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Adsorbing and collapsing trees

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Abstract. Self-interacting branched polymers interacting with a wall can be modelled by lattice trees in a half-space with a nearest-neighbour contact-fugacity β and a visit-fugacity α conjugate to the number of visits the tree makes to the wall (which is the boundary of the half-space). We show that there is a limiting free energy in this model, and that it is a non-analytic function of the visit-fugacity for every finite and fixed value of the contact-fugacity. This implies the existence of an adsorption transition in this model, and there is a critical curve $\alpha_c^+(\beta)$ in the phase diagram which separates the phase of desorbed trees from a phase of adsorbed trees. Moreover, we show that $\alpha_c^+(\beta) > 0$ for all finite values of the contact-fugacity, and the adsorption transition occurs at a strictly attractive value of the interaction between the tree and the wall.

1. Introduction

Branched polymers in dilute solution can be modelled by lattice trees which are connected and acyclic subgraphs of the lattice (usually the square or cubic lattice). Vertices represent *monomers* in the polymer, while edges represent the bonds between monomers. A branched polymer in dilute solution will undergo a collapse transition if the quality of its solvent deteriorates beyond a certain critical point, called the θ -point. The transition is an internal rearrangement of the monomers in the polymer, which occurs when the effective attractive interaction between the monomers overcomes the entropic repulsion (due to excluded volume) in the polymer (Mazur and McCrackin 1968, Mazur and McIntyre 1975). In a lattice tree, the monomer–monomer interaction is modelled by a fugacity conjugate to the number of *contacts* between nearest-neighbour vertices in the tree which are not adjacent in the tree. This model has been the subject of numerous studies in the last couple of decades, see for example Dickman and Shieve (1986), Lam (1988), Madras *et al* (1990), Gaunt and Flesia (1990, 1991), Flesia and Gaunt (1992), Janse van Rensburg and Madras (1996), Madras and Janse van Rensburg (1997).

In this paper we are interested in a lattice tree model of a self-interacting branched polymer interacting with a plane. This problem has been considered for self-avoiding walk models of linear polymers and ring polymers, see for example the papers by Finsky *et al* (1975), Hammersley *et al* (1982), Vanderzande (1995), Vrbová and Whittington (1996, 1998a, 1998b), Janse van Rensburg (1998). Related results for the adsorption of a copolymer were obtained by Whittington (1998). The scaling theory of the adsorption transition has been reviewed by De’Bell and Lookman (1993). In the lattice tree version of this problem we will work with bond- or edge-trees in \mathcal{Z}^d interacting with the $(d - 1)$ -dimensional hyperplane $z = 0$.

We consider two lattice trees (in general) to be equivalent if they can be made identical by a translation. The total number of lattice trees defined in this way will be denoted by T_n , where n is the number of edges in the trees. It is known that the limit

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log T_n = \log \lambda_d \quad (1.1)$$

exists, where λ_d is the growth constant of lattice trees (Klein 1981, Janse van Rensburg 1992). If the lattice tree interacts with the hyperplane $z = 0$, then the definition of T_n must to be changed as follows. We indicate coordinates of a vertex in a tree by (x, y, \dots, z) , where the d th coordinate will always be z . Two lattice trees are equivalent if one can be made identical to the other by a translation which leaves all z -coordinates unchanged (such a translation is parallel to the hyperplane $z = 0$). Since the trees should always be in the vicinity of the hyperplane $z = 0$, we also require that there is at least one vertex in each tree which has its z -coordinate in the set $\{-1, 0, 1\}$; these trees will be called *attached trees*. Let t_n be the number of attached trees. Notice that the growth constant of attached trees is also given by λ_d in equation (1.1). Obviously, $t_n \geq T_n$, since each tree counted by T_n can be translated to intersect the hyperplane $z = 0$. On the other hand, each attached tree can be translated in the z -direction to become a tree; since at most n attached trees can be translated to the same tree, $t_n \leq nT_n$. Thus,

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log t_n = \log \lambda_d. \quad (1.2)$$

There are two models of lattice trees interacting with the hyperplane $z = 0$. In the first model we will confine the tree to the half-space $z \geq 0$, in which case we have a model of a branched polymer interacting with an impenetrable wall. Such attached trees are called *positive trees*, and the number of these will be indicated by t_n^+ . In the second case we will not confine the tree to the half-space $z \geq 0$; this may be considered a model of a branched polymer interacting with the interface between two liquids. In this paper we are primarily interested in t_n^+ : the model of branched polymers adsorbing on a wall. However, we shall also find it useful to compare these two models.

The interaction between the attached tree and the adsorbing plane is modelled by counting the number of vertices in the tree with z -coordinate equal to zero. Such vertices are called *visits*, and the basic quantities in this paper will be $t_n(v, c)$ and $t_n^+(v, c)$, where $t_n(v, c)$ is the number of attached trees with v visits and c contacts, and $t_n^+(v, c)$ is the number of positive attached trees with v visits and c contacts. We introduce two fugacities into these models. The interaction with the adsorbing plane is modelled by introducing a *visit-fugacity* α , with α conjugate to the number of visits in the tree, and the self-interaction in the tree is modelled by introducing a *contact-fugacity* β , with β conjugate to the number of contacts. It is generally believed that there is a θ -transition at a critical value of β , where the tree undergoes a collapse transition from an expanded conformation to a collapsed conformation. We shall prove that there is an adsorption transition in these models at a critical value of the visit-fugacity. The partition function for the model of attached trees interacting with the hyperplane $z = 0$ is

$$Z_n(\alpha, \beta) = \sum_{v \geq 0} \sum_{c \geq 0} t_n(v, c) e^{\alpha v} e^{\beta c}. \quad (1.3)$$

A model of self-interacting branched polymers interacting with an impenetrable wall is defined by considering positive attached trees instead.

$$Z_n^+(\alpha, \beta) = \sum_{v \geq 0} \sum_{c \geq 0} t_n^+(v, c) e^{\alpha v} e^{\beta c}. \quad (1.4)$$

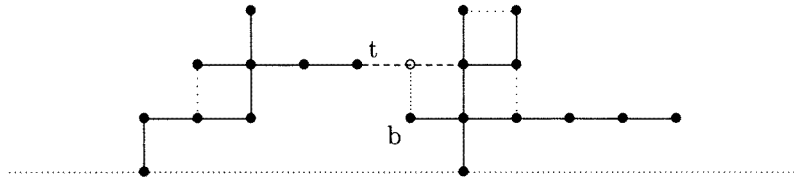


Figure 1. Concatenation of two positive trees. If the tree on the right is shifted two more steps towards the left, then there will be an intersection between them. The trees are concatenated by adding the vertex \circ and an edge to each tree. This may create as many as $2(d-1)$ new contacts in d dimensions, as well as an extra visit, if \circ is in the wall. The top vertex and bottom vertex are indicated by t and b respectively.

At small (or negative) values of the parameters (α, β) we expect the trees to be desorbed and expanded in a phase which we call the DE-phase. Increasing α should lead to an adsorption into an adsorbed and expanded phase (AE-phase). Similarly, increasing β will give a desorbed and collapsed phase (DC-phase). In three and higher dimensions increasing both α and β should give a collapse and adsorbed phase (AC-phase). Available data in directed walk models suggest that the AC-phase is not present in two dimensions (see for example Foster 1990, Foster and Yeomans 1991, Foster *et al* 1992).

In the next section we show that the limiting free energies of these models exist. In section 3 we consider primarily the phase diagram of positive attached trees. We prove that the limiting free energy is a non-analytic function of α for each $\beta < \infty$. This corresponds to the adsorption transition in this model. We then turn our attention to attached trees interacting with a defect plane, and prove that there is an adsorption transition in that model as well. These results prove that there are critical curves in the phase diagrams of these models which separate the desorbed and adsorbed phases. We also observe that the limiting free energy is independent of the visit-fugacity in the desorbed phase in both models. A consequence is that if there is a collapse transition in these models, then the phase boundaries separating the DE-phase from the DC-phase are straight lines. In section 4 we turn our attention to the nature of the adsorbed phase in positive attached trees. We prove that there is a connection between the density functions of visits in the models, and the location of the adsorption transition. This gives a proof that positive trees adsorb only at a strictly positive value of the visit-fugacity. A second proof of this fact is given using a different approach, and we also examine the density of excursions in the adsorbed phase.

2. The limiting free energies of adsorbing and collapsing trees

In this section we examine the limiting free energies of the models defined in equations (1.3) and (1.4). Let Z^d be the d -dimensional hypercubic lattice. The *bottom* and *top* vertices of a tree are its lexicographic least and most vertices.

Theorem 2.1. There exist functions \mathcal{F}_d and \mathcal{F}_d^+ such that

$$\mathcal{F}_d(\alpha, \beta) = \lim_{n \rightarrow \infty} \frac{1}{n} \log Z_n(\alpha, \beta)$$

$$\mathcal{F}_d^+(\alpha, \beta) = \lim_{n \rightarrow \infty} \frac{1}{n} \log Z_n^+(\alpha, \beta)$$

for all $\alpha < \infty$ and $\beta < \infty$. Moreover, $\mathcal{F}_d(\alpha, \beta)$ and $\mathcal{F}_d^+(\alpha, \beta)$ are convex functions in both their arguments, and are non-decreasing, continuous, and differentiable almost everywhere.

Proof. We prove this for the model of positive trees. A similar proof will show the existence of the limiting free energy $\mathcal{F}_d(\alpha, \beta)$. Let T_1 and T_2 be two positive trees with n edges, v_1 visits and c_1 contacts, and m edges, $v - v_1$ visits and $c - c_1$ contacts, respectively. Translate T_2 parallel to the $z = 0$ hyperplane until its bottom vertex has the same coordinates as the top vertex of T_1 , except for the x - and z -coordinates. Translate T_2 in the x -direction until the x -coordinate of its bottom vertex is two steps bigger than the x -coordinate of the top vertex of T_1 . Next translate T_2 in the negative x -direction, until there is a vertex in T_2 which is within a distance of two steps from a vertex in T_1 (see figure 1). At this point, there are no contacts between vertices in T_1 and in T_2 . Let w_1 in T_1 and w_2 in T_2 be two vertices which are exactly two steps apart. We concatenate T_1 and T_2 by adding two new edges and one vertex between w_1 and w_2 . The new vertex may be adjacent to at most $2d$ vertices in the two trees, and so as many as $2(d - 1)$ new contacts may be created. In addition, if the new vertex is in the wall, then there is also a new visit. Thus, a new tree with $n + m + 2$ edges and $v + i$ visits ($i = 0$ or $i = 1$) and $c + j$ contacts ($j \in \{0, 1, \dots, 2(d - 1)\}$) is created. Each distinct pair of trees will give a different outcome, therefore

$$\sum_{v_1, c_1} t_n^+(v_1, c_1) t_m^+(v - v_1, c - c_1) \leq \sum_{i=0}^1 \sum_{j=0}^{2(d-1)} t_{n+m+2}^+(v + i, c + j).$$

In other words, $t_n^+(v, k)$ is a generalized supermultiplicative function, of the kind discussed in Tesi *et al* (1997). Multiply this equation by $e^{\alpha v + \beta c}$, and sum over v and c . Then

$$Z_n^+(\alpha, \beta) Z_m^+(\alpha, \beta) \leq \left[\sum_{i=0}^1 \sum_{j=0}^{2(d-1)} e^{-\alpha i - \beta j} \right] Z_{n+m+2}^+(\alpha, \beta).$$

Thus, $Z_{n-2}^+(\alpha, \beta) / [\sum_{i=0}^1 \sum_{j=0}^{2(d-1)} e^{-\alpha i - \beta j}]$ is a supermultiplicative function. In addition, since there are at most $n + 1$ visits and $(d - 1)n$ contacts in a tree,

$$Z_n^+(\alpha, \beta) \leq \begin{cases} t_n^+ & \text{if } \alpha \leq 0 \text{ and } \beta \leq 0 \\ t_n^+ e^{\alpha(n+1)} & \text{if } \alpha > 0 \text{ and } \beta \leq 0 \\ t_n^+ e^{(d-1)\beta n} & \text{if } \alpha \leq 0 \text{ and } \beta > 0 \\ t_n^+ e^{\alpha(n+1) + (d-1)\beta n} & \text{if } \alpha > 0 \text{ and } \beta > 0. \end{cases}$$

But there is a finite constant $K > 0$ such that $t_n^+ < K^n$, thus, $Z_n^+(\alpha, \beta)$ is bounded exponentially in n for all finite values of α and β . Thus, the claimed limit exists (Hille 1948). \square

We define $\mathcal{F}_d^+(0, 0) = \log \lambda_d^+$, where λ_d^+ is the growth constant of positive attached trees in d dimensions. If λ_d is the growth constant of attached trees in d dimensions, then the following inequalities relate λ_d^+ and λ_d .

Lemma 2.2. $\lambda_{d-1} < \lambda_d^+ = \lambda_d$.

Proof. We first prove the inequality $\lambda_{d-1} < \lambda_d^+$. Let $T_n^{(d-1)}$ be the number of trees, counted up to translation, in the $(d - 1)$ -dimensional lattice defined by the hyperplane $z = 0$. Let T be one of these trees. Then we can add an edge at any vertex of T in the z -direction to create a positive tree. If k vertices are added to the tree in this way in $\binom{n}{k}$ ways, then

$$\binom{n}{k} T_n^{(d-1)} \leq t_{n+k}^+.$$

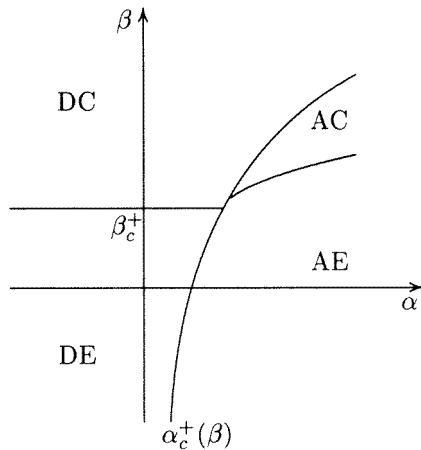


Figure 2. The hypothetical phase diagram for adsorbing and collapsing positive attached trees in three and more dimensions.

Let $k = \lfloor \epsilon n \rfloor$ in this, take the $1/n$ -power, and let $n \rightarrow \infty$. This gives

$$\left[\frac{(\lambda_d^+)^{-\epsilon}}{\epsilon^\epsilon (1-\epsilon)^{(1-\epsilon)}} \right] \lambda_{d-1} \leq \lambda_d^+.$$

The factor in the square brackets is equal to its maximum $(1 + 1/\lambda_d^+)$ when $\epsilon = 1/(1 + \lambda_d^+)$. This proves the inequality.

On the other hand, each attached tree counted by t_n can be translated normal to the plane $z = 0$ until it is a positive tree. Since at most n such trees can be translated to the same positive tree, we find that $t_n^+ \leq t_n \leq n t_n^+$, and by equation (1.2) we get the equality. \square

Non-analyticities in the free energy will signal thermodynamic phase transitions in the models above. In particular, we expect critical lines in the phase diagram which correspond to a collapse transition (these are the θ -points), and to an adsorption transition. The θ -points are believed to be tricritical, and if $\alpha = 0$, then the singularity in $\mathcal{F}_d(0, \beta)$ is expected to have the general form $\mathcal{F}_d(0, \beta) \sim |\beta - \beta_c|^{2-\alpha_\theta}$ (where β_c is the critical value of the β and α_θ is the specific heat exponent associated with the θ -transition). More generally, it is not unreasonable to expect that the θ -transition will occur for all values of the visit-fugacity α corresponding to a phase of desorbed trees. In three and higher dimensions we can also expect a line of θ -points corresponding to collapse transitions, but, in analogy with walks, this should not be present in two dimensions (Foster 1990, Foster and Yeomans 1991, Foster *et al* 1992). The phase diagram for adsorbing and collapsing trees is presented in figure 2, and is similar to the diagram proposed for walks and polygons (Vrbová and Whittington 1996, 1998a, b, Janse van Rensburg 1998).

3. The phase diagram of adsorbing and collapsing trees

In this section we examine the proposed phase diagram in figure 2 more closely. In the first instance we will prove below that there is an adsorption transition in this model at a critical visit fugacity $\alpha = \alpha_c^+(\beta)$ for any $\beta < \infty$. Secondly, the critical curve between the DE-phase and the DC-phase is a straight line. We shall see that if we assume that there is a collapse transition at $\beta = \beta_c^+$ for any (one) $\alpha \leq 0$, then there is a collapse transition at $\beta = \beta_c^+$ for all $\alpha \leq 0$ (theorem 3.1). If we also assume that $\alpha_c^+(\beta)$ is continuous at β_c^+ , then there is a collapse transition at $\beta = \beta_c^+$ for all $\alpha < \alpha_c^+(\beta_c^+)$ (theorem 3.4). These

results justify some of the features in the phase diagram in figure 2. The existence of an adsorption transition at $\alpha = \alpha_c^+(\beta)$ is shown in theorems 3.2 and 3.3.

If $\alpha = 0$ in $\mathcal{F}_d^+(\alpha, \beta)$, then we have a model of self-interacting positive trees. Arguments similar to those preceding equation (1.2) show that $t^+(c) \leq t(c) \leq nt^+(c)$ (where $t(c) = \sum_v t_n(v, c)$, etc), with the result that

$$\mathcal{F}_d^+(0, \beta) = \mathcal{F}_d(0, \beta) = \mathcal{F}_d(\beta) \quad (3.1)$$

where $\mathcal{F}_d(\beta)$ is the limiting free energy if a model of self-interacting lattice trees (see Janse van Rensburg and Madras (1996) and Madras and Janse van Rensburg (1997) for numerical results on the collapse transition in this model).

Theorem 3.1. For every value of $\beta < \infty$, the limiting free energy $\mathcal{F}_d^+(\alpha, \beta)$ is independent of α for all $\alpha \leq 0$ (that is, $\mathcal{F}_d^+(\alpha, \beta) = \mathcal{F}_d(\beta)$ for all $\alpha \leq 0$).

Proof. Consider any positive attached tree with v visits and c contacts. Such a tree can be translated one step in the z -direction to find a positive attached tree with zero visits, and c contacts. Thus $t_n^+(v, c) \leq t_n^+(0, c)$. Use this, and the fact that $\alpha \leq 0$, in the following string of inequalities:

$$\sum_c t_n^+(0, c)e^{\beta c} \leq Z_n^+(\alpha, \beta) \leq \sum_{v,c} t_n^+(0, c)e^{\alpha v + \beta c} \leq n \sum_c t_n^+(0, c)e^{\beta c}.$$

Take logarithms, divide by n and let $n \rightarrow \infty$. This shows that there is a limiting free energy $\mathcal{F}_d(\beta) = \mathcal{F}_d^+(0, \beta)$ for a model of self-interacting trees, and that $\mathcal{F}_d^+(\alpha, \beta) = \mathcal{F}_d(\beta)$ for all $\alpha \leq 0$. \square

Suppose now that there is a collapse transition in this model at $\beta = \beta_c^+$ for a given $\alpha \leq 0$. Then theorem 3.1 implies that there is a collapse transition at $\beta = \beta_c^+$ for all values of $\alpha \leq 0$; the critical curve of θ -points $\beta_c^+(\alpha)$ is a straight line for all $\alpha \leq 0$. Theorem 3.1 also suggests that there may be an adsorption transition in this model. Since $\mathcal{F}_d^+(\alpha, \beta)$ is a constant function of $\alpha \leq 0$, we only need to show that it is a non-constant function of α for some value of $\alpha > 0$ to prove that it is a non-analytic function of α .

Lemma 3.2. For $\alpha > 0$

$$\max\{\mathcal{F}_d(\beta), \mathcal{F}_{d-1}(\beta) + \alpha\} \leq \mathcal{F}_d^+(\alpha, \beta) \leq \mathcal{F}_d(\beta) + \alpha.$$

Proof. Since $Z_n^+(\alpha, \beta)$ is a non-decreasing function of α , we have $\mathcal{F}_d^+(0, \beta) \leq \mathcal{F}_d^+(\alpha, \beta)$, for all positive α . By picking out only those terms in the sum of $Z_n^+(\alpha, \beta)$ with $v = n + 1$, we have a completely adsorbed tree (there are $t_n^{(d-1)}(c)$ such trees with c contacts in $(d - 1)$ dimensions) and

$$\sum_c t_n^{(d-1)}(c)e^{\alpha(n+1) + \beta c} \leq Z_n^+(\alpha, \beta).$$

If we take logarithms of the above, divide by n and let $n \rightarrow \infty$, then we obtain

$$\mathcal{F}_{d-1}(\beta) + \alpha \leq \mathcal{F}_d^+(\alpha, \beta).$$

The upper bound is obtained by noting that the maximum value of v is $n + 1$, and that $\alpha > 0$. Thus, put $v = n + 1$ in $e^{\alpha v}$ in equation (1.4), then

$$Z_n^+(\alpha, \beta) \leq e^{\alpha(n+1)} \sum_c t_n^+(c)e^{\beta c}.$$

The bound follows on taking logarithms, dividing by n and letting $n \rightarrow \infty$. \square

Notice that

$$\mathcal{F}_d^+(0, 0) = \mathcal{F}_d(0, 0) = \mathcal{F}_d(0) = \log \lambda_d \tag{3.2}$$

by equations (1.2) and (3.1). The lower bound on $\mathcal{F}_d^+(\alpha, \beta)$ in lemma 3.2 indicates that the free energy becomes dependent on α for some value of α (indicated by $\alpha_c^+(\beta)$) in the interval $[0, \mathcal{F}_d(\beta) - \mathcal{F}_{d-1}(\beta)]$; there is a non-analyticity in $\mathcal{F}_d^+(\alpha, \beta)$ in this interval. The density of visits in positive trees is zero if $\alpha < \alpha_c^+(\beta)$. This we see by noting that $\frac{\partial}{\partial \alpha} \mathcal{F}_d^+(\alpha, \beta) = 0$ for all finite β , and all $\alpha < \alpha_c^+(\beta)$. Since $\mathcal{F}_d^+(\alpha, \beta)$ is convex in α , the density of visits is a non-decreasing function, and moreover, if $\alpha > \alpha_c^+(\beta)$, then the density of visits is non-zero. In other words, a non-zero fraction of the vertices in the polygon is adsorbed in the wall, and we can refer to $\alpha_c^+(\beta)$ as the critical fugacity of the adsorption transition. In theorem 3.3 we derive some bounds on the location of the critical visit-fugacity.

Theorem 3.3. The limiting free energy of self-interacting positive trees interacting with a surface, $\mathcal{F}_d^+(\alpha, \beta)$, is a non-analytic function of α for every value of $\beta < \infty$. Moreover, the phase boundary $\alpha_c^+(\beta)$ is in the interval $[0, \log \lambda_d - \frac{1}{2} \log \lambda_{d-1}]$ if $\beta < 0$ and in the interval $[0, \log \lambda_d - \log \lambda_{d-1} + (d - 1)\beta]$ if $\beta \geq 0$.

Proof. From theorem 3.1 and lemma 3.2, and from equation (3.2), for every $\beta < \infty$ there must be a non-analyticity in $\mathcal{F}_d^+(\alpha, \beta)$ at

$$\alpha_c^+(\beta) = \sup\{\alpha | \mathcal{F}_d^+(\alpha, \beta) = \mathcal{F}_d(\beta)\}.$$

In addition, the location of $\alpha_c^+(\beta)$ is in the interval $[0, \mathcal{F}_d(\beta) - \mathcal{F}_{d-1}(\beta)]$. If $\beta \geq 0$, then the maximum number of contacts in the tree is $(d - 1)n$, so that we note that $Z_n^+(0, \beta) \leq \sum_c t_n^+(c) e^{(d-1)\beta n} = t_n^+ e^{(d-1)\beta n}$. Thus, $\mathcal{F}_d(\beta) \leq \log \lambda_d + (d - 1)\beta$. In addition, $Z_n^+(0, \beta) \geq \sum_c t_n^+(c) = t_n^+$. Thus, $\mathcal{F}_{d-1}(\beta) \geq \log \lambda_{d-1}$. These bounds give the result if $\beta \geq 0$. Thus, $\mathcal{F}_d(\beta) - \mathcal{F}_{d-1}(\beta) \leq \log \lambda_d - \log \lambda_{d-1} + (d - 1)\beta$.

If $\beta < 0$, then $Z_n^+(0, \beta) = \sum_c t_n^+(0, c) e^{\beta c} \leq t_n^+$, so that $\mathcal{F}_d(\beta) \leq \log \lambda_d$. On the other hand, if every edge in the trees counted by t_n^+ is subdivided, then $t_n^+ \leq t_{2n}^+(0)$, since the resulting trees will have no contacts. Thus, $Z_n^+(0, \beta) \geq t_n^+(0)$ implies that $\mathcal{F}_{d-1}(\beta) \geq \frac{1}{2} \log \lambda_{d-1}$. This completes the proof if $\beta < 0$. \square

We can now show that the critical curve separating the DE-phase and the DC-phase is independent of α for all values of $\alpha \leq \alpha_c^+(\beta_c^+)$, provided that $\alpha_c^+(\beta)$ is a continuous function of β at $\beta = \beta_c^+$. In other words, the critical line of collapse transitions is a straight line for all values of $\alpha \leq \alpha_c^+(\beta_c^+)$. This observation justifies the straight line of collapse transitions separating the DE-phase from the DC-phase in figure 2.

Theorem 3.4. Assume that $\mathcal{F}_d^+(0, \beta)$ is singular at $\beta = \beta_c^+$, and that the phase boundary $\alpha_c^+(\beta)$ is continuous at $\beta = \beta_c^+$. Then $\mathcal{F}_d^+(\alpha, \beta)$ is singular at $\beta = \beta_c^+$ for every $\alpha \leq \alpha_c^+(\beta_c^+)$.

Proof. Let $\epsilon > 0$ and choose α_d by

$$\alpha_d < \inf\{\alpha_c^+(\beta) | \beta \in [\beta_c^+ - \epsilon, \beta_c^+ + \epsilon]\}.$$

Since $\mathcal{F}_d^+(\alpha, \beta)$ is analytic for all such α_d , as long as $\beta \neq \beta_c^+$ and $\beta \in [\beta_c^+ - \epsilon, \beta_c^+ + \epsilon]$, we conclude that $\mathcal{F}_d^+(\alpha_d, \beta) = \mathcal{F}_d^+(0, \beta)$ for $\beta \in [\beta_c^+ - \epsilon, \beta_c^+ + \epsilon]$ (if this is not so, then we will have a phase boundary at (α_d, β_d^+) with β_d^+ some point in $[\beta_c^+ - \epsilon, \beta_c^+ + \epsilon]$; this is a contradiction). By taking ϵ small we can choose α_d to approach $\alpha_c^+(\beta_c^+)$, and the result follows. \square

We can now show that the free energy and the critical curves of the model of attached trees interacting with a defect plane satisfies the same bounds as above. In theorem 2.1 we proved that there exists a limiting free energy in this model. Since $t_n^+(v, c) \leq t_n(v, c)$ for each value of n , we have that

$$\mathcal{F}_d^+(\alpha, \beta) \leq \mathcal{F}_d(\alpha, \beta). \quad (3.3)$$

In addition, we will see in theorem 3.5 that $\mathcal{F}_d(\alpha, \beta) = \mathcal{F}_d(0, \beta)$ for all fixed β and $\alpha \leq 0$. That there is an adsorption transition in this model as well is seen by finding a lower bound on $\mathcal{F}_d(\alpha, \beta)$ for positive α , as we did in the case of positive trees in theorem 3.3.

Theorem 3.5. The limiting free energy of attached trees is a non-analytic function of α for every fixed $\beta < \infty$, and the phase boundary $\alpha_c(\beta)$ is bounded by $\alpha_c(\beta) \in [0, \log \lambda_d - \frac{1}{2} \log \lambda_{d-1}]$ if $\beta < 0$ and $\alpha_c(\beta) \in [0, \log \lambda_d - \log \lambda_{d-1} + (d-1)\beta]$ if $\beta \geq 0$.

Proof. We first show that $\mathcal{F}_d(\alpha, \beta) = \mathcal{F}_d(0, \beta)$ for all fixed $\beta < \infty$ and $\alpha \leq 0$. By equation (3.3) and theorem 3.1, we note that $\mathcal{F}_d(\beta) = \mathcal{F}_d^+(\alpha, \beta) \leq \mathcal{F}_d(\alpha, \beta) \leq \mathcal{F}_d(0, \beta) = \mathcal{F}_d(\beta)$. Thus

$$\mathcal{F}_d(\alpha, \beta) = \mathcal{F}_d(\beta) \quad \text{for all } \alpha \leq 0.$$

On the other hand, if $\alpha > 0$, then by only retaining terms in $Z_n(\alpha, \beta)$ with n visits, we get $\sum_c t_n(n, c) e^{\alpha n + \beta c} \leq Z_n(\alpha, \beta)$. This implies that $\mathcal{F}_{d-1}(\beta) + \alpha \leq \mathcal{F}_d(\alpha, \beta)$, and for α large enough, $\mathcal{F}_d(\alpha, \beta) > \mathcal{F}_d(\beta)$. In other words, for each $\beta < \infty$ there is a non-analyticity in $\mathcal{F}_d(\alpha, \beta)$. Let the critical curve in this model be $\alpha_c(\beta)$:

$$\alpha_c(\beta) = \sup\{\alpha \mid \mathcal{F}_d(\alpha, \beta) = \mathcal{F}_d(\beta)\}.$$

The critical curve is in fact in the interval given by $0 \leq \alpha_c(\beta) \leq \mathcal{F}_d(\alpha, \beta) - \mathcal{F}_{d-1}(0, \beta)$, and the same arguments in the proof of theorem 3.3 can be used to find the bounds claimed above. \square

4. The location of the adsorption transition

In this section we prove that positive attached trees adsorb at a critical fugacity $\alpha_c^+(\beta) > \alpha_c(\beta) \geq 0$ for $\beta \in (-\infty, \infty)$. In particular, we will prove that there exists a non-increasing function $K(\beta) > 0$ such that

$$\alpha_c^+(\beta) - \alpha_c(\beta) > K(\beta) > 0. \quad (4.1)$$

The proof will rely on the use of *density functions*. The essentials are reviewed in appendix A.

4.1. The density of visits

Let $t_n^+(\lfloor \epsilon n \rfloor, c)$ be the number of positive attached trees with $\lfloor \epsilon n \rfloor$ visits and c contacts. Then ϵ is the density of visits as a fraction of the number of edges in the tree. Obviously $\epsilon \geq 0$, and $\max\{\epsilon\} = (n+1)/n$, so that we should consider $\epsilon \in [0, 1]$ asymptotically. The partition function of positive attached trees with a density ϵ of visits is

$$Z_n^+(\lfloor \epsilon n \rfloor, \beta) = \sum_c t_n^+(\lfloor \epsilon n \rfloor, c) e^{\beta c} \quad \epsilon \in [0, (n+1)/n]. \quad (4.2)$$

Concatenation of these trees as in the proof of theorem 2.1 gives

$$Z_n^+(\lfloor \epsilon n \rfloor, \beta) Z_m^+(\lfloor \epsilon m \rfloor, \beta) \leq \left[\sum_{j=0}^{2(d-1)} e^{-\beta j} \right] \sum_{i=0}^1 Z_{n+m+2}^+(\lfloor \epsilon n \rfloor + \lfloor \epsilon m \rfloor + i, \beta). \tag{4.3}$$

Comparison of equation (4.3) to equation (A.3) and theorem A.1 proves the following lemma:

Lemma 4.1. There exists a density function $\mathcal{P}^+(\epsilon; \beta)$ for every finite value of β , defined by

$$\log \mathcal{P}^+(\epsilon; \beta) = \mathcal{F}^+(\epsilon; \beta) = \lim_{n \rightarrow \infty} \frac{1}{n} \log Z_n^+(\lfloor \epsilon n \rfloor, \beta) \quad \epsilon \in [0, 1].$$

Moreover, $\log \mathcal{P}^+(\epsilon; \beta)$ is concave in ϵ and convex in β for $\beta \in (-\infty, \infty)$.

The concavity in lemma 4.1 follows from theorem A.1, and the convexity is a consequence of the Cauchy–Schwarz inequality:

$$Z_n^+(\lfloor \epsilon n \rfloor, \beta_1) Z_n^+(\lfloor \epsilon n \rfloor, \beta_2) \geq [Z_n^+(\lfloor \epsilon n \rfloor, (\beta_1 + \beta_2)/2)]^2. \tag{4.4}$$

In addition, $\mathcal{P}^+(\epsilon; \beta)$ has a dual character: in the first instance $\mathcal{P}^+(\epsilon; \beta)$ is the density function of visits, and $\mathcal{F}^+(\epsilon; \beta) = \log \mathcal{P}^+(\epsilon; \beta)$ is the free energy of a model of self-interacting positive attached trees at a contact fugacity β , and with a fixed density of visits equal to ϵ . The connection to the free energy of theorem 2.1 is through the Legendre transform in theorem A.2:

$$\begin{aligned} \log \mathcal{P}^+(\epsilon; \beta) &= \inf_{-\infty < \alpha < \infty} \{ \mathcal{F}^+(\alpha, \beta) - \epsilon \alpha \} \\ \mathcal{F}^+(\alpha, \beta) &= \sup_{0 < \epsilon < 1} \{ \log \mathcal{P}^+(\epsilon; \beta) + \epsilon \alpha \}. \end{aligned} \tag{4.5}$$

From theorem 3.1 and equation (3.1) lemma 4.2 follows.

Lemma 4.2.

$$\lim_{\epsilon \searrow 0} \log \mathcal{P}^+(\epsilon; \beta) = \mathcal{F}^+(0, \beta) = \mathcal{F}(\beta).$$

In the adsorption model in this paper there is an important connection between the critical curve $\alpha_c^+(\beta)$ of adsorbing positive attached trees and the density function $\mathcal{P}^+(\epsilon; \beta)$. Notice that for every fixed and finite β , $\log \mathcal{P}^+(\epsilon; \beta)$ is concave for $\epsilon \in [0, 1]$, and so has a right derivative everywhere in $(0, 1)$. We redefine

$$\log \mathcal{P}^+(0; \beta) = \lim_{\epsilon \searrow 0} \log \mathcal{P}^+(\epsilon; \beta) = \sup_{\epsilon} \log \mathcal{P}^+(\epsilon; \beta) = \mathcal{F}(\beta). \tag{4.6}$$

In that case, $\log \mathcal{P}^+(\epsilon; \beta)$ has a right derivative at $\epsilon = 0$ as well. The fact that the supremum of $\log \mathcal{P}^+(\epsilon; \beta)$ is equal to $\log \mathcal{P}^+(0; \beta)$ follows from $t_n^+(v) \leq t_n^+(0)$.

Lemma 4.3. The critical curve of adsorbing positive attached trees is given by

$$\alpha_c^+(\beta) = - \left[\frac{d^+}{d\epsilon} \log \mathcal{P}^+(\epsilon; \beta) \right]_{\epsilon=0}$$

where $\frac{d^+}{d\epsilon}$ is the right-derivative, and where we evaluate the right-derivative at $\epsilon = 0$. Since $\alpha_c^+(\beta)$ is finite for every finite β , $\log \mathcal{P}^+(\epsilon; \beta)$ has a finite right derivative to ϵ at $\epsilon = 0$.

Proof. Redefine $\log \mathcal{P}^+(0; \beta)$ as in equation (4.6), then $\log \mathcal{P}^+(\epsilon; \beta)$ has a right derivative at $\epsilon = 0$. Let $Q(\epsilon) = \log \mathcal{P}^+(\epsilon; \beta) + \epsilon \alpha$. By equation (4.5), $\mathcal{F}^+(\alpha, \beta) = \sup_{0 < \epsilon < 1} Q(\epsilon)$. Moreover, $Q(\epsilon)$ is concave, and its right derivative at $\epsilon = 0$ is

$$\left[\frac{d^+}{d\epsilon} Q(\epsilon) \right]_{\epsilon=0} = \left[\frac{d^+}{d\epsilon} \log \mathcal{P}^+(\epsilon; \beta) \right]_{\epsilon=0} + \alpha.$$

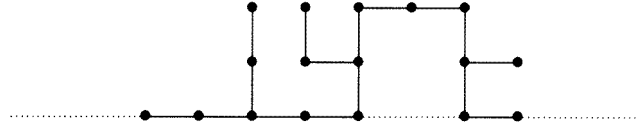


Figure 3. This attached tree has seven visits to which we may add an edge in the negative z -direction to find an attached tree. If we add edges only on non-adjacent visits, then no new contacts are created.

If $\alpha < -[\frac{d^+}{d\epsilon} \log \mathcal{P}^+(\epsilon; \beta)]_{\epsilon=0}$, then $Q(\epsilon)$ is strictly decreasing, and its supremum is achieved at $\epsilon = 0$, so that $\mathcal{F}^+(\alpha, \beta) = \log \mathcal{P}^+(0; \beta) = \mathcal{F}(\beta)$ by lemma 4.2. On the other hand, if $\alpha > -[\frac{d^+}{d\epsilon} \log \mathcal{P}^+(\epsilon; \beta)]_{\epsilon=0}$, then $Q(\epsilon)$ is strictly increasing in an interval $[0, \epsilon_c]$ for some $\epsilon_c > 0$, and $Q(\epsilon)$ has a global maximum at some $\epsilon_1 > 0$. Then equation (4.5) indicates that $\mathcal{F}^+(\alpha, \beta) = \log \mathcal{P}^+(\epsilon_1, \beta) + \epsilon_1 \alpha > \log \mathcal{P}^+(0, \beta) = \mathcal{F}(\beta)$. In other words, there is a non-analyticity in $\mathcal{F}^+(\alpha, \beta)$ at $\alpha = -[\frac{d^+}{d\epsilon} \log \mathcal{P}^+(\epsilon; \beta)]_{\epsilon=0}$. \square

We can use similar arguments to those in lemma 4.3 to show that the result for adsorbing attached trees is analogous.

Lemma 4.4. The critical curve of adsorbing attached trees is given by

$$\alpha_c(\beta) = - \left[\frac{d^+}{d\epsilon} \log \mathcal{P}(\epsilon; \beta) \right]_{\epsilon=0}.$$

Since $\alpha_c(\beta)$ is finite for every finite β , $\mathcal{P}(\epsilon; \beta)$ has a finite right derivative to ϵ at $\epsilon = 0$.

In addition to lemma 4.3 and 4.4, we can use equation (3.3), lemma 4.2 and the definition of the derivative to show the following.

Theorem 4.5. For every finite value of β ,

$$\alpha_c^+(\beta) - \alpha_c(\beta) = e^{-\mathcal{F}(\beta)} \lim_{\epsilon \searrow 0} \frac{1}{\epsilon} (\mathcal{P}(\epsilon, \beta) - \mathcal{P}^+(\epsilon, \beta)).$$

We can compare the critical curves in these models if more could be shown about the density functions. This is the next step in the proof that $\alpha_c^+(\beta) > 0$. We will find a lower bound of the right-hand side in theorem 4.5.

4.2. A relation between $\mathcal{P}(\epsilon, \beta)$ and $\mathcal{P}^+(\epsilon, \beta)$

Consider a tree counted by $t_n^+(\lfloor \epsilon n \rfloor, c)$ (see figure 3). These are all positive attached trees, and we can change them into attached trees by adding new edges in the negative z -direction on the visits. However, we cannot add edges on adjacent visits: this will increase the number of contacts, and complicate the discussion. Instead, we will choose from those visits whose coordinates add to either an odd number, or to an even number (whichever is more), in each tree. This means that we will have at least $\lfloor \epsilon n / 2 \rfloor$ visits to choose from. If we choose $\lfloor \delta n \rfloor$ visits from $\lfloor \epsilon n / 2 \rfloor$ visits, then

$$\binom{\lfloor \epsilon n / 2 \rfloor}{\lfloor \delta n \rfloor} t_n^+(\lfloor \epsilon n \rfloor, c) \leq t_{n+\lfloor \delta n \rfloor}(\lfloor \epsilon n \rfloor, c). \quad (4.7)$$

Multiply this by $e^{\beta c}$, sum over c , take the $1/n$ th power, and let $n \rightarrow \infty$:

$$\left[\frac{(\epsilon/2)^{\epsilon/2}}{\delta^\delta (\epsilon/2 - \delta)^{\epsilon/2 - \delta}} \right] \mathcal{P}^+(\epsilon; \beta) \leq \left[\mathcal{P}\left(\frac{\epsilon}{1+\delta}; \beta\right) \right]^{1+\delta}. \quad (4.8)$$

Notice that the free energy of collapsing trees is given by

$$\mathcal{F}(\beta) = \sup_{\epsilon} \log \mathcal{P}(\epsilon; \beta) \geq \log \mathcal{P}(\epsilon; \beta). \tag{4.9}$$

We may therefore write (4.8) as

$$\left[\frac{(\epsilon/2)^{\epsilon/2} e^{-\delta \mathcal{F}(\beta)}}{\delta^{\delta} (\epsilon/2 - \delta)^{\epsilon/2 - \delta}} \right] \mathcal{P}^+(\epsilon; \beta) \leq \mathcal{P}\left(\frac{\epsilon}{1 + \delta}; \beta\right). \tag{4.10}$$

The factor in square brackets is a maximum if

$$\delta = \frac{\epsilon/2}{1 + e^{\mathcal{F}(\beta)}} \tag{4.11}$$

in which case (4.10) becomes

$$(1 + e^{-\mathcal{F}(\beta)})^{\epsilon/2} \mathcal{P}^+(\epsilon; \beta) \leq \mathcal{P}\left(\frac{\epsilon}{1 + \delta}; \beta\right). \tag{4.12}$$

Thus, we obtain the following lemma.

Lemma 4.6. The density function of visits in self-interacting positive attached trees, and in self-interacting attached trees, are related by

$$(1 + e^{-\mathcal{F}(\beta)})^{\epsilon/2} \mathcal{P}^+(\epsilon; \beta) \leq \mathcal{P}\left(\frac{\epsilon}{1 + \delta}; \beta\right)$$

where $\mathcal{F}(\beta)$ is the free energy of trees with a contact fugacity.

The result in lemma 4.6 can now be used to show that positive trees adsorb at a strictly positive value of the visit-fugacity.

Theorem 4.7. For every finite value of β ,

$$\alpha_c^+(\beta) - \alpha_c(\beta) \geq \frac{1}{2} \log(1 + e^{-\mathcal{F}(\beta)}) > 0.$$

Proof. From theorem 4.5 and lemma 4.6 we note that

$$\alpha_c^+(\beta) - \alpha_c(\beta) \geq e^{-\mathcal{F}(\beta)} \mathcal{P}(0, \beta) \lim_{\epsilon \searrow 0} \frac{1}{\epsilon} \left(1 - \frac{\mathcal{P}(\frac{\epsilon}{1+\delta}; \beta)}{\mathcal{P}(\epsilon; \beta)} (1 + e^{-\mathcal{F}(\beta)})^{-\epsilon/2} \right) \tag{A}$$

where we used lemma 4.2, and where δ is given by equation (4.11). If $\epsilon > 0$ is given, then we can find an $\eta > 0$ such that (if $\mathcal{P}'(0; \beta) < 0$)

$$\mathcal{P}(0; \beta) + \epsilon(1 + \eta)\mathcal{P}'(0; \beta) \leq \mathcal{P}(\epsilon; \beta) \leq \mathcal{P}(0; \beta) + \epsilon(1 - \eta)\mathcal{P}'(0; \beta)$$

where we can take $\eta \rightarrow 0$ of $\epsilon = 0$, and where $\mathcal{P}'(0; \beta)$ is the right derivative of $\mathcal{P}(\epsilon; \beta)$ at $\epsilon = 0$. These bounds can now be used to show that there exists a finite number η_2 (possibly dependent on β), such that

$$\frac{\mathcal{P}(\frac{\epsilon}{1+\delta}; \beta)}{\mathcal{P}(\epsilon; \beta)} \leq 1 - \epsilon \left(2\eta + \frac{\delta}{1 + \delta} \right) \frac{\mathcal{P}'(0; \beta)}{\mathcal{P}(0; \beta)} + \eta_2 \epsilon^2.$$

Notice that $\mathcal{P}'(0; \beta) \leq 0$, and that $\delta \leq \epsilon/2$ in equation (4.11). Thus,

$$\frac{\mathcal{P}(\frac{\epsilon}{1+\delta}; \beta)}{\mathcal{P}(\epsilon; \beta)} \leq 1 - 2\epsilon\eta \frac{\mathcal{P}'(0; \beta)}{\mathcal{P}(0; \beta)} + \left(\eta_2 - \frac{\mathcal{P}'(0; \beta)}{2\mathcal{P}(0; \beta)} \right) \epsilon^2.$$

Substitute this last bound in equation (A), simplify and take the limit. This gives

$$\alpha_c^+(\beta) - \alpha_c(\beta) \geq \frac{1}{2} \log(1 + e^{-\mathcal{F}(\beta)}) + 2\eta \frac{\mathcal{P}'(0; \beta)}{\mathcal{P}(0; \beta)}.$$

We can now safely take $\eta \searrow 0$ to finish the proof. If $\mathcal{P}'(0; \beta) = 0$ then we use $\mathcal{P}(\epsilon; \beta) = \mathcal{P}(0; \beta) + O(\epsilon^2)$ instead. \square

Choose $K(\beta) = \frac{1}{2} \log(1 + e^{-\mathcal{F}(\beta)})$ to find equation (4.1).

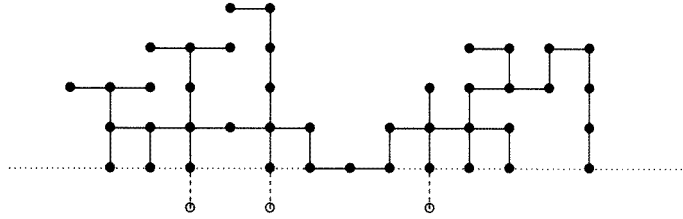


Figure 4. A positive tree with 11 visits, 10 roots and two excursions. By appending the broken edges, and translating the entire tree one step in the z -direction, we obtain a tree with three visits and three roots.

4.3. Roots

Those maximal subtrees with every edge (but not every vertex) in the half-space $z > 0$ are called *excursions*. A maximal subtree which is completely contained in the wall $z = 0$ is an *incursion*. The edges of an excursion which are incident with visits are called *roots*. In this section we will see that there is a density of roots in a tree, if there is a density of visits.

Let $t_n^+(v, c, r)$ be the number of positive trees with v visits, c contacts and r roots. Then $v \geq r$ and r of the v visits are incident with a root. Since we are interested in trees with a density of visits and of roots, we define the density function

$$\mathcal{P}^+(\epsilon; \beta; \rho) = \limsup_{n \rightarrow \infty} [Z_n^+(\lfloor \epsilon n \rfloor; \beta; \lfloor \rho n \rfloor)]^{1/n} \tag{4.13}$$

where

$$Z_n^+(\lfloor \epsilon n \rfloor; \beta; \lfloor \rho n \rfloor) = \sum_{c \geq 0} t_n^+(\lfloor \epsilon n \rfloor, c, \lfloor \rho n \rfloor) e^{\beta c} \tag{4.14}$$

is the partition function of a model of interacting trees with $\lfloor \epsilon n \rfloor$ visits and $\lfloor \rho n \rfloor$ roots, and where the density function is only defined as a lim sup (concatenation of attached trees will show that $\mathcal{P}^+(\epsilon; \beta; \rho)$ exists as a limit, but that is not essential in the arguments below). We illustrate a tree counted by $t_n^+(v, c, r)$ in figure 4. Choose m of the visits and append m edges in the z -direction; after translating the tree one step in the z -direction, these edges will be roots. Thus

$$\binom{v}{m} t_n^+(v, c, r) \leq \sum_{i=0}^{2(d-1)m} t_{n+m}^+(m, c+i, m) \tag{4.15}$$

since each of the m new vertices may have as many as $2(d-1)$ contacts. Multiply equation (4.15) by $e^{\beta c}$ and sum over c ; this gives a relation between the partition functions:

$$\binom{v}{m} Z_n^+(v; \beta; r) \leq \left[\sum_{i=0}^{2(d-1)m} e^{-\beta i} \right] Z_{n+m}^+(m; \beta; m). \tag{4.16}$$

Let $v = \lfloor \epsilon n \rfloor$, $r = \lfloor \rho n \rfloor$ and $m = \lfloor \delta n \rfloor$, where $\epsilon \geq \rho$ and $\epsilon \geq \delta$. Take the $1/n$ power of the resulting equation, and let $n \rightarrow \infty$. This gives

$$\frac{\epsilon^\epsilon}{\delta^\delta (\epsilon - \delta)^{\epsilon - \delta}} \mathcal{P}^+(\epsilon; \beta; \rho) \leq \phi(\beta)^\delta \left[\mathcal{P}^+\left(\frac{\delta}{1 + \delta}; \beta; \frac{\delta}{1 + \delta}\right) \right]^{1 + \delta} \tag{4.17}$$

and since $\mathcal{P}^+(\epsilon; \beta; \delta) \leq e^{\mathcal{F}(\beta)}$ we finally obtain

$$\frac{\epsilon^\epsilon}{\delta^\delta (\epsilon - \delta)^{\epsilon - \delta}} \mathcal{P}^+(\epsilon; \beta; \rho) \leq \phi(\beta)^\delta e^{\delta \mathcal{F}(\beta)} \mathcal{P}^+\left(\frac{\delta}{1 + \delta}; \beta; \frac{\delta}{1 + \delta}\right) \tag{4.18}$$

where $\phi(z) = \max\{1, e^{-2d\beta}\}$, and having used equation (4.6).

Theorem 4.8. For every $\epsilon > 0$ in $(0, 1]$ and $\rho \in [0, \epsilon]$

$$(1 + \phi(\beta)^{-1} e^{-\mathcal{F}(\beta)})^\epsilon \mathcal{P}^+(\epsilon; \beta; \rho) \leq \mathcal{P}^+(\delta_*; \beta; \delta_*)$$

where

$$\delta_* = \frac{\delta}{1 + \delta} \quad \text{and} \quad \delta = \frac{\epsilon}{1 + \phi(\beta) e^{\mathcal{F}(\beta)}} < \epsilon.$$

Proof. Write equations (4.17) and (4.18) in the following form:

$$\frac{\epsilon^\epsilon \phi(\beta)^{-\delta} e^{-\delta \mathcal{F}(\beta)}}{\delta^\delta (\epsilon - \delta)^{\epsilon - \delta}} \mathcal{P}^+(\epsilon; \beta; \rho) \leq \mathcal{P}^+\left(\frac{\delta}{1 + \delta}; \beta; \frac{\delta}{1 + \delta}\right).$$

The maximum of the left-hand side of this inequality is obtained when $\delta = \epsilon / (1 + \phi(\beta) e^{\mathcal{F}(\beta)})$. \square

An immediate consequence of theorem 4.8 is that $\alpha_c(\beta) > 0$, for all finite β . To see this, suppose that $\alpha > \alpha_c(\beta)$, so that there is a density of visits. Then theorem A.2 implies that there is a $\rho_* \geq 0$ and an $\epsilon_* > 0$ such that

$$\mathcal{F}^+(\alpha, \beta) = \log \mathcal{P}^+(\epsilon_*; \beta; \rho_*) + \epsilon_* \alpha \geq \log \mathcal{P}^+(\delta_*; \beta; \delta_*) + \delta_* \alpha \quad (4.19)$$

where δ_* is defined in theorem 4.8. On the other hand, by theorem 4.8,

$$\log(\mathcal{P}^+(\epsilon_*; \beta; \rho_*) e^{\epsilon_* \alpha}) \leq \log\left(\mathcal{P}^+(\delta_*; \beta; \delta_*) e^{\delta_* \alpha} \left[\frac{e^{\alpha(\epsilon_* - \delta_*)}}{\Delta}\right]\right) \quad (4.20)$$

where $\Delta = (1 + \phi(\beta)^{-1} e^{-\mathcal{F}(\beta)})^{\epsilon_*}$. This is a contradiction if $e^{\alpha(\epsilon_* - \delta_*)} < \Delta$. Let $\delta_* = \gamma \epsilon_*$ where $\gamma < 1$, then this implies that the above is a contradiction if

$$\alpha < \frac{1}{1 - \gamma} \log(1 + \phi(\beta)^{-1} e^{-\mathcal{F}(\beta)}) \quad (4.21)$$

unless $\epsilon_* = 0$, in which case we are in the desorbed phase. But then $\alpha_c^+(\beta) \geq \frac{1}{1 - \gamma} \log(1 + \phi(\beta)^{-1} e^{-\mathcal{F}(\beta)}) > 0$. In other words, by examining the density of roots, we obtained a proof that the adsorption occurs at a strictly positive value of α , for all finite β .

4.4. Roots in adsorbed trees

In this section we show that there is a density of roots in adsorbed trees if the contact-fugacity is $\beta = 0$. The construction does not work if the contact-fugacity is switched on. This partial result indicates that the adsorbed phase along the $\beta = 0$ axis in the phase diagram is dominated by adsorbed trees with a density of roots and visits (incidentally, this construction will also show that there is a density of excursions, since each newly constructed root will also be an excursion). The construction is illustrated in figure 5. In the first step of the construction we subdivide every root. Once this step is completed, we can safely add roots to visits which do not already have a root, without creating cycles in the trees. Since $\beta = 0$, any contacts lost or made are irrelevant; we just sum over those.

In an adsorbed tree with v visits and r roots, we can choose $m \leq v - r$ visits for the construction of new roots. The new tree will have v visits, $m + r$ roots and $n + m$ edges; we sum over all contacts, so the number of those are irrelevant. This gives a relation between the partition functions

$$\binom{v - r}{m} Z_n^+(v; 0; r) \leq Z_{n+m}^+(v; 0; m + r). \quad (4.22)$$

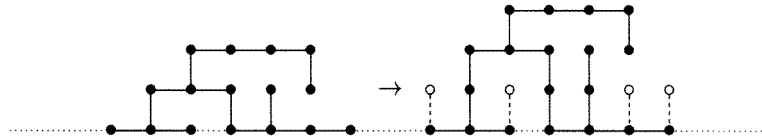


Figure 5. Construction new roots in an absorbed tree. The construction has two steps: first subdivide the roots; this creates room for the construction of roots on visits which are not incident with a root yet. Second, choose some visits from the set of visits not incident with a root, and construct new roots on those.

If we choose $v = \lfloor \epsilon n \rfloor$, $r = \lfloor \rho n \rfloor$, and $m = \lfloor \eta n \rfloor$, and use the fact that $\mathcal{F}^+(0) = \log \lambda_d$, then after taking the $1/n$ th power of equation (4.22), and taking $n \rightarrow \infty$, one obtains

$$\left[\frac{(\epsilon - \rho)^{\epsilon - \rho} \lambda_d^{-\eta}}{\eta^\eta (\epsilon - \rho - \eta)^{\epsilon - \rho - \eta}} \right] \mathcal{P}^+(\epsilon; 0; \rho) \leq \mathcal{P}^+\left(\frac{\epsilon}{1 + \eta}; 0; \frac{\rho + \eta}{1 + \eta}\right). \quad (4.23)$$

The factor in square brackets is a maximum if $\eta = (\epsilon - \rho)/(1 + \lambda_d)$, in which case

$$\frac{(1 + \lambda_d^{-1})^\epsilon}{(1 + \lambda_d^{-1})^\rho} \mathcal{P}^+(\epsilon; 0; \rho) \leq \mathcal{P}^+\left(\frac{\epsilon}{1 + \eta}; 0; \frac{\eta + \rho}{1 + \eta}\right). \quad (4.24)$$

This gives the following theorem if we choose $\rho = 0$.

Theorem 4.9.

$$(1 + \lambda_d^{-1})^\epsilon \mathcal{P}^+(\epsilon; 0; 0) \leq \mathcal{P}^+\left(\frac{\epsilon}{1 + \eta}; 0; \frac{\eta}{1 + \eta}\right)$$

where $\eta = \epsilon/(1 + \lambda_d)$.

We cannot yet fruitfully use theorem 4.9, the main problem is that the density of visits changes, which makes explicit calculation difficult. Instead, we first show that the density of visits can be increased in a density function without giving up too much:

Lemma 4.10.

$$\mathcal{P}^+(\epsilon; 0; \rho) \leq \left[\mathcal{P}^+\left(\frac{\epsilon + \delta}{1 + \delta}; 0; \frac{\rho}{1 + \delta}\right) \right]^{1 + \delta}.$$

Proof. Let $t_n^+(v, r)$ be the number of positive trees with v visits and r roots. Let τ be the lexicographic most visit in a tree, and add q edges in the first direction in the $z = 0$ hyperplane to τ one by one. This generates a tree with $v + q$ visits and $n + q$ edges, while there are still r roots. Let $v = \lfloor \epsilon n \rfloor$, $r = \lfloor \rho n \rfloor$ and $q = \lfloor \delta n \rfloor$. Take the $1/n$ power and let $n \rightarrow \infty$. This gives the result above. \square

Combining lemma 4.10 with theorem 4.9 (and using the fact that $\mathcal{P}^+(\epsilon; 0; \rho) \leq \lambda_d$) shows that

$$(1 + \lambda_d^{-1})^\epsilon \mathcal{P}^+(\epsilon; 0; 0) \leq \lambda_d^\delta \mathcal{P}^+\left(\epsilon; 0; \frac{\eta}{(1 + \eta)(1 + \delta)}\right) \quad (4.25)$$

where we have put

$$\delta = \frac{\epsilon \eta}{(1 - \epsilon)(1 + \eta)}. \quad (4.26)$$

But $\eta = \epsilon/(1 + \lambda_d)$ in theorem 4.9, so that

$$\mathcal{P}^+(\epsilon; 0; 0) \leq \frac{\lambda_d^{\frac{\epsilon^2}{(1+\lambda_d)(1-\epsilon)(1+\eta)}}}{(1 + \lambda_d^{-1})^\epsilon} \mathcal{P}^+\left(\epsilon; 0; \frac{\epsilon}{(1 + \lambda_d)(1 + \delta)(1 + \eta)}\right). \quad (4.27)$$

But for ϵ small enough (but not zero!) this implies that $\mathcal{P}^+(\epsilon; 0; 0) < \mathcal{P}^+(\epsilon; 0; \epsilon^\dagger)$ for some $\epsilon^\dagger > 0$. In other words, if the supremum in equation (4.5) is realized at a small value of ϵ , then there is a density of roots in the adsorbed phase. Incidentally, since the roots we construct in figure 5 are also excursions, this implies that there is also a density of excursions. This argument does not work if we include the contact-fugacity; the construction in figure 5 destroys too many contacts, and we cannot prove theorem 4.9.

Lastly, notice that if we multiply both sides of equation (4.27) with $e^{\epsilon\alpha} < (1 + \lambda_d^{-1})^\epsilon$, then by taking ϵ small enough we find that $\mathcal{P}^+(\epsilon; 0; 0)e^{\epsilon\alpha} < \mathcal{P}^+(\epsilon; 0; \epsilon^\dagger) \leq \mathcal{P}^+(0; 0; 0)$. Thus, $\mathcal{F}^+(\alpha, 0) < \mathcal{F}^+(0; 0)$. This is a contradiction, unless $\epsilon = 0$, which means that we are in the desorbed phase. Thus, $\alpha_c^+(0) \geq \log(1 + \lambda_d^{-1})$.

5. Conclusions

In this paper we considered the phase diagram of a model of collapsing and adsorbing trees. In particular, we paid attention to the existence and properties of a critical curve $\alpha_c^+(\beta)$ which corresponds to an adsorption of the tree onto a wall, where β is a contact fugacity. We showed that $\alpha_c^+(\beta) < \infty$, so that there is an adsorption transition for any value of the contact fugacity. Our most important result states that $\alpha_c^+(\beta) > 0$ for all $\beta \in (-\infty, \infty)$, and we conclude that the adsorption occurs at a strictly attractive value of the interaction between the tree and the wall.

We also showed that there is a critical curve $\alpha_c(\beta)$ in the phase diagram of trees interacting with a defect plane. We proved that $\alpha_c(\beta) \geq 0$, and that it is finite for all values of β , which means that the adsorption occurs for any value of the contact fugacity. We proved that $\alpha_c(\beta) < \alpha_c^+(\beta)$; this implies that these trees adsorb onto the defect plane before positive trees adsorb onto the wall. There are indications from other models that $\alpha_c(\beta) = 0$, at least for $\beta = 0$, but a proof of this fact is not known, and is a major outstanding issue.

The phase diagram in figure 2 proved to be similar to the phase diagram of collapsing and adsorbing walks, with four phases (presumably) present in three and higher dimensions (we know that there are at least two). If there is a collapse transition, then the phase boundary separating the expanded-desorbed phase from the collapsed-desorbed phase is a straight line, but it seems that this does not persist into the adsorbed phase. It remains a difficult challenge to show that there is a collapse transition in this model.

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Appendix

In this appendix we examine the relationship between limiting free energies and density functions. Let $T_n(k)$ be the number of trees with n edges and counted with respect to some property which occurs k times in each tree (such as the number of contacts, or the number of

visits, etc). We assume that $T_n(k) > 0$ if $a_n \leq k \leq b_n$, and define $\epsilon_m = \liminf_{n \rightarrow \infty} (a_n/n)$ and $\epsilon_M = \limsup_{n \rightarrow \infty} (b_n/n)$. The partition function of this model is

$$Z_n(\alpha_k) = \sum_{k \geq 0} T_n(k) e^{\alpha k}. \tag{A.1}$$

Suppose that $T_n(k)$ satisfies a supermultiplicative inequality of the following form:

$$\sum_{k_1 \leq k} T_n(k_1) T_m(k - k_1) \leq \sum_{i=-q}^q T_{n+m+p}(k + i) \tag{A.2}$$

for some constants q and p . If we put $k = \lfloor \epsilon n \rfloor + \lfloor \epsilon m \rfloor$ and $k_1 = \lfloor \epsilon n \rfloor$ in equation (A.2), then

$$T_n(\lfloor \epsilon n \rfloor) T_m(\lfloor \epsilon m \rfloor) \leq \sum_{i=-q}^q T_{n+m+p}(\lfloor \epsilon n \rfloor + \lfloor \epsilon m \rfloor + i). \tag{A.3}$$

The following theorem was proven by Tesi *et al* (1997).

Theorem A.1. (Theorem 4.1, Tesi et al (1997)). There exists a function $\mathcal{P}(\epsilon)$, log-concave in $[\epsilon_n, \epsilon_M]$, such that

$$\lim_{n \rightarrow \infty} [T_n(\lfloor \epsilon n \rfloor)]^{1/n} = \mathcal{P}(\epsilon).$$

The function $\mathcal{P}(\epsilon)$ is called a *density function*, and it is the density of the property counted by k in $T_n(k)$ in the $n \rightarrow \infty$ limit.

From equation (A.2) we note that the limiting free energy also exists in this model; in particular, if we multiply equation (A.2) by $e^{\alpha k}$ and sum over k , then

$$Z_{n-p}(\alpha_k) Z_{m-p}(\alpha_k) \leq \left[\sum_{i=-q}^q e^{\alpha k i} \right] Z_{n+m-p}(\alpha_k) \tag{A.4}$$

so that

$$\mathcal{F}(\alpha_k) = \lim_{n \rightarrow \infty} \frac{1}{n} \log Z_n(\alpha_k) \tag{A.5}$$

exists, and is a convex function on $(-\infty, \infty)$. An important relation between the logarithm of the density function and the limiting free energy is that they are Legendre transforms of one another.

Theorem A.2. (Madras et al 1988).

$$\begin{aligned} \mathcal{F}(\alpha_k) &= \sup_{\epsilon_m \leq \epsilon \leq \epsilon_M} \{ \log \mathcal{P}(\epsilon) + \epsilon \alpha_k \} \\ \log \mathcal{P}(\epsilon) &= \inf_{0 < \alpha_k < \infty} \{ \mathcal{F}(\alpha_k) - \epsilon \alpha_k \}. \end{aligned}$$

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