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Localization of a random copolymer at an interface

N Madras¹ and S G Whittington²

¹ Department of Mathematics and Statistics, York University, Toronto, Canada M3J 1P3

² Department of Chemistry, University of Toronto, Toronto, Canada M5S 3H6

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Abstract

We investigate the nature of the phase diagram for a self-avoiding walk model of a random copolymer at an interface between two immiscible solvents, when one monomer prefers to be in one solvent, the other monomer prefers to be in the other solvent, and both types of monomer have an attractive or repulsive interaction with the interface. Our results are all rigorous, and extend previous work of Maritan *et al* (1999) and Martin *et al* (2000).

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1. Introduction

Random copolymers are polymers with two or more types of comonomer where the distribution of comonomers along the polymer chain is determined by some random process but then fixed. They are an example of a system with quenched randomness (Brout 1959). These polymers can be modelled as self-avoiding walks with vertices coloured (say randomly and independently) A or B to represent two types of comonomer.

The problem which we shall examine in this paper is a random copolymer at an interface between two immiscible liquid phases, which we call α and β . It is energetically favourable for one of the two types of monomer (A , say) to be in phase α and for the other (B) to be in phase β . At high temperatures, the polymer delocalizes into the energetically preferred phase since this maximizes its entropy. At low temperatures, the polymer crosses the interface frequently to optimize the numbers of monomers in their preferred phases. The transition between these two types of behaviour is known as the *localization transition*.

There have been several previous treatments of this problem (Sinai and Spohn 1996, Bolthausen and den Hollander 1997, Maritan *et al* 1999, Biskup and den Hollander 1999, Martin *et al* 2000), in which the models considered differ in several ways. The first rigorous treatment of the problem was by Sinai and Spohn (1996). They considered a model with annealed randomness and found it necessary to include an interaction with the interface in order to obtain a localization transition. The remaining references all focussed on quenched randomness. Bolthausen and den Hollander (1997) and Biskup and den Hollander (1999) considered a directed walk model in two dimensions. Maritan *et al* (1999) considered both

random walk and self-avoiding walk models, and Martin *et al* (2000) considered a self-avoiding walk model. In addition, the models differed in the details of the potential functions used. There is general agreement about the existence of a localization transition in the system with quenched randomness but many details of the nature of the phase diagram are still unknown.

The model which we shall consider is a generalization of that introduced by Martin *et al* (2000). We shall work on the d -dimensional hypercubic lattice Z^d and we write a point of Z^d as $x = (x_1, \dots, x_d)$. The hyperplane $x_d = 0$ will play the role of the interface between the α and β phases. An N -step self-avoiding walk (SAW) is a sequence $\omega = (\omega(0), \omega(1), \dots, \omega(N))$ of $N + 1$ distinct points of Z^d such that $\omega(i + 1)$ is a nearest neighbour of $\omega(i)$ for each i . We write $\omega_i(k)$ to denote the i th coordinate of the point $\omega(k)$. Let c_N be the number of N -step SAWs with $\omega(0) = 0$. The limit $\lim_{N \rightarrow \infty} c_N^{1/N}$ is known to exist (see Madras and Slade (1993) for a review), and we call this limit μ_d , or μ where no confusion is likely to arise. A *half-space* SAW is a SAW with $\omega(0) = 0$ and $\omega_d(k) > 0$ for every $k \geq 1$. Thus a half-space SAW represents a polymer that is completely delocalized into the α phase. Let h_N be the number of N -step half-space SAWs. It is known (Whittington 1975) that

$$\lim_{N \rightarrow \infty} h_N^{1/N} = \mu_d. \tag{1.1}$$

The vertices of the walk are independently coloured A with probability p and B with probability $1 - p$. We write χ_i to denote the colour of the i th vertex (A or B). We take the 0th vertex of the walk to be at the origin, so its colour is irrelevant, and we write χ as a shorthand for the sequence of colours $\chi_1, \chi_2, \dots, \chi_N$. Let $c_N(v_A, v_B, w | \chi)$ be the number of N -step SAWs with colouring χ , having v_A A -vertices with $x_d > 0$, v_B B -vertices with $x_d < 0$ and $w + 1$ vertices with $x_d = 0$. We shall use the letter α as a parameter to denote the energy associated with each A monomer that lies in the α phase, and analogously for β . Define the partition function

$$Z_N(\alpha, \beta, \gamma | \chi) = \sum_{v_A, v_B, w} c_N(v_A, v_B, w | \chi) e^{\alpha v_A + \beta v_B + \gamma w} \tag{1.2}$$

and the corresponding free energy

$$\kappa_N(\alpha, \beta, \gamma | \chi) = N^{-1} \log Z_N(\alpha, \beta, \gamma | \chi). \tag{1.3}$$

Note that both A and B vertices have energy of interaction γ with the interfacial plane $x_d = 0$. Part of the interest in introducing the γ term is that such an interaction with the interface was considered by Sinai and Spohn (1996).

The results which are already known (Martin *et al* 2000) for this model are all for the special case $d = 3$ and $\gamma = 0$, though these results can easily be extended to general values of d . (We remark, however, that lemma 2.4 of Martin *et al* (2000) contains an error in the last step, where it essentially assumes that the expected value of the maximum of several random variables equals the maximum of the expected values, which is not generally true. The proof of the lemma can be repaired with some additional work, but fortunately there is an alternate route to the proof of self-averaging of the free energy using the methods of Madras and Whittington (2002) in the manner described below.) Theorem 2.3 of Martin *et al* (2000) says that the limiting quenched average free energy exists, i.e.

$$\bar{\kappa}(\alpha, \beta, 0) = \lim_{N \rightarrow \infty} \langle \kappa_N(\alpha, \beta, 0 | \chi) \rangle \tag{1.4}$$

where the angular brackets denote an average over colourings. The same method of proof works when $\gamma \neq 0$. The system is said to be *thermodynamically self-averaging* if for almost all χ

$$\lim_{N \rightarrow \infty} \kappa_N(\alpha, \beta, \gamma | \chi) = \bar{\kappa}(\alpha, \beta, \gamma). \tag{1.5}$$

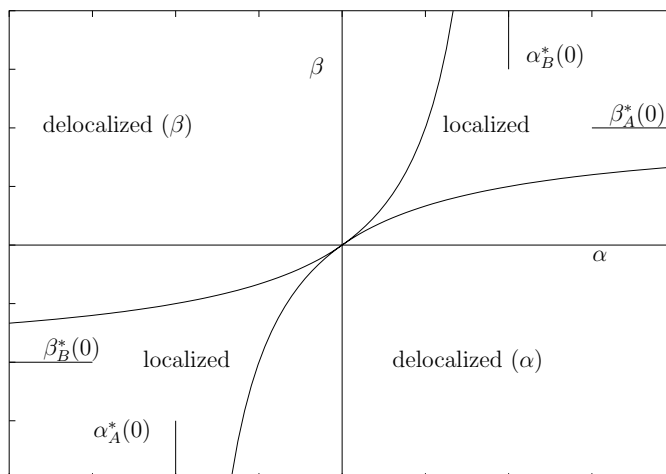


Figure 1. Sketch of phase diagram when $\gamma = 0$. The lines labelled $\alpha_A^*(0)$ and $\beta_A^*(0)$ (respectively, $\alpha_B^*(0)$ and $\beta_B^*(0)$) represent the asymptotes of the phase boundary of the region where the polymer is delocalized into the α (respectively, β) phase. See section 2 for the formal definitions.

The most direct proof of thermodynamic self-averaging uses a recent result about the extent of self-averaging for finite N (Madras and Whittington 2002) coupled with the existence of the limiting quenched average free energy. This is done in theorem 12 in section 3.

The following results were proved by Martin *et al* (2000), who only considered $\gamma = 0$. In the second quadrant ($\alpha \leq 0$ and $\beta \geq 0$), $\bar{\kappa}(\alpha, \beta, 0)$ equals $\log \mu_d + \beta(1 - p)$ (in particular, it is independent of α), and in the fourth quadrant ($\alpha \geq 0$ and $\beta \leq 0$) it equals $\log \mu_d + \alpha p$ (these proofs also hold for negative γ). As we shall discuss at the beginning of the next section, the value $\log \mu_d + \alpha p$ (respectively, $\log \mu_d + \beta(1 - p)$) for the free energy corresponds to the case that the polymer is delocalized into the α (respectively, β) phase. In the first quadrant ($\alpha, \beta \geq 0$) the free energy $\bar{\kappa}(\alpha, \beta, 0)$ is singular along two curves $\beta = f_1(\alpha)$ and $\alpha = f_2(\beta)$ such that $0 \leq f_1(\alpha) \leq \min\{\alpha p / (1 - p), C_1\}$ and $0 \leq f_2(\beta) \leq \min\{\beta(1 - p) / p, C_2\}$, where C_1 and C_2 are constants depending on p . In the third quadrant ($\alpha, \beta \leq 0$), $\bar{\kappa}(\alpha, \beta, 0)$ is singular on the curves $\beta = f_3(\alpha)$ and $\alpha = f_4(\beta)$, where $f_3(\alpha) \geq -(\log(\mu_d / \mu_{d-1})) / (1 - p)$ and $f_4(\beta) \geq -(\log(\mu_d / \mu_{d-1})) / p$. The f_1 and f_4 (respectively, f_2 and f_3) curves are on the boundary of the region where the copolymer is delocalized into the α (respectively, β) phase. The expected form of the phase diagram (in the (α, β) -plane for $\gamma = 0$) is sketched in figure 1.

The paper is organized as follows. Section 2 contains our results about the phase diagram for general (α, β, γ) , including monotonicity and convexity. For $\gamma \leq 0$, we prove several properties of the phase boundaries of figure 1, including the fact that the boundaries pass through the origin but are otherwise separated by the line $\alpha p = \beta(1 - p)$. For sufficiently large positive γ , however, we show that the origin is in the interior of the localized phase; indeed, the system is localized throughout the entire third quadrant for some positive values of γ , and it is localized everywhere when γ is very large. Additional results are presented in section 2. Some of the longer proofs are deferred to section 3. We remark that the system is localized whenever $\alpha p = \beta(1 - p) \neq 0$ (theorem 6) is a fully rigorous version of the proof of Maritan *et al* (1999). Section 4 is a discussion of our results, some extensions, and some open questions.

2. The form of the phase diagram

We begin by determining the free energy $\bar{\kappa}$ associated with the delocalized phase. Consider all N -step half-space self-avoiding walks, i.e. SAWs that are entirely delocalized into the α phase. The contribution to the partition function $Z_N(\alpha, \beta, \gamma|\chi)$ for these SAWs is $h_N e^{\alpha A(\chi)}$, where $A(\chi)$ is the number of A -vertices among the vertices of the walk. The strong law of large numbers tells us that $A(\chi)/N \rightarrow p$ as $N \rightarrow \infty$. With equation (1.1), this shows that

$$\lim_{N \rightarrow \infty} \frac{1}{N} \log(h_N e^{\alpha A(\chi)}) = \log \mu_d + \alpha p. \tag{2.1}$$

If this is the dominant term, then we will have $\bar{\kappa}(\alpha, \beta, \gamma) = \log \mu_d + \alpha p$. Thus, we shall say that the system is delocalized into the α phase if $\bar{\kappa}(\alpha, \beta, \gamma) = \log \mu_d + \alpha p$. Similarly, we say that the system is delocalized into the β phase if $\bar{\kappa}(\alpha, \beta, \gamma) = \log \mu_d + \beta(1 - p)$. These two expressions are always lower bounds for $\bar{\kappa}$. Thus we have the dichotomy that the system is either

$$\text{delocalized if } \bar{\kappa}(\alpha, \beta, \gamma) = \log \mu_d + \max\{\alpha p, \beta(1 - p)\}$$

or

$$\text{localized if } \bar{\kappa}(\alpha, \beta, \gamma) > \log \mu_d + \max\{\alpha p, \beta(1 - p)\}.$$

We define the following three regions of (α, β, γ) space:

$$\begin{aligned} \text{DELOC}_\alpha &= \{(\alpha, \beta, \gamma) : \bar{\kappa}(\alpha, \beta, \gamma) = \log \mu_d + \alpha p\} \\ &= \text{region of delocalization into } \alpha \text{ phase} \\ \text{DELOC}_\beta &= \{(\alpha, \beta, \gamma) : \bar{\kappa}(\alpha, \beta, \gamma) = \log \mu_d + \beta(1 - p)\} \\ &= \text{region of delocalization into } \beta \text{ phase} \\ \text{LOC} &= \{(\alpha, \beta, \gamma) : \bar{\kappa}(\alpha, \beta, \gamma) > \log \mu_d + \max\{\alpha p, \beta(1 - p)\}\} \\ &= \text{region of localization.} \end{aligned}$$

The union of these three regions is everything. Observe that DELOC_α is a subset of the half-space $\{(\alpha, \beta, \gamma) : \alpha p \geq \beta(1 - p)\}$, and DELOC_β is a subset of $\{(\alpha, \beta, \gamma) : \alpha p \leq \beta(1 - p)\}$. DELOC_α and DELOC_β could have common points only on the plane $\alpha p = \beta(1 - p)$.

We shall often consider regions of the (α, β) -plane for a fixed value of γ . For this reason we also define, for each real γ_0 ,

$$\begin{aligned} \text{DELOC}_\alpha(\gamma_0) &= \{(\alpha, \beta) : (\alpha, \beta, \gamma_0) \in \text{DELOC}_\alpha\} \\ \text{DELOC}_\beta(\gamma_0) &= \{(\alpha, \beta) : (\alpha, \beta, \gamma_0) \in \text{DELOC}_\beta\}. \end{aligned}$$

We begin with two straightforward results about the form of the three regions DELOC_α , DELOC_β and LOC .

Theorem 1. (i) If $(\alpha_1, \beta_1, \gamma_1)$ is in DELOC_α (i.e., the system is delocalized into the α phase at $(\alpha_1, \beta_1, \gamma_1)$), and if $\alpha_2 \geq \alpha_1, \beta_2 \leq \beta_1$ and $\gamma_2 \leq \gamma_1$ then $(\alpha_2, \beta_2, \gamma_2)$ is also in DELOC_α . In particular, DELOC_α contains the set of all (α, β, γ) such that $\alpha \geq 0, \beta \leq 0$ and $\gamma \leq 0$. (ii) If $(\alpha_1, \beta_1, \gamma_1)$ is in DELOC_β , and if $\alpha_2 \leq \alpha_1, \beta_2 \geq \beta_1$ and $\gamma_2 \leq \gamma_1$ then $(\alpha_2, \beta_2, \gamma_2)$ is also in DELOC_β . In particular, DELOC_β contains the set of all (α, β, γ) such that $\alpha \leq 0, \beta \geq 0$ and $\gamma \leq 0$.

Proof. We shall only prove (i), since the proof of (ii) is exactly analogous. Suppose that $(\alpha_1, \beta_1, \gamma_1) \in \text{DELOC}_\alpha$, and that $\alpha_2 \geq \alpha_1, \beta_2 \leq \beta_1$ and $\gamma_2 \leq \gamma_1$. Then $\bar{\kappa}(\alpha_1, \beta_1, \gamma_1) = \log \mu_d + \alpha_1 p$. We can write

$$\begin{aligned}
 Z_N(\alpha_2, \beta_2, \gamma_2 | \chi) &= \sum_{v_A, v_B, w} c_N(v_A, v_B, w | \chi) e^{\alpha_2 v_A + \beta_2 v_B + \gamma_2 w} \\
 &\leq \sum_{v_A, v_B, w} c_N(v_A, v_B, w | \chi) e^{(\alpha_2 - \alpha_1) v_A} e^{\alpha_1 v_A + \beta_1 v_B + \gamma_1 w} \\
 &\leq e^{(\alpha_2 - \alpha_1) A(\chi)} Z_n(\alpha_1, \beta_1, \gamma_1 | \chi).
 \end{aligned}
 \tag{2.2}$$

Hence $\bar{\kappa}(\alpha_2, \beta_2, \gamma_2) \leq \log \mu_d + \alpha_2 p$, which implies that the point $(\alpha_2, \beta_2, \gamma_2)$ is also in DELOC_α .

To prove the second statement of (i), it now suffices to show that $(0, 0, 0)$ is in DELOC_α , i.e. $\bar{\kappa}(0, 0, 0) = \log \mu_d$. This follows from the facts that $Z_N(0, 0, 0 | \chi) = c_N$ for every χ , and that $N^{-1} \log c_N$ converges to $\log \mu_d$ as $N \rightarrow \infty$. \square

Theorem 2. *The sets DELOC_α and DELOC_β are closed and convex.*

Proof. We shall only do the proof for DELOC_α , since the same argument works for DELOC_β . Observe that $\bar{\kappa}(\alpha, \beta, \gamma)$ is finite everywhere (i.e. for all finite values of α, β and γ). By standard methods (e.g. lemma 2.1 of Borgs *et al* (2000)), the function $\bar{\kappa}(\alpha, \beta, \gamma)$ is convex, hence continuous. Define

$$q(\alpha, \beta, \gamma) = \bar{\kappa}(\alpha, \beta, \gamma) - (\log \mu_d + \alpha p).$$

Then q is also a convex continuous function. The set of (α, β, γ) for which $q \leq 0$ is exactly DELOC_α . (Since q is never strictly negative, this is the same as the set where q equals 0.) But for any convex function q and any real number r , the set of points x for which $q(x) \leq r$ is a convex set. Hence DELOC_α is convex. Also, since q is continuous, the set of (α, β, γ) for which $q \leq 0$ is a closed set. \square

The *critical surface* of the delocalized region DELOC_α is the boundary of this region. The two previous results show that we can describe this surface by a function $\beta_c(\alpha, \gamma)$, defined by

$$\beta_c(\alpha, \gamma) = \sup\{\beta : (\alpha, \beta, \gamma) \in \text{DELOC}_\alpha\}.$$

This ‘critical value’ function takes on the value $-\infty$ if the set on the right-hand side is empty for some choice of α and γ . (The region DELOC_β can be handled analogously, so we shall usually not discuss it explicitly.) Theorems 1 and 2, together with the fact that DELOC_α is a subset of $\{(\alpha, \beta, \gamma) : \alpha p \geq \beta(1 - p)\}$, immediately imply the following.

Corollary 3. *The function $\beta_c(\alpha, \gamma)$ is nondecreasing in α and nonincreasing in γ . Also, it is a concave function, and hence continuous on the interior of the set of values for which it is finite. Also, $\beta_c(\alpha, \gamma) \leq \alpha p / (1 - p) < +\infty$ for all (α, γ) .*

In addition, we can deduce the following properties.

Corollary 4. *Fix $\gamma_0 \leq 0$. (i) The point $(0, 0, \gamma_0)$ is in DELOC_α and in DELOC_β . In particular, $\beta_c(0, \gamma_0) = 0$. (ii) For every fixed constant c such that $0 > c > -\infty$, the free energy $\bar{\kappa}(\alpha, \beta, \gamma_0)$ along the line $\beta = c\alpha$ is not differentiable at $(0, 0)$.*

Part (i) tells us that when $\gamma_0 \leq 0$ the boundaries of the regions $\text{DELOC}_\alpha(\gamma_0)$ and $\text{DELOC}_\beta(\gamma_0)$ must meet at the origin. We shall see in theorem 6 that for $\gamma_0 \leq 0$, the point $(0, 0)$ is the *only* point that is in both $\text{DELOC}_\alpha(\gamma_0)$ and $\text{DELOC}_\beta(\gamma_0)$. In contrast, for large (positive) γ_0 , theorem 5(v) will imply that $(0, 0, \gamma_0)$ is in LOC , and hence that the regions $\text{DELOC}_\alpha(\gamma_0)$ and $\text{DELOC}_\beta(\gamma_0)$ are disjoint. Part (ii) says that there is a first-order phase transition as we cross from one delocalized phase into the other through the origin.

Note, however, that the origin corresponds to a separate phase, and not to the coexistence of the two phases $\text{DELOC}_\alpha(\gamma_0)$ and $\text{DELOC}_\beta(\gamma_0)$.

Proof of corollary 4.

- (i) The first assertion follows directly from theorem 1. Since $(0, 0, \gamma_0) \in \text{DELOC}_\alpha$, we have $\beta_c(0, \gamma_0) \geq 0$. Also, for $\beta > 0$ we have $\bar{\kappa}(0, \beta, \gamma_0) \geq \log \mu_d + \beta(1 - p) > \log \mu_d$, so $(0, \beta, \gamma_0) \notin \text{DELOC}_\alpha$; hence $\beta_c(0, \gamma_0) \leq 0$. The second assertion now follows.
- (ii) Assume $0 > c > -\infty$. Theorem 1 tells us that

$$\bar{\kappa}(\alpha, c\alpha, \gamma_0) = \begin{cases} \log \mu_d + \alpha p & \text{for } \alpha \geq 0 \\ \log \mu_d + c\alpha(1 - p) & \text{for } \alpha \leq 0. \end{cases}$$

Since $p \neq c(1 - p)$, the function $\alpha \mapsto \bar{\kappa}(\alpha, c\alpha, \gamma_0)$ is not differentiable at 0. This proves (ii). □

Martin *et al* (2000) prove results about various horizontal and vertical asymptotes of the phase boundaries in the case $\gamma = 0$. To discuss these, we make the following definitions for each finite γ :

$$\begin{aligned} \beta_A^*(\gamma) &= \sup\{\beta : (\alpha, \beta) \in \text{DELOC}_\alpha(\gamma) \text{ for some finite } \alpha\} \\ \beta_B^*(\gamma) &= \inf\{\beta : (\alpha, \beta) \in \text{DELOC}_\beta(\gamma) \text{ for some finite } \alpha\} \\ \alpha_A^*(\gamma) &= \inf\{\alpha : (\alpha, \beta) \in \text{DELOC}_\alpha(\gamma) \text{ for some finite } \beta\} \\ \alpha_B^*(\gamma) &= \sup\{\alpha : (\alpha, \beta) \in \text{DELOC}_\beta(\gamma) \text{ for some finite } \beta\}. \end{aligned}$$

See figure 1. In particular, observe that $\beta_A^*(\gamma) = \lim_{\alpha \rightarrow \infty} \beta_c(\alpha, \gamma)$ by the monotonicity of β_c (corollary 3). In this sense, we regard the line $\beta = \beta_A^*(\gamma)$ as a horizontal asymptote for the curve $\alpha \mapsto \beta_c(\alpha, \gamma)$. Also observe that $\alpha_A^*(\gamma) = \inf\{\alpha : \beta_c(\alpha, \gamma) > -\infty\}$; we regard the line $\alpha = \alpha_A^*(\gamma)$ as a vertical asymptote of $\alpha \mapsto \beta_c(\alpha, \gamma)$. We shall see below that these four asymptote values are finite for every γ , unless the associated delocalized region is empty (see theorems 5(iv), 10 and 11).

We also define a critical value for the interfacial energy separating the localized region from the delocalized region(s):

$$\gamma_c(\alpha, \beta) = \inf\{\gamma : (\alpha, \beta, \gamma) \in \text{LOC}\}.$$

Theorems 1 and 2 imply that for a given α and β , the system is localized at (α, β, γ) if and only if $\gamma > \gamma_c(\alpha, \beta)$. The next theorem shows, among other things, that for any α and β the system can always be localized by making γ large enough. We shall also see that there is an upper bound for $\gamma_c(\alpha, \beta)$ that is uniform in α and β (theorem 11); when γ is above this value, everything is localized. In contrast, it is interesting to note that for fixed α and β the system cannot always be delocalized by making γ very negative (see corollary 7).

Theorem 5.

- (i) If $(\alpha, \beta, \gamma) \in \text{DELOC}_\alpha$ then $\gamma \leq \log(\mu_d/\mu_{d-1}) + \alpha p$.
- (ii) If $(\alpha, \beta, \gamma) \in \text{DELOC}_\beta$ then $\gamma \leq \log(\mu_d/\mu_{d-1}) + \beta(1 - p)$.
- (iii) For every finite α and β , we have

$$\gamma_c(\alpha, \beta) \leq \log(\mu_d/\mu_{d-1}) + \max\{\alpha p, \beta(1 - p)\} < +\infty.$$

- (iv) $\alpha_A^*(\gamma) \geq (\gamma - \log(\mu_d/\mu_{d-1}))/p$ and $\beta_B^*(\gamma) \geq (\gamma - \log(\mu_d/\mu_{d-1}))/(1 - p)$.
- (v) If $\gamma > \log(\mu_d/\mu_{d-1})$ then (α, β, γ) is in LOC for every nonpositive α and β .

Proof. We can obtain a lower bound on the quenched average free energy by considering the contribution to the partition function of those walks which lie entirely in the hyperplane $x_d = 0$. This gives

$$Z_N(\alpha, \beta, \gamma | \chi) \geq c_N(0, 0, N | \chi) e^{\gamma N} \tag{2.3}$$

so that

$$\bar{\kappa}(\alpha, \beta, \gamma) \geq \log \mu_{d-1} + \gamma. \tag{2.4}$$

If $(\alpha, \beta, \gamma) \in \text{DELOC}_\alpha$ then $\bar{\kappa}(\alpha, \beta, \gamma) = \log \mu_d + \alpha p$, so part (i) follows from equation (2.4). Part (ii) is similar. For part (iii), observe that if $\gamma > \log(\mu_d/\mu_{d-1}) + \max\{\alpha p, \beta(1-p)\}$ then (α, β, γ) cannot be in $\text{DELOC}_\alpha \cup \text{DELOC}_\beta$ (by parts (i) and (ii)), which implies that (α, β, γ) is in LOC. This proves (iii). The first inequality of part (iv) follows from the observation that if $(\alpha, \beta, \gamma) \in \text{DELOC}_\alpha$ then $\alpha \geq (\gamma - \log(\mu_d/\mu_{d-1}))/p$ (by part (i)). The second inequality of (iv) follows similarly from (ii). Finally, part (v) is a direct consequence of (iv). \square

For $\alpha = \beta = 0$, part (iii) of the preceding theorem can be improved by making use of results of Hammersley *et al* (1982). Their results imply that

$$0 \leq \gamma_c(0, 0) \leq 2 \log \mu_d - \log \mu_{d-1} - \sinh^{-1} \cosh \log \mu_d \tag{2.5}$$

so $(0, 0, \gamma)$ is in the localized phase if $\gamma > 2 \log \mu_d - \log \mu_{d-1} - \sinh^{-1} \cosh \log \mu_d$. Moreover, the system at $(0, 0, \gamma)$ is delocalized if $\gamma < 0$. It is conjectured that $\gamma_c(0, 0) = 0$ (see De'Bell and Lookman (1993)).

In the following results, we shall be interested in behaviour in the (α, β) -plane at fixed γ . We first consider the behaviour along the line $\beta = \alpha p/(1-p)$, and prove a rigorous version of a result first given (for a somewhat different model) by Maritan *et al* (1999).

Theorem 6. *For any fixed value of γ the system is localized at every point on the line $\beta = \alpha p/(1-p)$, except possibly at $\alpha = \beta = 0$.*

Corollary 7. *For every nonzero α we have $\gamma_c(\alpha, \alpha p/(1-p)) = -\infty$.*

Since the proof of theorem 6 is quite long we postpone it to the next section.

The next theorem uses an idea due to Maritan *et al* (1999) to bound the phase boundary in the first quadrant away from the axis.

Theorem 8. *If α and γ satisfy*

$$p e^{\gamma - \alpha} + (1-p) e^\gamma \leq 1 \tag{2.6}$$

or equivalently

$$\alpha \geq \log \left(\frac{p e^\gamma}{1 - (1-p) e^\gamma} \right) \tag{2.7}$$

then

$$\beta_c(\alpha, \gamma) \geq \log \left(\frac{1 - p e^{-\alpha}}{1-p} \right). \tag{2.8}$$

The proof of this result appears in the next section. We shall now deduce some useful consequences of this theorem.

Corollary 9. *(i) For every $\gamma \leq 0$ and every $\alpha > 0$, we have*

$$\beta_c(\alpha, \gamma) \geq \log \left(\frac{1 - p e^{-\alpha}}{1-p} \right) > 0. \tag{2.9}$$

(ii) For every $\gamma < -\log(1 - p)$ (note that $-\log(1 - p) > 0$), we have

$$\beta_A^*(\gamma) \geq -\log(1 - p) \quad \text{and} \quad \alpha_A^*(\gamma) \leq \log\left(\frac{p e^\gamma}{1 - (1 - p) e^\gamma}\right).$$

(iii) Fix $\gamma = \gamma_0 < 0$. In the (α, β) -plane, consider the curve $\alpha \mapsto \beta_c(\alpha, \gamma_0)$. This curve is differentiable at $\alpha = 0$, and its tangent line at that point is the line $\alpha p = \beta(1 - p)$.

Proof. (i) This follows directly from theorem 8. (ii) Observe that the condition $\gamma < -\log(1 - p)$ implies $(1 - p) e^\gamma < 1$, which says that inequality (2.6) holds for sufficiently large α . For the first bound, let $\alpha \rightarrow +\infty$ in theorem 8. To prove the second bound, assume $\alpha_0 > \log[p e^\gamma / (1 - (1 - p) e^\gamma)]$. By theorem 8, we know that $\beta_c(\alpha_0, \gamma) > -\infty$. Hence $\alpha_A^*(\gamma) \leq \alpha_0$. (iii) Let $\alpha_* = \log[p e^{\gamma_0} / (1 - (1 - p) e^{\gamma_0})]$. Since $\gamma_0 < 0$, we have $\alpha_* < 0$. Define the functions

$$h_1(\alpha) = \log\left(\frac{1 - p e^{-\alpha}}{1 - p}\right) \quad \text{and} \quad h_2(\alpha) = \left(\frac{p}{1 - p}\right)\alpha.$$

Theorems 8 and 6 imply that

$$h_1(\alpha) \leq \beta_c(\alpha, \gamma_0) \leq h_2(\alpha) \quad \text{for all} \quad \alpha \geq \alpha_*.$$

Since $h_1(0) = 0 = h_2(0)$ and $h_1'(0) = p/(1 - p) = h_2'(0)$, and since $\alpha_* < 0$, it follows that $\partial\beta_c(\alpha, \gamma_0)/\partial\alpha$ must exist and equal $p/(1 - p)$ at $\alpha = 0$. This proves (ii). \square

Our next result, theorem 10, shows that the phase boundary $\beta_c(\alpha, \gamma)$ has a horizontal asymptote in the first quadrant of the (α, β) -plane (provided that $\text{DELOC}_\alpha(\gamma)$ is nonempty). This is a straightforward generalization of theorem 3.3 of Martin *et al* (2000), using the same method of proof, so we do not present it here. Theorem 11 which follows it says that $\text{DELOC}_\alpha(\gamma)$ and $\text{DELOC}_\beta(\gamma)$ can be empty when γ is sufficiently large. That is, when the interfacial energy is sufficiently favourable, then even huge values of α and β cannot delocalize the copolymer. Theorem 11 will be proved at the end of section 3.

Theorem 10. For every finite γ , there exists a finite value $U(\gamma)$ such that $\beta_c(\alpha, \gamma) \leq U(\gamma)$ for every $\alpha > 0$. In particular, $\beta_A^*(\gamma)$ never equals $+\infty$ (and similarly, neither does $\alpha_B^*(\gamma)$).

Theorem 11. There is a finite value γ_L such that for every $\gamma > \gamma_L$, the region $\text{DELOC}_\alpha(\gamma) \cup \text{DELOC}_\beta(\gamma)$ is empty. Thus $\gamma_c(\alpha, \beta) \leq \gamma_L$ for every α and β . Moreover, $\gamma_L \leq \max\{p^{-2}, (1 - p)^{-2}\} \log \mu_d$.

3. Proofs of theorems

This section is devoted to the proofs of thermodynamic self-averaging (theorem 12 below), as well as theorems 6, 8 and 11 from the preceding section. In this section, we shall write μ for μ_d to improve readability of some large formulae.

We begin with the statement and proof of the self-averaging result.

Theorem 12. For every finite α, β and γ , and for almost all χ , we have

$$\lim_{N \rightarrow \infty} \kappa_N(\alpha, \beta, \gamma | \chi) = \bar{\kappa}(\alpha, \beta, \gamma).$$

Proof. As described in the introduction, we know that

$$\lim_{N \rightarrow \infty} \langle \kappa_N(\alpha, \beta, \gamma | \chi) \rangle = \bar{\kappa}(\alpha, \beta, \gamma). \tag{3.10}$$

We now follow the method of Madras and Whittington (2002). Let χ' and χ'' be two particular colourings that differ only in the colour of a single vertex. Then

$$|\kappa_N(\alpha, \beta, \gamma|\chi') - \kappa_N(\alpha, \beta, \gamma|\chi'')| \leq \frac{\max\{|\alpha|, |\beta|\}}{N}.$$

This is the analogue of equation (15) in Madras and Whittington (2002). Using the methods of that paper, we obtain

$$\limsup_{N \rightarrow \infty} \sqrt{\frac{N}{\log N}} |\kappa_N(\alpha, \beta, \gamma|\chi) - \langle \kappa_N(\alpha, \beta, \gamma|\chi) \rangle| \leq \sqrt{2} \max\{|\alpha|, |\beta|\} \tag{3.11}$$

with probability 1, which is the analogue of equation (19) in that paper. Combining this with our equation (3.10) proves our theorem. \square

We now proceed to the proof of theorem 6. The basic structure of the proof appears in Maritan *et al* (1999). However, that paper uses a scaling assumption which, as the authors acknowledge, cannot be proved rigorously. One of the main contributions of our paper is to fill this gap. To explain the situation, we need the following definition.

Definition 13. An N -step bridge is an N -step SAW ω such that $\omega_1(0) < \omega_1(i) \leq \omega_1(N)$ for every $i = 1, \dots, N$. Let b_N denote the number of N -step bridges with $\omega(0) = 0$.

An N -step positive excursion is an N -step bridge ω such that $\omega_d(0) = 0 = \omega_d(1) = \omega_d(N)$ and $\omega_d(i) > 0$ for $i = 2, \dots, N - 1$. A negative excursion is a positive excursion that has been reflected through the $x_d = 0$ plane (i.e. it has $\omega_d(i) < 0$ for $i = 2, \dots, N - 1$). Let L_N denote the number of N -step positive excursions with $\omega(0) = 0$.

The assumption of Maritan *et al* (1999) is that $L_n \sim Cn^t \mu^n$ for some constants C and t . In fact, their proof only uses the assumption that $L_n \geq Cn^t \mu^n$ for all sufficiently large n . Although this assumption is probably correct, rigorous mathematics usually cannot prove lower bounds better than $\mu^n \exp[-Cn^{1/2}]$. This is not quite good enough for the method of Maritan *et al* (1999) to work. Fortunately, we can rigorously prove a slightly better bound for infinitely many values of n , rather than for all sufficiently large n , and it turns out that this is good enough. The bound is the following lemma.

Lemma 14. There exists a positive constant K such that

$$L_n \geq \mu^n \exp[-Kn^{1/3} \log n]$$

for infinitely many positive integers n .

Proof. For each N -step SAW ω with $\omega(0) = 0$, we define the ‘vertical radius’ of ω to be

$$V(\omega) = \max_{i=0, \dots, N} |\omega_d(i)|.$$

For each integer $v \geq 0$, let $b_N^{[\leq v]}$ (respectively, $b_N^{[\geq v]}$) be the number of N -step bridges ω with $\omega(0) = 0$ such that $V(\omega) \leq v$ (respectively, $V(\omega) \geq v$). For each N , there is an integer v_N such that

$$b_N^{[\leq v_N]} \geq \frac{1}{2} b_N \quad \text{and} \quad b_N^{[\geq v_N]} \geq \frac{1}{2} b_N. \tag{3.12}$$

That is, v_N is the median vertical radius of N -step bridges. Also, for $y \in \mathbb{Z}$, $N \geq 1$ and $v \geq 1$, let $b_N^{[\leq v]}(y)$ denote the number of N -step bridges ω with $\omega(0) = 0$ such that $V(\omega) \leq v$ and $\omega_d(N) = y$.

Next, let $\eta_{N,r}$ be the number of N -step bridges with $\omega(0) = 0$ and $r = \omega_d(N) \geq \omega_d(i) \geq 0$ for every $i = 0, \dots, N$. (In the notation of page 108 of Madras and Slade (1993), we have

$\eta_{N,r} = |\cup_L \hat{B}_{N,L,r}|$. Note that in Madras and Slade (1993), the coordinate ω_2 plays the role of ω_d in the present paper, but this difference is not consequential.) As in the proof of proposition 4.4.2 of Madras and Slade (1993), we observe that if ω is an arbitrary N -step bridge, then we can ‘unfold’ part of ω upwards (in the manner of Hammersley and Welsh (1962)), and unfold the rest of ω downwards, to obtain a bridge of the kind counted by $\eta_{N,r}$ (for some r). The argument of that proof yields

$$b_N^{[\geq v]} \leq 2 \sum_{r=v}^N \sum_{A=0}^r P_D(A) P_D(r-A+1) \eta_{N,r} \leq 2 \sum_{r=v}^N (N+1) K_0^2 \exp[3(N+1)^{1/2}] \eta_{N,r}$$

where $P_D(A)$ is the number of partitions of A into distinct integers (see theorem 3.1.4 of Madras and Slade (1993) for the definition and asymptotics of $P_D(\cdot)$, which will not be needed again in this paper). This implies that

$$\sum_{r=v}^N \eta_{N,r} \geq \frac{1}{2K_0^2(N+1)} \exp[-3(N+1)^{1/2}] b_N^{[\geq v]} \tag{3.13}$$

for every $N, v \geq 1$. From the above inequality, we see that for every v and N there exists an integer $r(v, N) \geq v$ such that

$$\eta_{N,r(v,N)} \geq \frac{1}{K'N^2} \exp[-3(N+1)^{1/2}] b_N^{[\geq v]} \quad \text{where } K' = 4K_0^2. \tag{3.14}$$

Next we describe a procedure for making long bridges from certain kinds of shorter bridges. For given $N \geq 1$ and $v \geq 1$, let ζ and ξ be bridges of the type counted by $\eta_{N,r(v,N)}$ (i.e. N -steps, $\zeta(0) = 0, r(v, N) = \zeta_d(N) \geq \zeta_d(i) \geq 0$ for every i , and similarly for ξ). Let $\hat{\xi}$ be the reflection of ξ through the plane $x_d = 0$ (so that $-r(v, N) = \hat{\xi}_d(N) \leq \hat{\xi}_d(i) \leq 0$ for every i). Also, for given $j \geq 0$ and $m \geq 1$, let $\varphi^1, \dots, \varphi^j$ be bridges of the type counted by $b_m^{[\leq v]}(0)$ (i.e. m steps, vertical radius at most v , and $\varphi_d^i(m) = 0$). Now construct the $(2N + jm + 3)$ -step walk θ from the following sequence of steps: $\theta(0) = 0$, then one step in the $+x_1$ direction, one step in the $+x_d$ direction, then $\zeta, \varphi^1, \varphi^2, \dots, \varphi^j$, then $\hat{\xi}$, and finally one step in the $-x_d$ direction. Observe that θ is a bridge. Also, the part of θ that comes from ζ has $\theta_d(\cdot) \geq 1$, and ends with $\theta_d(N+2) = r(v, N) + 1 \geq v + 1$. The part of θ coming from the φ^i s has $\theta_d(\cdot) \geq r(v, N) + 1 - v \geq 1$, and ends with $\theta_d(N+2+jm) = r(v, N) + 1$. The part of θ coming from $\hat{\xi}$ has $\theta_d(\cdot) \geq 1$, and ends with $\theta_d(N+2+jm+N) = r(v, N) + 1 - r(v, N) = 1$. Hence the last step in the $-x_d$ direction ensures $\theta_d(2N + jm + 3) = 0$. Thus we see that θ is a positive excursion. This shows that the number of $(2N + jm + 3)$ -step positive excursions can be bounded below by the number of ways to choose ζ, ξ and the φ^i s. That is, for any $N, v, m \geq 1$ and $j \geq 0$, we have

$$L_{2N+jm+3} \geq (\eta_{N,r(v,N)})^2 (b_m^{[\leq v]}(0))^j. \tag{3.15}$$

Next, we need the following bound,

$$b_{2N+1}^{[\leq v]}(0) \geq \frac{(b_N^{[\leq v]})^2}{2N-1} \tag{3.16}$$

for every $N \geq 1$ and every $v \geq 1$. To prove (3.16), let y be an integer such that $|y| \leq v$, and consider two N -step bridges $\omega^{(k)}$ ($k = 1, 2$) with $\omega^{(k)}(0) = 0, \omega^{(k)}(N) = y$ and $V(\omega^{(k)}) \leq v$. Let ψ be the N -step SAW obtained by reflecting $\omega^{(2)}$ through the hyperplane $x_1 = 0$, and traversing it in the opposite order; that is,

$$\psi(t) = (-\omega_1^{(2)}(N-t), \omega_2^{(2)}(N-t), \dots, \omega_d^{(2)}(N-t)) \quad t = 0, \dots, N.$$

We can produce a $(2N + 1)$ -step SAW ω by adding one step in the $+x_1$ direction to the end of $\omega^{(1)}$, and then adding the steps of ψ . Then ω is a $(2N + 1)$ -step bridge with $\omega_d(2N + 1) = 0$ and $V(\omega) \leq v$. Moreover, ω uniquely determines $\omega^{(1)}$ and $\omega^{(2)}$, so we have

$$b_{2N+1}^{[\leq v]}(0) \geq \sum_y (b_N^{[\leq v]}(y))^2. \tag{3.17}$$

Since $b_N^{[\leq v]}(y)$ is nonzero only if $|y| < N$, an application of the Schwarz inequality gives

$$\sum_{y=-(N-1)}^{N-1} (b_N^{[\leq v]}(y))^2 (2N - 1) \geq \left(\sum_{y=-(N-1)}^{N-1} b_N^{[\leq v]}(y) \right)^2 = (b_N^{[\leq v]})^2. \tag{3.18}$$

Now equation (3.16) follows by combining equations (3.17) and (3.18).

For our next step, we define the subset of integers

$$\mathcal{N}^* = \left\{ N \geq 1 : b_N \geq \frac{1}{N^2} \mu^N \right\}.$$

Kesten (1963), see corollary 3.1.8 in Madras and Slade (1993), proved that $\sum_N b_N \mu^{-N}$ diverges, which implies that \mathcal{N}^* is an infinite set. For $N \in \mathcal{N}^*$, we have

$$b_N^{[\geq v_N]} \geq \frac{1}{2N^2} \mu^N \quad (\text{by (3.12)})$$

(recall the definition of $b_N^{[\geq v_N]}$ preceding equation (3.12)) (3.19)

$$b_N^{[\geq v_N]} \geq \frac{1}{2N^2} \mu^N \quad (\text{by (3.12)}) \tag{3.20}$$

$$b_{2N+1}^{[\leq v_N]}(0) \geq \frac{1}{8N^5} \mu^{2N} \quad (\text{by (3.16) and (3.19)}) \tag{3.21}$$

$$\eta_{N,r(v_N,N)} \geq \frac{\mu^N}{2K'N^4} \exp[-3(N + 1)^{1/2}] \quad (\text{by (3.14) and (3.20)}) \tag{3.22}$$

For any $j \geq 1$ and $N \in \mathcal{N}^*$, equations (3.15), (3.21) and (3.22) imply that

$$L_{2N+j(2N+1)+3} \geq \frac{\mu^{2N+2jN} \exp[-6(N + 1)^{1/2}]}{(8N^5)^j (2K')^2 N^8} \frac{\mu^{j+3}}{\mu^j \mu^3}. \tag{3.23}$$

Now let $N \in \mathcal{N}^*$. Define $j = j_N = \lfloor N^{1/2} \rfloor$ and $n = n_N = 2N + j(2N + 1) + 3$. Then for sufficiently large N , we have $n \geq (N + 1)^{3/2}$, which implies that

$$j \leq (N + 1)^{1/2} \leq n^{1/3} \quad \text{and} \quad N \leq n^{2/3}.$$

Using these inequalities in equation (3.23), we obtain

$$L_n \geq \frac{\mu^n \exp[-6n^{1/3}]}{\mu^3 (2K')^2 (8\mu)^{n^{1/3}} (n^{2/3})^{5n^{1/3}+8}} \geq \mu^n \exp[-Kn^{1/3} \log n]$$

(for some constant $K > 0$) for sufficiently large n of the form $n = n_N = 2N + j_N(2N + 1) + 3$ with $N \in \mathcal{N}^*$. This proves the lemma. □

The above lemma permits us to make the argument of Maritan *et al* (1999) completely rigorous, as we now show.

Proof of theorem 6. Fix a value of γ , and fix nonzero values of α and β satisfying $\alpha p = \beta(1 - p)$. It suffices to prove a lower bound on $\bar{\kappa}(\alpha, \beta, \gamma)$ which is strictly larger than $\log \mu + \alpha p$. We shall obtain such a lower bound by counting a particular subset of N -step SAWs in the sum defining Z_N .

Let σ be a large integer for which the inequality of lemma 14 holds. (Near the end of the proof we shall specify how large σ must be.) In our proof, we shall consider long SAWs that are made up of many shorter SAWs of length σ . In particular, consider a sequence of k σ -step SAWs, each of which is either a positive or a negative excursion. This sequence can always be concatenated in order to get a $k\sigma$ -step SAW ω starting at 0 that has exactly $2k + 1$ vertices in the $x_d = 0$ plane.

For a colouring χ and an integer $r \geq 1$, let $A_r(\chi)$ (respectively, $B_r(\chi)$) denote the number of As (respectively, Bs) among $\{\chi_i : i = (r - 1)\sigma + 2, \dots, r\sigma - 1\}$. (Note that in the scheme outlined in the previous paragraph, the vertices $\omega((r - 1)\sigma)$ and $\omega((r - 1)\sigma + 1)$ always lie in the $x_d = 0$ plane, so we do not care about their colours.) Then $A_1(\chi), A_2(\chi), \dots$ is a sequence of independent random variables, each binomially distributed with parameters p and $\sigma - 2$.

Consider SAWs of length $N = k\sigma$ for some large integer r . Given χ , consider the subset of N -step SAWs ω such that for each $r = 1, \dots, k$, the subwalk $(\omega((k - 1)\sigma), \dots, \omega(k\sigma))$ is a positive (respectively, negative) excursion if $\alpha A_r(\chi) \geq \beta B_r(\chi)$ (respectively, if $\alpha A_r(\chi) < \beta B_r(\chi)$). This shows that

$$Z_{k\sigma}(\alpha, \beta, \gamma|\chi) \geq e^{\gamma(2k+1)} \prod_{r=1}^k (L_\sigma \exp[\max\{\alpha A_r(\chi), \beta B_r(\chi)\}]). \tag{3.24}$$

This and lemma 14 imply that

$$\frac{\log Z_{k\sigma}(\alpha, \beta, \gamma|\chi)}{k\sigma} \geq \frac{\gamma(2k + 1)}{k\sigma} + \frac{\sum_{r=1}^k [\sigma \log \mu - K\sigma^{1/3} \log \sigma + \max\{\alpha A_r(\chi), \beta B_r(\chi)\}]}{k\sigma}.$$

Now we let $k \rightarrow \infty$. Using the self-averaging property (as described in section 1) and the strong law of large numbers, we obtain

$$\bar{\kappa}(\alpha, \beta, \gamma|\chi) \geq \frac{2\gamma}{\sigma} + \log \mu - K \frac{\log \sigma}{\sigma^{2/3}} + \frac{E(\max\{\alpha A_1(\chi), \beta B_1(\chi)\})}{\sigma}. \tag{3.25}$$

Using the identities $\max\{u, v\} = (u + v + |u - v|)/2$ and $B_1(\chi) = \sigma - 2 - A_1(\chi)$, as well as $\beta(1 - p) = \alpha p$, we obtain

$$\begin{aligned} & E(\max\{\alpha A_1(\chi), \beta B_1(\chi)\}) \\ &= \frac{E(\alpha A_1(\chi)) + E(\beta B_1(\chi)) + E|\alpha A_1(\chi) - \beta(\sigma - 2 - A_1(\chi))|}{2} \\ &= \frac{\alpha p(\sigma - 2) + \beta(1 - p)(\sigma - 2) + E|(\alpha + \beta)A_1(\chi) - \beta(\sigma - 2)|}{2} \\ &= \alpha p(\sigma - 2) + \frac{\beta}{2p} E|A_1(\chi) - p(\sigma - 2)| \quad \text{using } \alpha + \beta = \frac{\beta}{p}. \end{aligned} \tag{3.26}$$

Since the distribution of $A_1(\chi)$ is asymptotically normal with mean $p(\sigma - 2)$ and variance $p(1 - p)(\sigma - 2)$ as $\sigma \rightarrow \infty$, we obtain the asymptotic relation

$$\begin{aligned} E|A_1(\chi) - p(\sigma - 2)| &\sim \frac{\sqrt{p(1 - p)\sigma}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} |z| e^{-z^2/2} dz \\ &= \sqrt{\frac{2p(1 - p)}{\pi}} \sqrt{\sigma}. \end{aligned}$$

Using this and equation (3.26) in equation (3.25), we see that for large σ

$$\bar{\kappa}(\alpha, \beta, \gamma|\chi) \geq \log \mu + \alpha p + \beta \sqrt{\frac{1-p}{2p\pi}} \sigma^{-1/2} + o(\sigma^{-1/2}). \tag{3.27}$$

In particular, we can make the right-hand side of equation (3.27) strictly greater than $\log \mu + \alpha p$ by taking σ large enough. This shows that $\bar{\kappa}(\alpha, \beta, \gamma|\chi)$ is strictly greater than $\log \mu + \alpha p$. This completes the proof of delocalization. \square

We now proceed to the proof of theorem 8, the lower bound for $\beta_c(\alpha, \gamma)$.

Proof of theorem 8. It suffices to prove the following. Assume that (α, β, γ) satisfies

$$\alpha p > \beta(1 - p) \tag{3.28}$$

$$p e^{\gamma - \alpha} + (1 - p) e^{\gamma} \leq 1 \tag{3.29}$$

and

$$p e^{-\alpha} + (1 - p) e^{\beta} \leq 1. \tag{3.30}$$

Then (α, β, γ) is in DELOC_α .

Before proceeding, we shall introduce some new notation. For a colouring $\chi = (\chi_1, \dots, \chi_N)$ and a SAW $\omega = (\omega(0), \dots, \omega(N))$, define the sets

$$\begin{aligned} \chi_{[A]} &= \{i : \chi_i = A, 1 \leq i \leq N\} \\ \chi_{[B]} &= \{i : \chi_i = B, 1 \leq i \leq N\} \\ \omega_{[>]} &= \{i : \omega_d(i) > 0, 1 \leq i \leq N\} \\ \omega_{[<]} &= \{i : \omega_d(i) < 0, 1 \leq i \leq N\} \\ \omega_{[=]} &= \{i : \omega_d(i) = 0, 1 \leq i \leq N\}. \end{aligned}$$

Also, write $\langle \cdot \rangle$ to denote expectation over colourings, and write $|\cdot|$ to denote the cardinality of a set.

We can write the partition function (1.2) as a sum over all N -step SAWs ω , as follows:

$$Z_N(\alpha, \beta, \gamma|\chi) = \sum_{\omega} \exp(\alpha|\omega_{[>]} \cap \chi_{[A]}| + \beta|\omega_{[<]} \cap \chi_{[B]}| + \gamma|\omega_{[=]}|). \tag{3.31}$$

Writing $|\omega_{[>]} \cap \chi_{[A]}| = |\chi_{[A]}| - |\omega_{[<]} \cap \chi_{[A]}| - |\omega_{[=]} \cap \chi_{[A]}|$ and $|\omega_{[=]}| = |\omega_{[=]} \cap \chi_{[A]}| + |\omega_{[=]} \cap \chi_{[B]}|$, we obtain

$$\begin{aligned} Z_N(\alpha, \beta, \gamma|\chi) &= \exp(\alpha|\chi_{[A]}|) \sum_{\omega} [\exp((\gamma - \alpha)|\omega_{[=]} \cap \chi_{[A]}| + \gamma|\omega_{[=]} \cap \chi_{[B]}|) \\ &\quad \times \exp(-\alpha|\omega_{[<]} \cap \chi_{[A]}| + \beta|\omega_{[<]} \cap \chi_{[B]}|)]. \end{aligned}$$

We now take logarithms and expectations, and apply Jensen's inequality (since the logarithm is a concave function):

$$\begin{aligned} \langle \log Z_N(\alpha, \beta, \gamma|\chi) \rangle &= \langle \alpha|\chi_{[A]}| \rangle + \left\langle \log \sum_{\omega} [\exp((\gamma - \alpha)|\omega_{[=]} \cap \chi_{[A]}| + \gamma|\omega_{[=]} \cap \chi_{[B]}|) \right. \\ &\quad \left. \times \exp(-\alpha|\omega_{[<]} \cap \chi_{[A]}| + \beta|\omega_{[<]} \cap \chi_{[B]}|)] \right\rangle \\ &\leq \alpha p N + \log \sum_{\omega} (\exp((\gamma - \alpha)|\omega_{[=]} \cap \chi_{[A]}| + \gamma|\omega_{[=]} \cap \chi_{[B]}|) \\ &\quad \times \exp(-\alpha|\omega_{[<]} \cap \chi_{[A]}| + \beta|\omega_{[<]} \cap \chi_{[B]}|)). \end{aligned} \tag{3.32}$$

(Observe that the resulting upper bound can be thought of as a partial annealing.) For a random event E , we write $1\{E\}$ to denote the random variable that equals 1 when E occurs and equals 0 when E does not occur. Since the χ_i s are independent, for each ω we have that

$$\begin{aligned} & \langle \exp((\gamma - \alpha)|\omega_{[=]} \cap \chi_{[A]}| + \gamma|\omega_{[=]} \cap \chi_{[B]}|) \exp(-\alpha|\omega_{[<]} \cap \chi_{[A]}| + \beta|\omega_{[<]} \cap \chi_{[B]}|) \rangle \\ &= \left\langle \prod_{i \in \omega_{[=]}} \exp((\gamma - \alpha)1\{\chi_i = A\} + \gamma 1\{\chi_i = B\}) \right. \\ & \quad \left. \times \prod_{i \in \omega_{[<]}} \exp((- \alpha)1\{\chi_i = A\} + \beta 1\{\chi_i = B\}) \right\rangle \\ &= (p e^{\gamma - \alpha} + (1 - p) e^{\gamma})^{|\omega_{[=]}|} (p e^{-\alpha} + (1 - p) e^{\beta})^{|\omega_{[<]}|} \\ &\leq 1 \quad (\text{by equations (3.29) and (3.30)}). \end{aligned}$$

Inserting this into the right-hand side of (3.32) gives

$$\langle \log Z_N(\alpha, \beta, \gamma | \chi) \rangle \leq \alpha p N + \log \sum_{\omega} 1 = \alpha p N + \log c_N.$$

This implies that $\bar{\kappa}(\alpha, \beta, \gamma) \leq \alpha p + \log \mu$, i.e. that (α, β, γ) is in DELOC_{α} . This proves the italicized assertion in the first paragraph, and the theorem follows. \square

Finally, we prove that everything is localized for sufficiently large γ and, in fact, that $\gamma > \max\{p^{-2}, (1 - p)^{-2}\} \log \mu_d$ suffices.

Proof of theorem 11. The proof uses the idea of theorem 3.3 of Martin *et al* (2000). Consider a colouring χ for a given N . We will bound the free energy by considering the contribution of a single walk ω that depends on χ .

For each integer k , let $\mathcal{I}_k = \{x \in Z^d : x_d = k\}$. In particular, \mathcal{I}_0 is the interfacial hyperplane. We will describe an N -step SAW ω that lies entirely in $\mathcal{I}_0 \cup \mathcal{I}_1$, and only takes steps in the $+x_1, +x_d$ and $-x_d$ directions. Let $\omega(0) = 0$, and for each integer i such that $0 \leq 2i \leq N - 2$, put both of $\omega(2i + 1)$ and $\omega(2i + 2)$ in \mathcal{I}_0 if $\chi_{2i+1} = \chi_{2i+2} = B$, and put both of $\omega(2i + 1)$ and $\omega(2i + 2)$ in \mathcal{I}_1 otherwise. In this way all of the A -vertices of ω are in \mathcal{I}_1 . (It is easy to see that such an ω always exists for a given χ .)

Let $A(\chi)$ be the number of A s in χ_1, \dots, χ_N , and let $h(\chi)$ be the number of i s such that $\chi_{2i+1} = \chi_{2i+2} = B$. Then by considering the contribution of ω to the partition function Z_N , we find

$$Z_N(\alpha, \beta, \gamma | \chi) \geq \exp[2\gamma h(\chi) + \alpha A(\chi)]$$

and hence

$$\langle \kappa_N(\alpha, \beta, \gamma | \chi) \rangle \geq \frac{2\gamma \langle h(\chi) \rangle + \alpha \langle A(\chi) \rangle}{N}.$$

We have $\langle A(\chi) \rangle = pN$ and $\langle h(\chi) \rangle = \lfloor (N - 1)/2 \rfloor (1 - p)^2$, so letting $N \rightarrow \infty$ in the above inequality gives

$$\bar{\kappa}(\alpha, \beta, \gamma) \geq \gamma(1 - p)^2 + \alpha p. \tag{3.33}$$

A similar argument leads to the bound

$$\bar{\kappa}(\alpha, \beta, \gamma) \geq \gamma p^2 + \beta(1 - p). \tag{3.34}$$

From (3.33) and (3.34), we see that $\bar{\kappa}(\alpha, \beta, \gamma)$ is strictly greater than $\log \mu_d + \max\{\alpha p, \beta(1 - p)\}$ if $\gamma(1 - p)^2$ and γp^2 are both strictly greater than $\log \mu_d$, i.e. if $\gamma > \max\{p^{-2}, (1 - p)^{-2}\} \log \mu_d$. This proves the theorem. \square

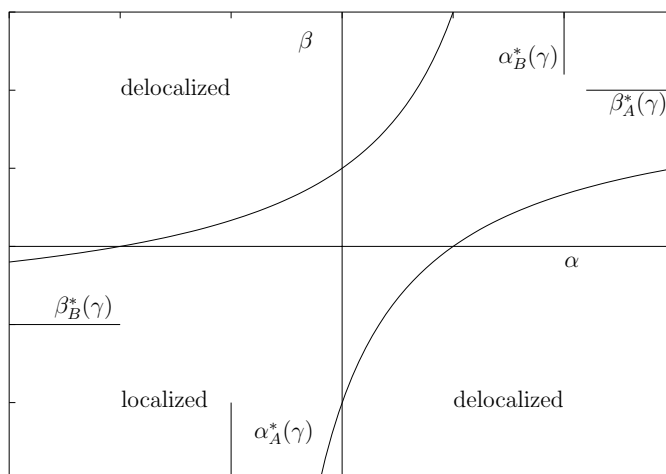


Figure 2. The expected form of the phase diagram when $\gamma > 0$. When γ is sufficiently large, the delocalized regions stay out of the third quadrant entirely, by theorem 5.

4. Discussion

We have shown that the shapes of the phase boundaries in the (α, β) -plane for $\gamma = 0$ are qualitatively those shown in figure 1. When γ is negative, we have shown that the picture does not change qualitatively. In contrast, for sufficiently positive γ , we have shown that the boundaries of the two delocalized phases no longer have a common point, as illustrated in figure 2. The general shape of each individual boundary is the same for all values of γ ; in particular, they are convex and continuous, with horizontal and vertical asymptotes. The exception to this occurs when γ is large enough that the phase boundaries disappear and the system is localized for every α and β .

For the special case $p = 1/2, d = 3$ and $\gamma = 0$, the locations of the phase boundaries have been estimated numerically by Martin *et al* (2000) (see figure 4 in that paper). In particular, they found that $\beta_c(\alpha, 0)$ tends to a value close to 1 for large α . This compares well with theorem 8 which gives a lower bound of $\log 2 = 0.693\dots$ for the location of the asymptote. The numerical asymptotes of Martin *et al* (2000) in the third quadrant also compare well with the rigorous bounds (theorem 2.3 in their paper, which is our theorem 5(iv) for $\gamma = 0$).

Our model can be extended by not requiring the first vertex of the walk to be at the origin but allowing it to be at any distance from the interface. Lemma 2.4 of Martin *et al* (2000) (extended to $\gamma \neq 0$ and suitably fixed) establishes that the quenched average free energy for walks without the constraint that they begin at the origin is equal to our $\bar{\kappa}(\alpha, \beta, \gamma)$ and so the original model and its extension have the same phase diagram. This means that, in the localized regime, the walk will find the interface and cross it frequently.

Many open questions remain. We have shown that the phase boundaries are differentiable at the origin when $\gamma \leq 0$, but are the phase boundaries smooth everywhere? We have shown that for fixed $\gamma_0 \leq 0$ there is a first-order transition as we cross from $\text{DELOC}_\alpha(\gamma_0)$ to $\text{DELOC}_\beta(\gamma_0)$ through the origin, but in general what is the order of the phase transition as we cross the phase boundaries? Is it true that $\gamma_c(0, 0) = 0$, i.e. does figure 2 hold for every small positive γ ? We have proved that the delocalized region in the (α, β) -plane is empty

for large γ , but does it vanish continuously as γ increases to the critical value γ_L (i.e., are $\text{DELOC}_\alpha(\gamma_L)$ and $\text{DELOC}_\beta(\gamma_L)$ both empty)?

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