\ &= \frac{2z^2}{2(1-z) + z(\sqrt{1-4a^2t^2} + \sqrt{1-4b^2t^2})}. \end{aligned} \tag{50}$$

If $z = 1$, the above reduces to

$$g_\infty = \frac{1}{1 - \frac{p^2}{1+p^2} - \frac{q^2}{1+q^2}} = \frac{2}{(\sqrt{1-4a^2t^2} + \sqrt{1-4b^2t^2})}, \tag{51}$$

which has branch-points in the ab-plane along the lines $t = 1/2a$ and $t = 1/2b$. The free energy in this case is given by

$$F_\infty(a, b) = \max\{\log(2a), \log(2b)\}, \tag{52}$$

Note that these critical lines ($t = 1/2a$ and $t = 1/2b$) correspond to an A- and a B-phase, respectively. If $a > b$, the walk has free energy determined by paths localized in the A-layer. On the other hand, if $b > a$, the walk has free energy determined by paths localized in the B-layer.

Consider next the case where $0 < z < 1$, in which case $2(1 - z) > 0$. Hence, the singularities in g_∞ in equation (50) are still lines of branch points due to the square root terms, and the free energy is given by equation (52).

Finally, consider the case $1 < z$. In this case, the radius of convergence of the generating function g_∞ is given by the zeros of the denominator in equation (50). One can rewrite the denominator in this case and solve for t from

$$(\sqrt{1-4a^2t^2} + \sqrt{1-4b^2t^2}) = \frac{2(z-1)}{z}. \tag{53}$$

The left-hand side takes values between 0 and 2 as t varies between 0 and $\min\{1/2a, 1/2b\}$. If $a < b$, then there are solutions to (53) if $\sqrt{1-(a/b)^2} \leqslant 2(z-1)/z \leqslant 2$. Thus, if $a < b$, there are solutions if

$$z \geqslant \frac{2}{2 - \sqrt{1-(a/b)^2}}. \tag{54}$$

More generally, we define

$$z_c = \begin{cases} \dfrac{2}{2-\sqrt{1-(a/b)^2}}, & \text{if} \quad a \leqslant b, \\ \dfrac{2}{2-\sqrt{1-(b/a)^2}}, & \text{if} \quad a > b. \end{cases} \tag{55}$$

Therefore, if $a \neq b$ and $z \geqslant z_c$ the solutions to equation (53) are given by

$$t_c^2 = \frac{(z-1)((1-z)(a^2+b^2)+\sqrt{z^2(a^2+b^2)^2+4(1-2z)a^2b^2})}{z^2(a^2-b^2)^2}. \tag{56}$$

If $z \to z_c^+$, this becomes $t_c^2 = \min\{1/4a^2, 1/4b^2\}$.

Hence, the free energy of this model in the limit $w \to \infty$ is given by

$$\mathcal{F}_\infty = \begin{cases} \max\{\log 2a, \log 2b\}, & \text{if} \quad z \leqslant z_c; \\ -\log t_c, & \text{if} \quad z > z_c, \end{cases} \tag{57}$$

where t_c and z_c are defined in equations (56) and (55), respectively. In the abz-parameter space this model has several critical surfaces. One critical surface is a first-order phase transition given by $a = b$ and $z \leqslant z_c$. A second critical surface is given by $z = z_c$, which is a transition from the localized phases (with the path localized to the A-phase or the B-phase) to an adsorbed phase where the path adsorbs onto the AB- or BA-interfaces. These critical surfaces meet on the curve $a = b$ and $z = z_c$, which is a curve of multicritical points.

In the case that $a = b$ as well, then $z_c = 1$, and if $z > 1$ the solutions for t_c are obtained by solving

$$4a^2t^2 = 1 - \left(\frac{z-1}{z}\right)^2. \tag{58}$$

This has real solutions given by $t_c = \sqrt{1-((z-1)/z)^2}/2a$. Observe that as $z \to 1^+$, $t_c \to 1/2a$. This shows that the free energy is given by

$$F_\infty(a,a) = \begin{cases} \log 2a, & \text{if} \quad z \leqslant 1, \\ \log 2a + \log\sqrt{\dfrac{2z-1}{z^2}}, & \text{if} \quad z > 1. \end{cases} \tag{59}$$

Increasing z from $z < 1$ shows that branch point singularities in the generating function give way to simple poles for $z > 1$. In other words, there is a phase change in this model, from phases dominated by paths localized in either the A- or B-layers for ($z < 1$), to a phase of paths pinned onto the AB- or BA-interfaces with free energy containing a term dependent on the value of z (and therefore a positive density of visits to the interfaces).

4. The general model

In this section we consider the general model (see figure 11) of directed paths in a layered square lattice with two types of layers alternating in the Y-direction: an A-layer of width w_a and a B-layer of width w_b.

This is the model in figures 1 and 11 of a path starting at the origin and ending at an interface between the A- and B-layers (or alternatively, starting at an interface between the two layers, and having its final vertex on the X-axis). The X-axis will be chosen to be at a BA-interface, as in figure 2. This is also a model of directed paths in a bilayered slit of width $w_a + w_b$ with periodic boundaries, as depicted in figure 11.

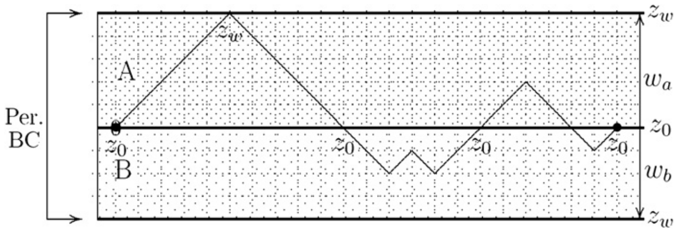

Figure 11. The general model: a bilayered lattice with two alternating layers of thicknesses w_a and w_b, and two different interactions with the interfaces given by z_0 and z_w. By introducing periodic boundary conditions as indicated by the arrows on the left, the model wraps around on a cylinder of circumference $w_a + w_b$ with two defect lines along the interfaces between the layers.

As before we have generating variables for edges (t), weights for edges in the A-layers (a) and in the B-layers (b), for vertices at a BA-interface (z_0), and for vertices at an AB-interface (z_w).

Let $w \equiv (w_a, w_b)$ and introduce the following generating functions of paths starting at an interface on the Y-axis and ending at a prescribed height:

g_0 = paths ending on the X-axis;

g_w = paths ending at height w_a (or w_b by periodicity);

h_j = paths ending at height j, $j = 1, 2, \ldots, w_a - 1$;

k_j = paths ending at height $-j$, $j = 1, 2, \ldots, w_b - 1$,

where we designate $h_{w_a} \equiv k_{w_b} \equiv g_w$ and $h_0 \equiv k_0 \equiv g_0$ in what follows.

Recurrences for these generating functions can be determined by considering the equivalent periodic bilayered lattice, similar to the situation in figures 5 and 6. We obtain a system of linear equations given by

$$
\begin{aligned}
g_0 &= z_0 + z_0 a h_1 + z_0 b k_1, \\
g_w &= z_w + z_w a h_{w_a-1} + z_w b k_{w_b-1},
\end{aligned}
\tag{60}
$$

where h_i and k_j are solutions of

$$
\begin{aligned}
h_1 &= a g_0 + a h_2, & k_1 &= b g_0 + b k_2; \\
h_2 &= a h_1 + a h_3, & k_2 &= b k_1 + b k_3; \\
\ldots &= \ldots, & \ldots &= \ldots; \\
h_{w_a-1} &= a h_{w_a-2} + a g_w, & k_{w_b-1} &= b k_{w_a-2} + b g_w.
\end{aligned}
$$

The solutions to these recurrences are given by the following theorem:

Theorem 4.1. *Define the functions*

$$
c_s = \frac{p^2 - p^{2w_a}}{(1+p^2)(1-p^{2w_a})} + \frac{q^2 - q^{2w_b}}{(1+q^2)(1-q^{2w_b})}
\tag{61}
$$

and

$$
c_o = \frac{p^{w_a}(1-p^2)}{(1+p^2)(1-p^{2w_a})} + \frac{q^{w_b}(1-q^2)}{(1+q^2)(1-q^{2w_b})}
\tag{62}
$$

where we define p and q via the transformations

$$
a \to at = \frac{p}{1+p^2}, \qquad b \to bt = \frac{q}{1+q^2}.
\tag{63}
$$

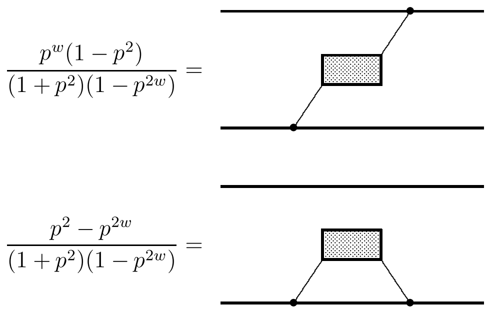

Figure 12. The term $p^w(1-p^2)/(1+p^2)(1-p^{2w})$ in (62) generates paths in a slit of width w, from the origin, and terminating on the first intersection with the top wall of the slit, without visiting the bottom wall. The term $(p^2-p^{2w})/(1+p^2)(1-p^{2w})$ in (61) generates paths in a slit of width w, from the origin, and terminating on the first intersection with the bottom wall of the slit, without visiting the top wall. Summing these terms produces figure 7.

Then the solutions for g_0 and g_w in equations (60) are given by

$$g_0 = \frac{z_0(1-z_w(c_s-c_o))}{1-(z_w+z_0)c_s+z_0z_w\left(c_s{}^2-c_o{}^2\right)}, \tag{64}$$

and

$$g_w = \frac{z_w\,(1-z_0\,(c_s-c_o))}{1-(z_w+z_0)\,c_s+z_0z_w\left(c_s{}^2-c_o{}^2\right)}. \tag{65}$$

The solutions for h_i and k_i in equations (60) are

$$h_i = \frac{z_w(1-z_0(c_s-c_o))(p^i-p^{-i})+z_0(1-z_w(c_s-c_o))(p^{w_a-i}-p^{-(w_a-i)})}{(p^{w_a}-p^{-w_a})\left(1-(z_w+z_0)c_s+z_0z_w\left(c_s{}^2-c_o{}^2\right)\right)}, \tag{66}$$

and

$$k_i = \frac{z_w(1-z_0(c_s-c_o))(q^i-q^{-i})+z_0(1-z_w(c_s-c_o))(q^{w_b-i}-q^{-(w_b-i)})}{(q^{w_b}-q^{-w_b})(1-\left(z_w+z_0)c_s+z_0z_w\left(c_s{}^2-c_o{}^2\right)\right)}. \tag{67}$$

Proof. The theorem can be verified by direct substitution and simplification of the expressions into the recurrences in equations (60). □

Observe that the first term in c_s counts paths that start at the origin, step into the A-layer, and terminate on first return to the X-axis before reaching the AB-interface at w_a. The edges of these paths remain entirely inside the A-layer, and the paths have only two vertices at the interfaces between layers: both vertices are on the X-axis. These are *loops* in the A-layer. Similarly, the second term in c_s counts loops in the B-layer. We illustrate this in figure 12.

Note also that the first term in c_o counts paths that start at the origin, step into the A-layer, and terminate on first intersection with the AB-interface at w_a without visiting the X-axis again. The edges of these paths remain entirely inside the A-layer, and the paths have only two vertices at the interfaces between layers: the initial vertex is on the X-axis and the final vertex is at the AB-interface. This is a *bridge* in the A-layer. Similarly, the second term in c_o counts bridges in the B-layer. We illustrate this in figure 12.

Let g_0 and g_w be defined as above. Then each path ending on the X-axis (the BA-interface) is either a single vertex (z_0), or is a bridge from the BA- to the AB-interface followed by a

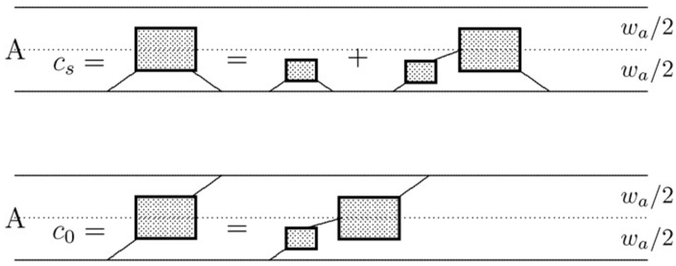

Figure 13. A proof by picture that $c_s(w_a, w_b) - c_o(w_a, w_b) = c_s(w_a/2, w_b/2)$. This illustrates the identity for path confined to the A-layer. Similar more general drawings prove it generally.

path counted by g_w (crossing back to the BA-interface), or is a loop starting and ending in the BA-interface followed by a path counted by g_0. Hence

$$g_0 = z_0 + z_0 c_o g_w + z_0 c_s g_0.$$

Similarly, a path ending in the AB-interface is either a single vertex (z_w), or is a bridge from the AB-interface to the BA-interface followed by a path counted by g_0, or is a loop starting and ending in the AB-interface, followed by a path counted by g_w. This shows that

$$g_w = z_w + z_w c_o g_0 + z_w c_s g_w.$$

Solving simultaneously for g_0 and g_w gives the expressions claimed. Similar arguments give solutions for the h_i and k_i.

It is interesting to note that for even values of w_a and w_b,

$$c_s(w_a, w_b) - c_o(w_a, w_b) = c_s(w_a/2, w_b/2). \tag{68}$$

In other words, the number of loops in layers of widths (w_a, w_b) minus the number of bridges in layers of widths (w_a, w_b) is equal to the number of loops in layers of width $(w_a/2, w_b/2)$. In figure 13 we give a proof by picture.

This model has a rich mathematical structure, and we next investigate some special cases. In the case $z_0 = z_w = z$, the generating function g_0 reduces to

$$g_0|_{z_0=z_w=z} = \frac{1}{1 - z(c_s + c_o)}, \tag{69}$$

and this is identical to the solution in equation (28) when $w_a = w_b = w$ as well. For general values of w_a and w_b this shows that paths are generated by multiplying together the factors in figure 12, since

$$g_0|_{z_0=z_w=z} = 1 + z(c_s + c_o) + z^2(c_s + c_o)^2 + \cdots. \tag{70}$$

In the case $b = 0$ and $a = 1$, the model reduces to that of a fully directed path in a slit of width w_a and interacting with the walls of the slit via the activities z_0 and z_w. This model was examined in great detail in [3], and we show that the generating function above reduces to that model if $b = 0$ and $a = 1$. We focus on this model in section 4.1.

A different model is obtained when $z_w = 0$. In this case the path is confined to a bilayer with a BA-interface (or a defect line) on the X-axis separating the A-layer of thickness w_a and the B-layer of thickness w_b. In this case there are several models to consider, namely, the case $a = b$ and $w_a = w_b = w$ (section 4.2), the cases that $a = b$ with $w_b = w_a + m$ (section 4.3) and $a = b$ and $w_b = m w_a = m w$ (section 4.4).

The model with a finite A-layer between two infinite B-layers is obtained when $w_b \to \infty$. We examine this case in section 4.5. The general case is complex, and we give only partial

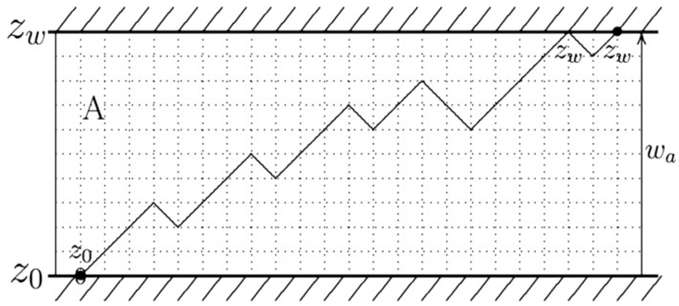

Figure 14. A directed path in a slit of width w_a with hard walls. This model is obtained from the general model by setting $b = 0$ in theorem 4.1. This is also the model solved in [3].

results. In several special cases in this model we give asymptotic expressions for the free energy and entropic forces.

More generally, one may use the arguments in this section to study paths in layered environments with more than one layer. Consider a model with N layers repeating periodically and of thicknesses w_i, $i = 0, 1, 2, \ldots, N-1$, where each edge of the path in an ith layer is weighted by a factor a_i; each vertex of the path at an interface between layers $(i-1)$ and i is weighted by a factor z_i, and in the interface between layer $N-1$ and layer 0 weighted by z_0.

For $i = 0, 1, \ldots, N-1$, let g_i be the generating function of paths starting at a given interface between layers $i-1$ and i, and terminating at an interface between any two layers, and define

$$a_i t = \frac{p_i}{1+p_i^2}, \qquad c_o^{(i)} = \frac{p_i^{w_i}\left(1-p_i^2\right)}{\left(1+p_i^2\right)\left(1-p_i^{2w_i}\right)}, \qquad \text{and} \qquad c_s^{(i)} = \frac{p_i^2 - p_i^{2w_i}}{\left(1+p_i^2\right)\left(1-p_i^{2w_i}\right)}.$$

Then the generating functions $g_0, g_1, \ldots, g_{(N-1)}$ are the solutions of the linear system

$$\begin{aligned}
&\left(1 - z_0\left(c_s^{(0)} + c_s^{(N-1)}\right)\right)g_0 = z_0 + z_0\left(c_o^{(0)} g_1 + c_o^{(N-1)} g_{(N-1)}\right);\\
&\left(1 - z_1\left(c_s^{(1)} + c_s^{(0)}\right)\right)g_1 = z_1 + z_1\left(c_o^{(1)} g_2 + c_o^{(0)} g_0\right);\\
&\left(1 - z_2\left(c_s^{(2)} + c_s^{(1)}\right)\right)g_2 = z_2 + z_2\left(c_o^{(2)} g_3 + c_o^{(1)} g_1\right);\\
&\ldots = \ldots\\
&(1 - z_{N-1}\left(c_s^{(N-1)} + c_s^{(N-2)}\right))g_{(N-1)} = z_{N-1} + z_{N-1}\left(c_o^{(N-1)} g_N + c_o^{(N-2)} g_{(N-2)}\right),
\end{aligned}$$

where $g_N \equiv g_0$. Rewriting the linear system as $DG = Z + AG$ with D and A being matrices, whose entries are the coefficients of the vector $(g_0, g_1, \ldots, g_{(N-1)})^t$ and $Z = (z_0, z_1, z_2, \ldots, z_{N-1})^t$, shows that the solution is $G = (D-A)^{-1}Z$, and the singularities in G which determine the free energy are found by considering $\det(D-A) = 0$.

4.1. A directed path in a slit

Consider the case where $b = 0$, which implies $q = 0$. Then the directed path is confined to a slit of width w_a interacting with the hard walls with activities z_0 and z_w, and having each edge weighted by a factor a, as illustrated in figure 14. This model was considered in [3], and we examine it here briefly by considering the generating function g_0:

$$g_0|_{q=0} = \frac{z_0(1+p^2)((1+p^2-z_w p^2) - (1+p^2-z_w)p^{2w_a}) + z_0 z_w p^{w_a}(1-p^4)}{(1+p^2-z_0p^2)(1+p^2-z_wp^2) - (1+p^2-z_0)(1+p^2-z_w)p^{2w_a}}. \tag{71}$$

In [3] the generating functions $B(w_a)$ of *bridges* (paths starting and ending at opposite walls of the slit) and $L(w_a)$ of *loops* (paths starting and ending at the same wall of the slit)[5]

$$B(w_a) = \frac{z_0 z_w p^{w_a}(1-p^4)}{(1+p^2-z_0p^2)(1+p^2-z_wp^2)-(1+p^2-z_0)(1+p^2-z_w)p^{2w_a}}, \tag{72}$$

$$L(w_a) = \frac{z_0(1+p^2)[(1+p^2-z_wp^2)-(1+p^2-z_w)p^{2w_a}]}{(1+p^2-z_0p^2)(1+p^2-z_wp^2)-(1+p^2-z_0)(1+p^2-z_w)p^{2w_a}}. \tag{73}$$

One may check that

$$g_0|_{q=0} = B(w_a) + L(w_a) \tag{74}$$

as expected because $g_0|_{q=0}$ generates paths starting on the X-axis, which corresponds to the bottom wall in a slit of width w_a, and ending either at the X-axis (it is a loop) or at the AB-interface (it is a bridge), which corresponds to the top wall of the slit.

Similarly, if $z_w = q = 0$ then the generating function g_0 reduces to the generating function of loops in a slit of width $w_a - 1$ adsorbing at the X-axis with activity z_0. Thus,

$$g_0|_{\substack{z_w=0,\\ q=0}} = L(w_a)|_{z_w=0} = L(w_a-1)|_{z_w=1} \tag{75}$$

because loops in a slit of width $w_a - 1$ (and not interacting with the top bounding line) are generated by $L(w_a)|_{z_w=0}$ or by $L(w_a-1)|_{z_w=1}$.

Singularities in the generating function in this model are given by branch points in p, and by zeros of the denominators in $B(w_a)$ and $L(w_a)$, namely, by solutions of

$$p^{2w_a} = \frac{(1+p^2-z_0p^2)(1+p^2-z_wp^2)}{(1+p^2-z_0)(1+p^2-z_w)} \tag{76}$$

in the t-plane if $p = (1-\sqrt{1-4a^2t^2})/2t$. The free energy can be determined from these singularities, and asymptotic expressions in w have been determined in [3]. These are

$$\mathcal{F}_{w_a} \simeq \begin{cases} \log\left(\frac{az_0}{\sqrt{z_0-1}}\right) + \frac{(z_0-2)^2(z_0z_w-z_0-z_w)}{2(z_0-z_w)(z_0-1)^{w_a+1}} & \\ \quad + O(w_a(z_0-1)^{-2w_a}), & \text{if} \quad z_0 > 2 \quad \text{and} \quad z_0 > z_w; \\ \log\left(\frac{az_0}{\sqrt{z_0-1}}\right) + \frac{(z_0-2)^2}{2(z_0-1)^{\frac{w_a}{2}+1}} & \\ \quad + O(w_a(z_0-1)^{-w_a}), & \text{if} \quad z_0 \geqslant 2 \quad \text{and} \quad z_0 = z_w; \\ \log(2a) - \frac{\pi^2}{2w_a^2} - \frac{2\pi^2(z_0z_w-z_0-z_w)}{(2-z_0)(2-z_w)w_a^3} & \\ \quad + O\left(w_a^{-4}\right), & \text{if} \quad z_0 < 2 \quad \text{and} \quad z_w < 2; \\ \log(2a) - \frac{\pi^2}{8w_a^2} + \frac{\pi^2 z_w}{4(2-z_w)w_a^3} + O\left(w_a^{-4}\right), & \text{if} \quad z_0 = 2 \quad \text{and} \quad z_w < 2. \end{cases} \tag{77}$$

In the case that $z_w > z_0$, then $z_0 \leftrightarrow z_w$ in the above expressions. The phase diagram of this model was discussed in [3], and we only point out the essential elements here. We reproduce the phase diagram in figure 15. In the $w_a \to \infty$ limit there are several critical curves in the diagram. These are given in solid lines in figure 15: the lines $z_0 = 2$ and $z_w < 2$ and $z_w = 2$

[5] These loops and bridges are defined differently from our earlier definition. In this case the paths may visit vertices in the walls of the slit numerous times before terminating in a vertex in one of the two walls.

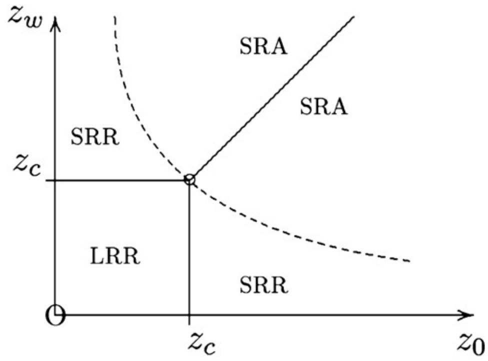

Figure 15. The phase and force diagram of a directed path in a slit with hard walls in the limit that $w_a \to \infty$. In this model, $z_c = 2$. There are three phases: for $z_0 > 2$ and $z_0 > z_w$ the path is adsorbed at the bottom wall of the slit. For $z_w > 2$ and $z_w > z_0$ the path is adsorbed at the top wall of the slit. For both $z_0 < 2$ and $z_w < 2$ the path is desorbed. There is a zero force curve denoted by a dashed curve in the diagram, given by $z_0z_w - z_0 - z_w = 0$. For values of z_0 and z_w on the large z_0 and z_w side of this curve the forces are attractive and short ranged (SRA). For values of z_0 and z_w on the small z_0 and z_2 side of the curve, the forces are repulsive, and either short ranged (SRR) if either $z_0 > 2$ or $z_w > 2$, and long ranged if both $z_0 < 2$ and $z_w < 2$ (LRR).

and $z_0 < 2$ are the lines of adsorption transitions, while the line $z_0 = z_w > 2$ is a line of first-order transitions separating two adsorbed phases on either the bottom or top wall. For finite values of w_a there are no phase transitions, but the entropic forces in the model changes along the phase boundaries in figure 15, as well as along a line of zero forces.

Forces on the walls of the slit can be determined by taking the derivative of $\mathcal{F}_{w_a}$ with respect to w_a. This gives

$$f_{w_a} \simeq \begin{cases} -\dfrac{(z_0-2)^2(z_0z_w - z_0 - z_w)\log(z_0-1)}{2(z_0-z_w)(z_0-1)^{w_a+1}} & \\ \quad + O((z_0-1)^{-2w_a}), & \text{if} \quad z_0 > 2 \quad \text{and} \quad z_0 > z_w; \\ -\dfrac{(z_0-2)^2\log(z_0-1)}{4(z_0-1)^{\frac{w_a}{2}+1}} + O((z_0-1)^{-w_a}), & \text{if} \quad z_0 \geqslant 2 \quad \text{and} \quad z_0 = z_w; \\ \dfrac{\pi^2}{w_a^3} + \dfrac{6\pi^2(z_0z_w - z_0 - z_w)}{(2-z_0)(2-z_w)w_a^4} + O\left(w_a^{-5}\right), & \text{if} \quad z_0 < 2 \quad \text{and} \quad z_w < 2; \\ \dfrac{\pi^2}{4w_a^3} - \dfrac{3\pi^2 z_w}{4(2-z_w)w_a^4} + O\left(w_a^{-5}\right), & \text{if} \quad z_0 = 2 \quad \text{and} \quad z_w < 2. \end{cases} \tag{78}$$

In the case that $z_w > z_0$, then $z_0 \leftrightarrow z_w$ in these expressions for the forces as well.

The phase and force diagram of this model is given in figure 15. For values of z_0 larger than 2 such that $z_0z_w > z_0 + z_w$, there are attractive forces between the walls of the slit. These forces decay exponentially in w_a with increasing width of the slit (they are short-ranged forces). For values $z_0 > 2$ and z_w small enough so that $z_0z_w < z_0+z_w$ the forces are repulsive, but remain short ranged. The curve $z_0z_w = z_0 + z_w$ is a zero force curve in the force diagram.

For values $z_0 > 2$ and $z_0 = z_w$ the forces are attractive and decay at a different exponential rate in w_a with increasing width of the slit. In this regime the forces are also short ranged. For values of $z_0 < 2$ and $z_w < 2$ or $z_0 = 2$ and $z_w < 2$, the forces are repulsive, but decay as a cubic power in w_a. These are long-ranged forces.

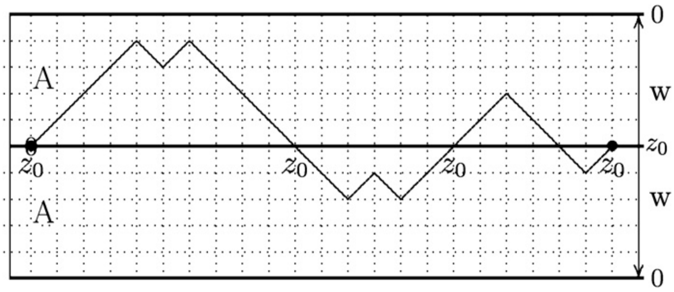

Figure 16. A path in a slit of width $2w - 2$ with hard walls and with a centered defect line. The path terminates on the defect line. This model is obtained by setting $b = a$, $w_b = w_a$ and $z_w = 0$ in the general model.

In the limit $w_a \to \infty$, the generating function g_0/z_0 reduces to

$$\lim_{w_a\to\infty} \frac{g_0}{z_0}\bigg|_{q=0} = \frac{1+p^2}{1+p^2-z_0p^2} = \frac{2z_0}{2-z_0(1-\sqrt{1-4t^2})}, \tag{79}$$

which is the generating function of a Dyck path adsorbing on the X-axis.

4.2. *A directed path in a slit with a centered defect line*

Consider the case where $z_w = 0, a = b$ and $w_a = w_b = w$. Then the directed path starts at the origin and ends on the X-axis, which is a defect line with activity z_0, as illustrated in figure 16. The path cannot intersect the AB-interfaces because $z_w = 0$, so that it is effectively confined in a slit of width $2w - 2$ with hard walls given by $Y = \pm(w - 1)$.

The generating function of interest in this case becomes

$$g_0 = \frac{z_0\,(1 - z_w\,(c_s - c_o))}{1 - (z_w + z_0)\,c_s + z_0 z_w\left({c_s}^2 - {c_o}^2\right)} = \frac{z_0}{1 - z_0 c_s} \tag{80}$$

where we have used the fact that $z_w = 0$, and

$$c_s = \frac{p^2 - p^{2w_a}}{(1+p^2)(1-p^{2w_a})} + \frac{q^2 - q^{2w_b}}{(1+q^2)(1-q^{2w_b})} = \frac{2(p^2 - p^{2w})}{(1+p^2)(1-p^{2w})} \tag{81}$$

because $w_a = w_b = w$ and $p = q$ (due to the fact that $a = b$).

The denominator of g_0 is given by

$$(1+p^2)(1-p^{2w}) - 2z_0(p^2 - p^{2w}) = 0 \tag{82}$$

which can be rewritten as

$$p^{2+2w} + (1-2z_0)p^{2w} - (1-2z_0)p^2 - 1 = 0. \tag{83}$$

This is a polynomial of degree $2w + 2$ in p, and if $w \to \infty$ with $0 \leqslant p < 1$, then it simplifies to

$$(1-2z_0)p^2 + 1 = 0. \tag{84}$$

The solution is

$$p_0 = \frac{1}{\sqrt{2z_0 - 1}} \tag{85}$$

which is real if $z_0 > 1/2$, and we note that $0 < p_0 < 1$ if $z_0 > 1$.

To develop an asymptotic formula for p for large but finite w, we again use the approach in [1]. If $z_0 > 1$, in which case $0 < p_0 < 1$, we assume that for some function C, independent of w, we have the following asymptotic expansion of p in terms of p_0:

$$p = p_0 + C p_0^{2w} + O\left(p_0^{3w}\right). \tag{86}$$

To determine C, substitute (86) into (83), and compare coefficients of p_0 with powers less than $3w$. This shows that

$$C = \frac{2z_0\,(z_0 - 1)}{(2z_0 - 1)^{3/2}}. \tag{87}$$

The asymptotics for the critical value of t can be obtained from the transformation $at = p/(1 + p^2)$ and the asymptotic expansion for p. This is given by

$$at_c = \frac{\sqrt{2z_0 - 1}}{2z_0} + \frac{(z_0 - 1)^2}{z_0\sqrt{2z_0 - 1}}\left(\frac{1}{2z_0 - 1}\right)^w + O(w(2z_0 - 1)^{-3w/2}). \tag{88}$$

These asymptotics are only valid if $|p| < 1$, which is the case if $z_0 > 1$.

Otherwise $z_0 < 1$ and we approximate p by a root of unity by assuming

$$p = e^{\pi i/w}\left(1 + \frac{c_1}{w} + \frac{c_2}{w^2} + \frac{c_3}{w^3} + O(1/w^4)\right). \tag{89}$$

Substituting this into the denominator in equation (83), expanding in inverse powers of w, and determining the values of the c_i, then gives the solutions

$$c_1 = 0, \qquad c_2 = \frac{\pi i z_0}{z_0 - 1}, \qquad \text{and} \qquad c_3 = \frac{\pi i z_0^2}{(z_0 - 1)^2}. \tag{90}$$

The critical value of t can again be determined from these results:

$$at_c = \frac{1}{2} + \frac{\pi^2}{4w^2} - \frac{\pi^2 z_0}{2(1 - z_0)w^3} + O(w^{-4}). \tag{91}$$

If $z_0 = 1$, the denominator reduces to $(p^2 - 1)(p^{2w} - 1)$ so that $p = e^{\pi i/2w}$. Determining the asymptotics from this solution shows that

$$at_c = \frac{1}{2} + \frac{\pi^2}{16w^2} + \frac{5\pi^4}{768w^4} + O(w^{-6}). \tag{92}$$

The free energy $\mathcal{F}_w = -\log t_c$ can be determined from (88), (91) and (92):

$$\mathcal{F}_w \simeq \begin{cases} \log\left(\dfrac{2z_0 a}{\sqrt{2z_0 - 1}}\right) - \dfrac{2(z_0 - 1)^2}{(2z_0 - 1)^{w+1}} + O(w(2z_0 - 1)^{-3w/2}), & \text{if} \quad z_0 > 1; \\ \log(2a) - \dfrac{\pi^2}{8w^2} - \dfrac{\pi^4}{192w^4} + O(w^{-6}), & \text{if} \quad z_0 = 1; \\ \log(2a) - \dfrac{\pi^2}{2w^2} + \dfrac{z_0\pi^2}{(1 - z_0)w^3} + O(w^{-4}), & \text{if} \quad z_0 < 1. \end{cases} \tag{93}$$

In the $w \to \infty$ limit this model reduces to a path near a defect line. If $z_0 < 1$, the path is delocalized, but when $z > z_0$ the path has a positive density of visits to the defect line and it is pinned. This transition has an effect on the entropic forces on the walls of the slit for finite values of w.

The entropic forces on the walls of the slit can be determined by taking the derivative of $\mathcal{F}_w$ with respect to w. The asymptotic formula for the force is given by

$$f_w \simeq \begin{cases} \dfrac{2(z_0 - 1)^2 \log(2z_0 - 1)}{(2z_0 - 1)^{w+1}} + O((2z_0 - 1)^{-3w/2}), & \text{if} \quad z_0 > 1; \\ \dfrac{\pi^2}{4w^3} + \dfrac{\pi^4}{48w^5} + O(w^{-7}), & \text{if} \quad z_0 = 1; \\ \dfrac{\pi^2}{w^3} - \dfrac{3\pi^2 z_0}{(1 - z_0)w^4} + O(w^{-5}), & \text{if} \quad z_0 < 1. \end{cases} \tag{94}$$

The force regimes in this model are characterized by both a long-range repulsive force when $z_0 < 1$, and a short-range repulsive force when $z_0 \geqslant 1$. In the event that $z_0 < 1$, the walk is not pinned on the defect line, and its steric repulsion on the walls is long ranged. For $z_0 > 1$ the walk is pinned on the defect line, and its effects on the walls decays exponentially with w; it is short ranged.

4.3. A directed path in a slit with an off-centered defect line I

In this section we consider a variant of the model in section 4.2. Assume once again that $z_w = 0$ and $a = b$, so that $p = q$, but this time consider the case where $w_a = w$ and $w_b = w + m$ for a non-negative integer $m \ll w$. This is a model where w_a and w_b are not equal, but are comparable in size. The directed path starts at the origin and ends on the X-axis, without reaching the AB-interface (because $z_w = 0$). Therefore, the path is confined to a slit of total width $2w + m - 2$ with hard walls at $Y = -(w + m) + 1$ and $Y = (w - 1)$.

In the limit that $w \to \infty$, the denominator of g_0 becomes $2p^2z_0-(1+p^2)$. This is the same as obtained in section 4.2 since $a = b$ and $z_w = 0$ in both models. Thus $p_0 = 1/\sqrt{2z_0 - 1}$. To determine the asymptotics in this model, consider the three cases: $z_0 > 1$, $z_0 = 1$ and $z_0 < 1$.

If $z_0 > 1$ then asymptotic expansion of p in powers of p_0 is given by equation (86). To determine C we substitute this ansatz for p into the denominator of g_0 and compare coefficients of p_0 with powers less than $3w$. This shows that

$$C = \frac{z_0(z_0 - 1)(1 + (2z_0 - 1)^{-m})}{(2z_0 - 1)^{3/2}}. \tag{95}$$

This solution for C reduces to that in equation (87) if $m \to 0^+$. One may again determine a critical value for t from this solution for p:

$$at_c = \frac{\sqrt{2z_0 - 1}}{2z_0} + \frac{(z_0 - 1)^2(1 + (2z_0 - 1)^{-m})}{2z_0(2z_0 - 1)^{w+1/2}} + O(w(2z_0 - 1)^{-3(w+m)/2}). \tag{96}$$

If $z_0 < 1$ then we assume instead that p is approximated by

$$p = \mathrm{e}^{\mathrm{i}\pi/(w+m)}\left(1 + \frac{c_1}{w} + \frac{c_2}{w^2} + \frac{c_3}{w^3} + \frac{c_4}{w^4} + O(w^{-5})\right). \tag{97}$$

Determining c_i as in section 4.2 gives

$$c_1 = 0, \qquad c_2 = \frac{\pi\mathrm{i}\left(z_0 + m(z_0 - 1) + \sqrt{m^2(z_0 - 1)^2 + z_0^2}\right)}{2(z_0 - 1)}, \tag{98}$$

and a complicated expression for c_3 which we omit for brevity. The critical value of t in this case can be determined as

$$at_c = \frac{1}{2} + \frac{\pi^2}{4w^2} + \frac{\pi^2\left(z_0 - m(z_0 - 1) + \sqrt{m^2(z_0 - 1)^2 + z_0^2}\right)}{4(z_0 - 1)w^3} + O(w^{-4}). \tag{99}$$

This reduces to equation (91) when $m \to 0^+$, as one would expect.

If $z_0 = 1$ then the denominator of the generating function reduces to $(p^2 - 1)(p^{4w+2m} - 1)$ with solutions which are roots of unity. Determining t_c from these roots shows that

$$at_c = \frac{1}{2} + \frac{\pi^2}{16w^2} - \frac{\pi^2 m}{16w^3} - \frac{\pi^2(5\pi^2 + 36m^2)}{768w^4} + O(w^{-5}). \tag{100}$$

These results for t_c give us the asymptotic behavior of the free energy as

$$\mathcal{F}_w \simeq \begin{cases} \log\left(\dfrac{2z_0 a}{\sqrt{2z_0-1}}\right) - \dfrac{(z_0-1)^2(1+(2z_0-1)^{-m})}{(2z_0-1)^{w+1}} \\ \qquad + O(w(2z_0-1)^{-3(w+m)/2}), & \text{if} \quad z_0 > 1; \\ \log(2a) - \dfrac{\pi^2}{8w^2} + \dfrac{\pi^2 m}{w^3} + O(w^{-4}), & \text{if} \quad z_0 = 1; \\ \log(2a) - \dfrac{\pi^2}{2w^2} \\ \qquad - \dfrac{\pi^2\left(z_0 + m(1-z_0) + \sqrt{z_0^2 + m^2(1-z_0)^2}\right)}{2(1-z_0)w^3} + O(w^{-4}), & \text{if} \quad z_0 < 1. \end{cases} \tag{101}$$

If $w \to \infty$ in this model, then a model of a path at a defect line is obtained. The critical point is at $z_0 = 1$, and the path is pinned at the defect line if $z_0 > 1$, while the path is delocalized when $z_0 \leqslant 1$. Note that setting $m = 0$ we recover the expressions in equation (93).

The asymptotic formula for the force is given by

$$f_w \simeq \begin{cases} \dfrac{(z_0-1)^2 \log(2z_0-1)(1+(2z_0-1)^{-m})}{(2z_0-1)^{w+1}} \\ \qquad + O((2z_0-1)^{-3(w+m)/2}), & \text{if} \quad z_0 > 1; \\ \dfrac{\pi^2}{4w^3} - \dfrac{3\pi^2 m}{8w^4} + O(w^{-5}), & \text{if} \quad z_0 = 1; \\ \dfrac{\pi^2}{w^3} + \dfrac{3\pi^2\left(z_0 + m(1-z_0) + \sqrt{z_0^2 + m^2(1-z_0)^2}\right)}{2(1-z_0)w^4} + O(w^{-5}), & \text{if} \quad z_0 < 1. \end{cases} \tag{102}$$

There are two force regimes: in the event that $z_0 < 1$, the walk is not pinned on the defect line, and its steric repulsion on the walls is long ranged. For $z_0 > 1$ the walk is pinned on the defect line, and its effects on the walls decays exponentially with w; it is short ranged. This is the same situation as in section 4.2, which is not surprising because even though in this model the widths of the layers are not equal, they are comparable in size.

4.4. A directed path in a slit with an off-centered defect line II

In this section we consider another variant of the model in figure 16 and section 4.2. Assume again that $z_w = 0$ and $a = b$, so that $p = q$, but this time assume that $w_a = w$ and $w_b = mw$ for some large integer $m \geqslant 1$. In this case the width of the layers are not comparable in size, like they were in sections 4.2 and 4.3, in this case one layer is much larger than the other. This is a model where the directed path starts at the origin and ends on the X-axis without reaching the AB-interface (because $z_w = 0$). The path is therefore confined to a slit of total width $(m+1)w - 2$ with hard walls at $Y = -(mw-1)$ and $Y = (w-1)$, and with a defect line close to one wall.

In this model we proceed similarly to sections 4.2 and 4.3. First, consider the case where $z_0 > 1$. Then p_0 is again given by equation (85) because we get the same denominator for the generating function g_0 as we did in section 4.2. This is due to the fact that $a = b$ and $z_w = 0$ in both models. Assuming that p is approximated by equation (86). One can determine C by substitution of this ansatz for p into the denominator of g_0 and comparing coefficients of p_0 with powers less than that of $3w$. This gives

$$C = \frac{z_0(z_0-1)}{(2z_0-1)^{3/2}}. \tag{103}$$

Determining t_c from p then shows that

$$at_c = \frac{\sqrt{2z_0-1}}{2z_0} + \frac{(z_0-1)^2}{2z_0\sqrt{2z_0-1}^{2w+1}} + O(w(2z_0-1)^{-3w/2}). \tag{104}$$

If $z_0 < 1$ then we assume instead that p is approximated by equation (89). Substituting this ansatz for p into the denominator of g_0, expanding in inverse powers of w, and solving for c_i gives the solutions

$$c_1 = 0, \qquad c_2 = \frac{\mathrm{i}\pi z_0}{2m^2(z_0-1)}, \tag{105}$$

and a complicated expression for c_3 which we omit for brevity. Determining t_c from these results yields

$$at_c = \frac{1}{2} + \frac{\pi^2}{4m^2w^2} + \frac{z_0\pi^2}{4m^3(z_0-1)w^3} + O(w^{-4}). \tag{106}$$

We note that this formula is valid for large w and m and that it breaks down as $m \to 1^+$ when we compare it to equation (91); there is a factor of 2 discrepant in the $O(w^{-3})$ term which is the result of different contributions to the asymptotics by the two layers depending on whether $m = 1$ or $m \neq 1$.

If $z_0 = 1$ the denominator of the generating function g_0 reduces to $(p^2-1)(p^{2w(m+1)}-1)$ with solutions which are roots of unity. Determining t_c from these roots shows that

$$at_c = \frac{1}{2} + \frac{\pi^2}{4(m+1)^2w^2} + \frac{5\pi^4}{48(m+1)^4w^4} + O(w^{-5}). \tag{107}$$

The free energy in this model can be determined from the asymptotic formulae for t_c above:

$$\mathcal{F}_w \simeq \begin{cases} \log\left(\dfrac{2z_0a}{\sqrt{2z_0-1}}\right) - \dfrac{(z_0-1)^2}{(2z_0-1)^{w+1}} + O(w(2z_0-1)^{-3w/2}), & \text{if} \quad z_0 > 1; \\ \log(2a) - \dfrac{\pi^2}{2(m+1)^2w^2} - \dfrac{\pi^4}{12(m+1)^4w^4} + O(w^{-6}), & \text{if} \quad z_0 = 1; \\ \log(2a) - \dfrac{\pi^2}{2m^2w^2} + \dfrac{z_0\pi^2}{2(1-z_0)m^3w^3} + O(w^{-4}), & \text{if} \quad z_0 < 1. \end{cases} \tag{108}$$

There is again a critical point at $z_0 = 1$ if $w \to \infty$. If $z_0 > 1$, then the path is pinned in the defect line, but if $z_0 \leqslant 1$, the path is delocalized in the slab.

By taking the derivative of the free energy with respect to w we obtain the asymptotic formula for the forces exerted on the walls of the slit

$$f_w \simeq \begin{cases} \dfrac{(z_0-1)^2\log(2z_0-1)}{(2z_0-1)^{w+1}} + O((2z_0-1)^{-3w/2}), & \text{if} \quad z_0 > 1; \\ \dfrac{\pi^2}{(m+1)^2w^3} + \dfrac{\pi^4}{3(m+1)^4w^5} + O(w^{-7}), & \text{if} \quad z_0 = 1; \\ \dfrac{\pi^2}{m^2w^3} - \dfrac{3\pi^2z_0}{2m^3(1-z_0)w^4} + O(w^{-5}), & \text{if} \quad z_0 < 1. \end{cases} \tag{109}$$

In the event that $z_0 < 1$, the walk is not pinned on the defect line, and its steric repulsion on the walls is long ranged. For $z_0 > 1$ the walk is pinned on the defect line, and its effects on the walls decays exponentially with w; it is short ranged.

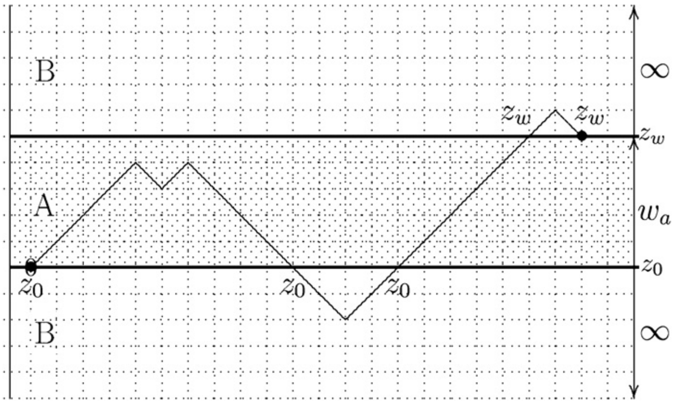

Figure 17. A path in a layered lattice with an A-layer of width w_a between two infinite B-layers. This model is obtained when $w_b \to \infty$, as in section 4.5. The path interacts with the two interfaces via z_0 and z_w respectively.

4.5. *The case* $w_b = \infty$

This is a model of a path in a layered lattice with an A-layer of width w_a between two B-layers of infinite width, as illustrated in figure 17. This is a model of finite membrane (the A-layer) in (for example) a lipid–water membrane system.

In this case the generating function is given by

$$g_0 = \frac{z_0(1 - z_w(c_s - c_o))}{1 - (z_0 + z_w)c_s + z_0 z_w\left(c_s^2 - c_o^2\right)}, \tag{110}$$

$$c_s = \frac{p^2 - p^{2w_a}}{(1+p^2)(1-p^{2w_a})} + \frac{q^2}{1+q^2}, \tag{111}$$

$$c_o = \frac{p^{w_a}(1-p^2)}{(1+p^2)(1-p^{2w_a})}. \tag{112}$$

Zeros in the denominator of g_0 determine singular behavior in the generating function, and we seek in particular the values of p which determine these zeros. First we determine the value of $p = p_0$ in the case where $w_a \to \infty$, and then expand p about p_0. If $w_a \to \infty$, then g_0 reduces to

$$\lim_{w_a \to \infty} g_0 = \frac{z_0}{1 - z_0\left(\frac{p^2}{1+p^2} + \frac{q^2}{1+q^2}\right)}. \tag{113}$$

Singularities in this generating function are given by zeros of the denominator, that is when $p = p_0$, and p_0 is a solution of

$$(1+p^2)(1+q^2) = z_0(p^2(1+q^2) + q^2(1+p^2)). \tag{114}$$

Solving for $p^2 = p_0^2$ shows that

$$p_0^2 = \frac{q^2(z_0 - 1) - 1}{1 + q^2 - z_0(1 + 2q^2)}. \tag{115}$$

However, this is not an explicit expression for the solution of p_0 in the $w_a \to \infty$ case. This is because q depends on t and t depends on p, so q is an implicit function of p_0 in the above. To determine p_0, we use the facts that $q = (1 - \sqrt{(1-4b^2t^2)})/2bt$ and that $at = p/(1+p^2)$ to determine $q(p) \equiv q(t(p))$ given by

$$q(p) = \frac{a(1+p^2) - \sqrt{a^2(1+p^2)^2 - 4p^2b^2}}{2pb}. \tag{116}$$

Substituting this into equation (115) we find the solution for p_0 given by

$$p_0^2 = -\frac{z_0^2 - 4z_0 + 2}{2(2z_0-1)(z_0-1)} - \frac{z_0\left(z_0b^2 \pm \sqrt{z_0^2(a^2+b^2)^2 + 4a^2b^2(1-2z_0)}\right)}{2a^2(2z_0-1)(z_0-1)}. \tag{117}$$

One may similarly solve for q_0^2:

$$q_0^2 = -\frac{z_0^2 - 4z_0 + 2}{2(2z_0-1)(z_0-1)} - \frac{z_0\left(z_0a^2 \pm \sqrt{z_0^2(a^2+b^2)^2 + 4a^2b^2(1-2z_0)}\right)}{2b^2(2z_0-1)(z_0-1)}. \tag{118}$$

Observe that $p_0(a,b) = q_0(b,a)$. In addition, if $a = b = 1$, then p_0 reduces to $1/\sqrt{2z_0-1}$ and if $a = 1$ and $b = 0$, then p_0 reduces to $1/\sqrt{z_0-1}$.

In the case that z_0 is large, asymptotics can be determined generally for this model. The denominator of the generating function (110) is too large to reproduce here. An asymptotic expression for p is determined by assuming that

$$p = p_0 + Cp_0^{2w_a} + O\left(p_0^{3w_a}\right) \tag{119}$$

where p_0 is given in equation (117), and then determining C. Substituting this ansatz for p into the denominator of g_0 in equation (110), expanding in powers of p_0, collecting terms, enables one to compute C from the coefficients of powers of p_0 less than $3w_a$. C is independent of w_a but for arbitrary values of a and b its expression is quite large. We reproduce it in the appendix (see equation (A.1)).

For small values of z_0 and z_w, the asymptotics are determined by assuming that

$$p = \mathrm{e}^{\mathrm{i}\pi/w_a}\left(1 + \frac{c_1}{w_a} + \frac{c_2}{w_a^2} + \frac{c_3}{w_a^3} + O\left(w_a^{-4}\right)\right). \tag{120}$$

For general values of a and b (assuming that $a \geqslant b$) the values of c_i are determined by substituting this ansatz for p into the denominator of equation (110). Expanding asymptotically allows the determination of c_i term by term. This shows that $c_1 = 0$, while c_2 and c_3 are given by complicated expressions. We reproduce c_2 in the appendix (see equation (A.2)).

4.5.1. The case $z_0 = z_w = 1$. If $a \gg b$ in this model, then we assume that p can be approximated by a root of unity and its asymptotics can be determined by assuming that p is approximated by equation (120). Substituting $z_0 = z_1 = 1$ in c_i shows that $c_1 = 0$ and c_2 is given in the appendix (equation (A.2) with $z_0 = z_w = 1$:

$$c_2 = \frac{2\pi\mathrm{i}a((b^2-2a^2)\sqrt{a^2-b^2} + 2a(a^2-b^2))}{(a^2-b^2)(2a^2-b^2-2a\sqrt{a^2-b^2})}. \tag{121}$$

A more complicated expression for c_3 can also be determined. The asymptotic behavior of the critical value t_c can then be obtained from $at = p/(1+p^2)$:

$$at_c \simeq \frac{1}{2} + \frac{\pi^2}{4w_a^2} + \frac{\pi^2a((b^2-2a^2)\sqrt{a^2-b^2} + 2a(a^2-b^2))}{(a^2-b^2)(2a^2-b^2-2a\sqrt{a^2-b^2})w_a^3} + O\left(w_a^{-4}\right). \tag{122}$$

For fixed b (this sets a zero point in the free energy in the model), it follows that $t_c < 1/2b$ for all values of $a > b$.

On the other hand, if $b \gg a$, then the critical value of t must be determined from the denominator of the generating function. The roots of the denominator of the generating function are given by solving for p in

$$(q^2 - p^2)p^{w_a} + p^2q^2 - 1 = 0, \tag{123}$$

where q is an implicit function of p. This is done as in section 3.3. Write the last equation as

$$p - \left(\frac{p^2q^2 - 1}{p^2 - q^2}\right)^{\frac{1}{w_a}} = 0, \tag{124}$$

substitute for q by using equation (116). Assume that p is approximated in equation (120) and determine c_i by expanding asymptotically in w_a, and solving for c_i term by term. This shows that

$$c_0 = \frac{b \pm \sqrt{b^2 - a^2}}{a} \tag{125}$$

and $c_1 = -\mathrm{i}\pi c_0/2$, $c_2 = -\pi^2 c_0/8$, $c_3 = \mathrm{i}\pi^3 c_0/48$ and $c_4 = \pi^4 c_0/384$. The resulting value of t_c is given by

$$at_c = \frac{a}{2b}. \tag{126}$$

Finally, if $a \lessapprox b$, then we use the approximation $bp = aq$ and the arguments in section 3.3 to observe that

$$bt_c \simeq \frac{\sqrt{ab}}{a+b}. \tag{127}$$

These are similar results to that obtained in section 3.3 (see equation (48), and the same comments made there apply to this case. Observe that there are no dependencies on w in these results in equations (126) and (127), except that with increasing w_a the regime given by equation (127) decreases in size, as argued in section 3.3.

Generally, for $b \gg a$ the path delocalizes in the infinite B-layer, and for $b \gtrapprox a$ it delocalizes over both the B- and the A-layers. If $b \ll a$ the path will localize to the A-layer.

In other words, the critical value of t in the large a and in the large b regimes are determined by two different asymptotic regimes of the generating function. These correspond to a phase where paths are localized in the A-layer, and a phase where paths are delocalized in the B-layer. By comparing equations (122) and (127), one can determine asymptotically (for large a and b) the location of the crossover regime in the ab-plane. If we assume that for large values of w_a the crossover regime is given by $b_c(a) = \hat{c}_0 + \hat{c}_1/w_a + \hat{c}_2/w_a^2 + \cdots$, then $\hat{c}_i$ can again be determined by equating equations (122) and (127), expanding asymptotically in w_a and then analyzing term by term. Simplification of the results show that

$$b_c(a) \simeq a\left(1 - \frac{\pi^2}{2w_a^2}\right) + O\left(w_a^{-3}\right). \tag{128}$$

Observe that $b_c(a) \to a$ in the limit $w_a \to \infty$, as one would expect.

The free energy of this model can be determined from the values of t_c obtained above:

$$\mathcal{F}_w \simeq \begin{cases} \log 2b, & \text{if} \quad b \gg b_c(a); \\ \log b - \log\left(\dfrac{\sqrt{ab}}{a+b}\right), & \text{if} \quad b \gtrapprox b_c(a); \\ \log 2a - \dfrac{\pi^2}{2w_a^2} - \dfrac{2\pi^2 a((b^2-2a^2)\sqrt{a^2-b^2} + 2a(a^2-b^2))}{(a^2-b^2)(2a^2-b^2-2a\sqrt{a^2-b^2})w_a^3} & \\ \qquad + O\left(w_a^{-4}\right), & \text{if} \quad b < b_c(a). \end{cases} \tag{129}$$

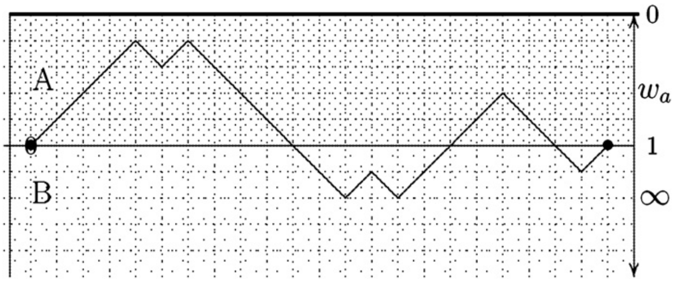

Figure 18. A path in a bilayered lattice with hard walls, obtained by setting $z_0 = 1$ and $z_w = 0$ in figure 17. The central defect line is the BA-interface between the two layers.

In the $w_a \to \infty$ limit, $b_c(a) \to a$ and $\mathcal{F}_w \to \min\{\log 2a, \log 2b\}$, as one would expect. For finite values of w_a the free energy is either determined by paths in the infinite B-layer if $b \gg b_c(a)$, or crosses over into the more complicated expressions above for $b < b_c(a)$.

The force exerted on the interfaces can be determined by taking the derivative of the free energy with respect to w_a:

$$f_w \simeq \begin{cases} 0, & \text{if} \quad b > b_c(a); \\ \dfrac{\pi^2}{w_a^3} + \dfrac{6\pi^2 a((b^2-2a^2)\sqrt{a^2-b^2}+2a(a^2-b^2))}{(a^2-b^2)(2a^2-b^2-2a\sqrt{a^2-b^2})w_a^4)} + O\left(w_a^{-5}\right), & \text{if} \quad b < b_c(a). \end{cases} \tag{130}$$

In this model there are two phase and force regimes. If $b < b_c(a)$ the path exerts a long-ranged repulsive force on the walls of the A-layer for finite values of w_a, and if $w_a \to \infty$ limit there is a localization of the path at the A-layer. For values of $b > b_c(a)$ there is a zero net force on the walls of the A-layer for finite values of w_a, and if $w_a \to \infty$ the path is delocalized from the A-layer (it explores the B-layer).

4.5.2. The case $z_0 = 1$ and $z_w = 0$. Setting $z_w = 0$ introduces a hard wall in the model, which is illustrated in figure 18. If $b > a$, the model will again be dominated by paths in the infinite B-layer (below the X-axis). If $a \gg b$, an asymptotic expansion for p can again be determined by using the ansatz in equation (120). In this case $c_1 = 0$ and c_2 is given in the appendix (equation (A.2). When $z_0 = 1$ and $z_w = 0$, then c_2 is given by

$$c_2 = \frac{\pi \mathrm{i} a(2a\sqrt{a^2-b^2}+2a^2-b^2)}{(\sqrt{a^2-b^2}(b^2-2a^2)+2a(a^2-b^2))}. \tag{131}$$

The critical value of t can be determined to be

$$at_c = \frac{1}{2} + \frac{\pi^2}{4w_a^2} + \frac{\pi^2 a(2a\sqrt{a^2-b^2}+2a^2-b^2)}{2(\sqrt{a^2-b^2}(b^2-2a^2)+2a(a^2-b^2))w_a^3} + O\left(w_a^{-4}\right). \tag{132}$$

To estimate t_c for the case where $b \gg a$, we use the same arguments as in the previous section. The roots denominator of the generating function are given by solving for q in

$$(p^2-q^2)p^{2w_a} + p^2q^2 - 1 = 0, \tag{133}$$

where p is an implicit function of q. Arguing as above shows that

$$at_c = \frac{a}{2b} \tag{134}$$

in this regime.

If $b \gtrsim a$, we again approximate $bp \approx aq$, and use the arguments above. This shows that

$$bt_c \simeq \frac{ab}{a^2+b^2}. \tag{135}$$

This is a similar result to that obtained in sections 3.3 and 4.5.1 (see equations (48) and (127), and the same comments made there apply to this case.

The curve $b_c(a)$ describing the crossover regime can again be determined by equating equations (132) and (135). The result is

$$b_c(a) \simeq a\left(1-\frac{\pi^2}{2w_a^2}\right)+O\left(w_a^{-3}\right). \tag{136}$$

Observe that $b_c(a) \simeq a$ as $w_a \to \infty$, as one would expect. This is the same crossover behavior observed in the previous section.

The free energy of this model can be determined from the values of t_c:

$$\mathcal{F}_w \simeq \begin{cases} \log 2b, & \text{if} \quad b \gg b_c(a); \\ \log b - \log\left(\dfrac{ab}{a^2+b^2}\right), & \text{if} \quad b \gtrsim b_c(a); \\ \log(2a) - \dfrac{\pi^2}{2w_a^2} - \dfrac{\pi^2 a(2a\sqrt{a^2-b^2}+2a(a^2-b^2))}{((b^2-2a^2)\sqrt{a^2-b^2}+2a(a^2-b^2))w_a^3} & \\ \qquad + O\left(w_a^{-4}\right), & \text{if} \quad b < b_c(a). \end{cases} \tag{137}$$

For finite values of w_a the free energy is either determined by paths in the infinite B-layer if $b \gg b_c(a)$, or crosses over into the more complicated expressions above for $b < b_c(a)$.

The force exerted on the interfaces can be determined by taking the derivative of the free energy with respect to w_a:

$$f_w \simeq \begin{cases} 0, & \text{if} \quad b > b_c(a); \\ \dfrac{\pi^2}{w_a^3} + \dfrac{3\pi^2 a(2a\sqrt{a^2-b^2}+2a^2-b^2)}{((b^2-2a^2)\sqrt{a^2-b^2}+2a(a^2-b^2))w_a^4} + O\left(w_a^{-5}\right), & \text{if} \quad b < b_c(a). \end{cases} \tag{138}$$

In this model there are again two phases and force regimes. If $b < b_c(a)$ the path exerts a long-ranged repulsive force on the walls of the A-layer for finite values of w_a, and if $w_a \to \infty$ limit there is a localization of the path at the A-layer. For values of $b > b_c(a)$ there is a zero net force on the walls of the A-layer for finite values of w_a, and if $w_a \to \infty$ the path is delocalized from the A-layer (it explores the B-layer).

4.5.3. The case $a = b$. In this section we consider the model as a function of the adsorption parameters z_0 and z_w, which is depicted in figure 17 with $a = b$. There are several regimes to be considered, depending on whether the adsorption parameters are large or small. We shall assume that $z_0 \geqslant z_w$ in all cases; interchanging z_0 and z_w will give expressions for the case $z_w > z_0$.

In the case that z_0 is large, asymptotics are determined by assuming that p is given by equation (119) with p_0 is given in equation (117) with $a = b$. Then C is given by equation (A.1) in the appendix with $a = b$. If $a = b$, $z_0 > z_w$, and $z_0 > 1$, then the results are $p_0 = 1/\sqrt{2z_0-1}$ and

$$p \simeq \frac{1}{\sqrt{2z_0-1}} - \frac{z_0^2(z_w-1)(z_0-1)}{(z_0-z_w)(2z_0-1)^{3/2}}\left(\frac{1}{2z_0-1}\right)^{w_a} + O(w_a(2z_0-1)^{-2w_a}). \tag{139}$$

If $a = b$ and $z_0 = z_w > 1$ the asymptotics change to

$$p \simeq \frac{1}{\sqrt{2z_0-1}} - \frac{z_0(z_0-1)}{(2z_0-1)^{3/2}}\left(\frac{1}{2z_0-1}\right)^{w_a/2} + O(w_a(2z_0-1)^{-w_a}). \tag{140}$$

Asymptotics for the critical value of t can be determined to be

$$at_c \simeq \begin{cases} \dfrac{\sqrt{2z_0-1}}{2z_0} - \dfrac{(z_w-1)(z_0-1)^2}{2(z_0-z_w)\sqrt{2z_0-1}}\left(\dfrac{1}{2z_0-1}\right)^{w_a} \\ \quad + O(w_a(2z_0-1)^{-2w_a}), & \text{if} \quad a=b, \quad z_0>z_w \quad \text{and} \quad z_0>1; \\ \dfrac{\sqrt{2z_0-1}}{2z_0} - \dfrac{(z_0-1)^2}{2z_0\sqrt{2z_0-1}}\left(\dfrac{1}{2z_0-1}\right)^{w_a/2} \\ \quad + O(w_a(2z_0-1)^{-w_a}), & \text{if} \quad a=b, \quad z_0=z_w>1. \end{cases} \tag{141}$$

For small values of z_0 and z_w, the asymptotics are determined by assuming that p is given by equation (120), with $c_1=0$ and c_2 given in equation (A.2) in the appendix. Putting $a=b$ gives

$$c_2 = \frac{\pi \mathrm{i}(2z_0z_w - z_0 - z_w)}{2(1-z_0)(1-z_w)}. \tag{142}$$

Determining t_c from p gives the asymptotic formula

$$at_c \simeq \frac{1}{2} + \frac{\pi^2}{4w_a^2} + \frac{\pi^2(2z_0z_w - z_0 - z_w)}{4(1-z_0)(1-z_w)w_a^3} + O\left(w_a^{-4}\right), \qquad \text{if} \quad z_0<1 \quad \text{and} \quad z_w<1. \tag{143}$$

If $z_0=1$, $z_w<z_0$ and $a=b$, then the free energy can be computed by putting $a=b$ and taking the limit $z_0\to 1$ in equation (A.2) using L'Hospital's rule to obtain

$$at_c \simeq \frac{1}{2} + \frac{\pi^2}{4w_a^2} + \frac{\pi^2(2-3z_w)}{2(1-z_w)w_a^3} + O\left(w_a^{-4}\right), \qquad \text{if} \quad z_0=1 \quad \text{and} \quad z_w<1. \tag{144}$$

Finally, if $z_0=z_w=1$, the critical value of t is given by $t_c=1/2a$, as seen in equation (127).

These results can be used to determine the free energy in this case:

$$\mathcal{F}_w \simeq \begin{cases} \log\left(\dfrac{2z_0a}{\sqrt{2z_0-1}}\right) + \dfrac{z_0(z_w-1)(z_0-1)^2}{(z_0-z_w)(2z_0-1)} \\ \quad \times \left(\dfrac{1}{2z_0-1}\right)^{w_a} + O(w_a(2z_0-1)^{-2w_a}), & \text{if} \quad a=b, z_0>z_w \quad \text{and} \quad z_0>1; \\ \log\left(\dfrac{2z_0a}{\sqrt{2z_0-1}}\right) + \dfrac{(z_0-1)^2}{2z_0-1}\left(\dfrac{1}{2z_0-1}\right)^{w_a/2} \\ \quad + O(w_a(2z_0-1)^{-w_a}), & \text{if} \quad a=b, z_0=z_w \geqslant 1; \\ \log 2a - \dfrac{\pi^2}{2w_a^2} - \dfrac{\pi^2(2z_0z_w - z_0 - z_w)}{2(1-z_0)(1-z_w)w_a^3} \\ \quad + O\left(w_a^{-4}\right), & \text{if} \quad a=b, z_0<1 \quad \text{and} \quad z_w<1; \\ \log 2a - \dfrac{\pi^2}{2w_a^2} - \dfrac{\pi^2(2-3z_w)}{(1-z_w)w_a^3} + O\left(w_a^{-4}\right), & \text{if} \quad a=b, z_0=1 \quad \text{and} \quad z_w<1. \end{cases} \tag{145}$$

There are numerous phases in this model in the $w_a\to\infty$ limit. For $z_0>1$ the path is pinned at the AB-interface (provided that $z_0>z_w$), and similarly for $z_w>1$. If $z_0<1$ and $z_w<1$, then the path is in an expanded phase delocalized over the lattice. This does not change when $z_0=1$ and $z_w<1$; the path remains delocalized.

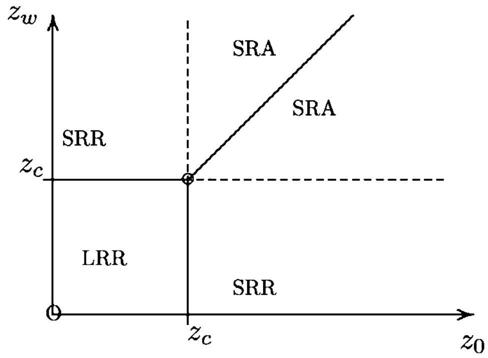

Figure 19. The phase diagram of the model in section 4.5.3, with $a = b = 1$ in figure 17. In this model $z_c = 1$. The phase boundaries are denoted by the solid lines and separate a desorbed phase for $z_0 < 1$ and $z_w < 1$. If $z_0 > 1$ and $z_0 > z_w$, then the path is adsorbed on the BA-interface, and if $z_w > 1$ and $z_w > z_0$, then the path is adsorbed on the AB-interface. If both $z_w > 1$ and $z_0 > 1$, then there is a short-ranged attractive (SRA) force between the interfaces. When $z_w \to 1^+$ for $z_0 > 1$ the force vanishes (along the dashed lines in figure 19) and then changes sign to become repulsive and short ranged (SRR). Finally, for both $z_0 < 1$ and $z_w < 1$, the forces are long ranged and repulsive (LRR).

The force exerted by the path on the bounding walls of the A-layer are obtained by taking the derivative of the free energy with respect to w_a:

$$f_w \simeq \begin{cases} -\dfrac{z_0(z_w-1)(z_0-1)^2\log(2z_0-1)}{(z_0-z_w)(2z_0-1)}\left(\dfrac{1}{2z_0-1}\right)^{w_a} & \\ \qquad + O((2z_0-1)^{-2w_a}), & \text{if} \quad a=b, z_0 > z_w \quad \text{and} \quad z_0 > 1; \\ -\dfrac{(z_0-1)^2\log(2z_0-1)}{2(2z_0-1)}\left(\dfrac{1}{2z_0-1}\right)^{w_a/2} & \\ \qquad + O((2z_0-1)^{-w_a}), & \text{if} \quad a=b, \quad z_0 = z_w \geqslant 1; \\ \dfrac{\pi^2}{w_a^3} + \dfrac{3\pi^2(2z_0z_w - z_0 - z_w)}{2(1-z_0)(1-z_w)w_a^4} + O\left(w_a^{-5}\right), & \text{if} \quad a=b, \quad z_0 < 1 \quad \text{and} \quad z_w < 1; \\ \dfrac{\pi^2}{w_a^3} + \dfrac{3\pi^2(2-3z_w)}{(1-z_w)w_a^4} + O\left(w_a^{-5}\right), & \text{if} \quad a=b, z_0 = 1 \quad \text{and} \quad z_w < 1, \end{cases} \tag{146}$$

where we note that the expressions are symmetric in z_w and z_0. In other words, if $z_w > z_0$ instead, then we exchange $z_0 \leftrightarrow z_w$ to obtain the expressions for the force and for the free energy above. Observe the zero force lines give by $z_0 = 1$ and $z_w \geqslant 1$, and $z_w = 1$ and $z_0 < 1$.

The force and phase diagram of this model is given in figure 19. There are three phases in the model in the limit that $w_a \to \infty$: a desorbed phase for small values of $z_0 < 1$ and $z_w < 1$, and two adsorbed or pinned phases when either $z_0 > 1$ and $z_0 > z_w$ or $z_w > 1$ and $z_w > z_0$. The phase boundaries are denoted by the solid lines in figure 19.

For finite values of w_a the path exerts a force on the two interfaces separating the A-layer from the B-layers. If both $z_w > 1$ and $z_0 > 1$, then the paths are pinned on the interfaces and equation (146) indicates a short-ranged attractive (SRA) force between the interfaces due to the pinning of paths on both interfaces. When $z_w \to 1^+$ for $z_0 > 1$ or $z_w > 1$ and $z_0 \to 1^+$ these forces vanish (along the dashed lines in figure 19) and then changes sign to become repulsive and short ranged (SRR). In this regime the path is pinned on one interface but is repelled by the other, and the resulting forces are repulsive and short ranged. Finally, for both $z_0 < 1$ and $z_w < 1$ the paths are desorbed in the A-layer. The forces are long ranged and repulsive (LRR).

4.5.4. The case $b = 0$. The case $b = 0$ introduces a hard wall on the AB- and BA-interfaces and the model reduces to the model in [3] and section 4.1. It can be verified that the solution here gives the same expressions.

5. Conclusions

In this paper we examined the properties of a directed path model of a polymer in a layered environment composed of two alternating layers. The model has a rich thermodynamic structure, with several distinct phases, including localized, adsorbed or pinned and delocalized phases which give rise to several long-ranged or short-ranged attractive or repulsive force regimes.

We solved for the generating function of the general model in section 4, and for a simpler case (the 'diagonal model') in section 3. Exact solutions for small values of the widths of the layers are given in section 2.2. Even for these cases (small values of the width in the diagonal model) the exact solutions increase quickly in complexity, and for $w = 3$ the free energy of the model can only be determined by solving for the roots of a cubic.

While we give general expressions for the generating function of these models in both the diagonal and general cases in sections 3 and 4, determining free energies and phase regimes cannot in general be done exactly, and only asymptotic regimes were identified for large values of the width. In the diagonal model, we determined asymptotics for the free energy in several cases, including the cases that $b = 0$ in section 3.1 (this is the slit model), and $a = b$ in section 3.2. These models are characterized by two force regimes, namely, a long-ranged repulsive force on the interfaces for small values of the parameter z, and a short-ranged attractive force for large values of z. See equations (33) and (36). The effects of the parameters a and b on the free energy are examined in section 3.3. We identified two distinct cases, namely $a \approx b$ and the cases that $a \gg b$ or $a \ll b$. The free energy is approximated in equation (49).

Asymptotics for the general model in section 4 have only been done in a number of special cases. A notable case is presented in section 4.1, which is a directed path in a slit. Our solution reduces to that in [3], and we verify asymptotics of the free energy and force regimes by showing that we obtain the same expressions given in [3].

We proceeded by considering models of paths in a slits with centered and off-centered defect lines in sections 4.2, 4.3 and 4.4. In these models all forces are repulsive, but do fall into two regimes, namely, a long-ranged repulsive force on the walls of the slit for small values of z_0, and a short-ranged repulsive force for large values of z_0.

In section 4.5, a model with a finite A-layer between two infinite B-layers is examined as a model of a lipid–water membrane system. This model is obtained by $w_b \to \infty$. We give expressions for the general asymptotics in this case and present several subcases. In particular, we develop asymptotics for the models that $z_0 = z_w = 1$ and $z_0 = 1$ with $z_w = 0$, and for the cases $a = b$ and $b = 0$ (this last case reduces the model again to a path in a slit). These models exhibit a rich structure, and attractive and repulsive, and long- and short-ranged force regimes were uncovered. Further generalizations of this model to an ABC-layered model with an infinite width C-layer is possible, and is left for future exploration.

Acknowledgments

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Appendix A. Expressions for C in equation (119) and c_2 in equations (120)

The expression for C in the asymptotic formula for p in equation (119) is given by

$$C = \frac{N_1}{D_1}, \tag{A.1}$$

where

$$\begin{aligned}
N_1 = \big(&17{z_0}^2{z_w}^2 - 26{z_0}^2 z_w - 26 z_0 {z_w}^2 + 9{z_0}^2 + 44 z_0 z_w + 9{z_w}^2 - 16 z_0 \\
&- 16 z_w + 6\big)a^4 {p_0}^{11} + \big(\big(37{z_0}^2{z_w}^2 - 82{z_0}^2 z_w - 82 z_0 {z_w}^2 + 35{z_0}^2 \\
&+ 172 z_0 z_w + 35{z_w}^2 - 72 z_0 - 72 z_w + 30\big)a^4 + \big(16b^2{z_0}^2{z_w}^2 \\
&- 16b^2{z_0}^2 z_w - 16b^2 z_0 {z_w}^2 + 6b^2{z_0}^2 + 6b^2{z_w}^2\big)a^2\big){p_0}^9 + \big(6b^4{z_0}^2{z_w}^2 \\
&+ \big(32{z_0}^2{z_w}^2 - 100{z_0}^2 z_w - 100 z_0 {z_w}^2 + 52{z_0}^2 + 264 z_0 z_w \\
&+ 52{z_w}^2 - 128 z_0 - 128 z_w + 60\big)a^4 + \big(36b^2{z_0}^2{z_w}^2 - 40b^2{z_0}^2 z_w \\
&- 40b^2 z_0 {z_w}^2 + 18b^2{z_0}^2 + 18b^2{z_w}^2\big)a^2\big){p_0}^7 + \big(6b^4{z_0}^2{z_w}^2 \\
&+ \big(16{z_0}^2{z_w}^2 - 60{z_0}^2 z_w - 60 z_0 {z_w}^2 + 36{z_0}^2 + 200 z_0 z_w + 36{z_w}^2 \\
&- 112 z_0 - 112 z_w + 60\big)a^4 + \big(20b^2{z_0}^2{z_w}^2 - 32b^2{z_0}^2 z_w - 32b^2 z_0 {z_w}^2 \\
&+ 18b^2{z_0}^2 + 18b^2{z_w}^2\big)a^2\big){p_0}^5 + \big(\big(5{z_0}^2{z_w}^2 - 18{z_0}^2 z_w - 18 z_0 {z_w}^2 \\
&+ 11{z_0}^2 + 76 z_0 z_w + 11{z_w}^2 - 48 z_0 - 48 z_w + 30\big)a^4 + \big(-8b^2{z_0}^2 z_w \\
&- 8b^2 z_0 {z_w}^2 + 6b^2{z_0}^2 + 6b^2{z_w}^2\big)a^2\big){p_0}^3 + \big({z_0}^2{z_w}^2 - 2{z_0}^2 z_w - 2 z_0 {z_w}^2 \\
&+ {z_0}^2 + 12 z_0 z_w + {z_w}^2 - 8 z_0 - 8 z_w + 6\big)a^4 p_0, \\
D_1 = \big(&120{z_0}^2{z_w}^2 - 180{z_0}^2 z_w - 180 z_0 {z_w}^2 + 60{z_0}^2 + 270 z_0 z_w + 60{z_w}^2 \\
&- 90 z_0 - 90 z_w + 30\big)a^4 {p_0}^{10} + \big(\big(168{z_0}^2{z_w}^2 - 392{z_0}^2 z_w - 392 z_0 {z_w}^2 \\
&+ 168{z_0}^2 + 798 z_0 z_w + 168{z_w}^2 - 322 z_0 - 322 z_w + 126\big)a^4 \\
&+ \big(112b^2{z_0}^2{z_w}^2 - 84b^2{z_0}^2 z_w - 84b^2 z_0 {z_w}^2 + 28b^2{z_0}^2 + 28b^2{z_w}^2\big)a^2\big){p_0}^8 \\
&+ \big(26b^4{z_0}^2{z_w}^2 + \big(74{z_0}^2{z_w}^2 - 288{z_0}^2 z_w - 288 z_0 {z_w}^2 + 164{z_0}^2 \\
&+ 860 z_0 z_w + 164{z_w}^2 - 432 z_0 - 432 z_w + 204\big)a^4 + \big(100b^2{z_0}^2{z_w}^2 \\
&- 140b^2{z_0}^2 z_w - 140b^2 z_0 {z_w}^2 + 64b^2{z_0}^2 + 64b^2{z_w}^2\big)a^2\big){p_0}^6 \\
&+ \big(10b^4{z_0}^2{z_w}^2 + \big(10{z_0}^2{z_w}^2 - 84{z_0}^2 z_w - 84 z_0 {z_w}^2 + 64{z_0}^2 + 412 z_0 z_w \\
&+ 64{z_w}^2 - 264 z_0 - 264 z_w + 156\big)a^4 + \big(20b^2{z_0}^2{z_w}^2 - 64b^2{z_0}^2 z_w \\
&- 64b^2 z_0 {z_w}^2 + 44b^2{z_0}^2 + 44b^2{z_w}^2\big)a^2\big){p_0}^4 + \big(\big(-8{z_0}^2 z_w - 8 z_0 {z_w}^2 \\
&+ 8{z_0}^2 + 86 z_0 z_w + 8{z_w}^2 - 70 z_0 - 70 z_w + 54\big)a^4 + \big(-8b^2{z_0}^2 z_w \\
&- 8b^2 z_0 {z_w}^2 + 8b^2{z_0}^2 + 8b^2{z_w}^2\big)a^2\big){p_0}^2 + (6 z_0 z_w - 6 z_0 - 6 z_w + 6)a^4.
\end{aligned}$$

This shows that C is a rational function of p_0, its numerator a polynomial of degree 12 in p_0 and its denominator a polynomial of degree 10 in p_0, both with coefficients which are quadratic in z_0 and z_w multiplied by even powers of a less than or equal to 4. In each case p_0 is given by

$$p_0^2 = -\frac{z_0^2 - 4z_0 + 1}{2(2z_0 - 1)(z_0 - 1)} - \frac{z_0\left(2z_0b^2 \pm \sqrt{z_0^2(a^2+b^2)^2 + 4a^2b^2(1-2z_0)}\right)}{2a^2(2z_0 - 1)(z_0 - 1)}.$$

The solution for c_2 in equation (120) is given as

$$c_2 = \frac{Nc_2}{Dc_2} \tag{A.2}$$

where

$$Nc_2 = 4\pi \mathrm{i} a^3(a + \sqrt{a^2 - b^2})(3z_0z_w - z_w - z_0) - 2\pi \mathrm{i}(4z_0z_w - z_0 - z_w)a^2b^2 + 2\pi \mathrm{i} z_0z_w ab^2\sqrt{a^2 - b^2},$$

and

$$Dc_2 = 6a^3(a - \sqrt{a^2 - b^2})(3z_0z_2 - 2z_0 - 2z_w) + 8a^3(a - \sqrt{a^2 - b^2}) - a^2b^2(15z_0z_w - 8z_0 - 8z_w) + 2ab^2\sqrt{a^2 - b^2}(3z_0z_w - z_0 - z_w) - 4a^2b^2 + b^4z_0z_w.$$

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