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Critical behaviour of self-avoiding walks that cross a square

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Abstract. Consider the set of all self-avoiding walks in the square lattice which start at (0, 0), end at (L, L), and are entirely contained in the square $[0, L] \times [0, L]$. Associate a fugacity x with each step of the walk. Whittington and Guttmann (1990) showed that the dominant walks have $O(L)$ steps when x is small and $O(L^2)$ steps when x is large, and they conjectured that there is a single transition point at $x = \mu^{-1}$, where μ is the inverse of the connective constant for (unconstrained) self-avoiding walks. We present a rigorous proof of this conjecture (and its analogue in higher dimensions). We also discuss what can be said rigorously about two scaling exponents associated with this phase transition, and compare this with analogous results that have been obtained exactly (and rigorously) on the discrete Sierpinski gasket by Hattori, Hattori and Kusuoka (1990).

1. Introduction

The self-avoiding walk has long been a standard model of a long linear polymer molecule in a good solvent (Madras and Slade 1993). The usual setting is a single walk on an infinite lattice, which models a polymer in a dilute solution. If we consider instead a (large) finite region of a lattice, then the solution changes from dilute to dense as we increase the length of the walk (or the fugacity for the number of steps). In fact, Whittington and Guttmann (1990) proved the existence of a dilute-to-dense phase transition for the model described in the next paragraph. The aim of the present paper is to prove some rigorous results about this transition.

To fix ideas, let us begin with self-avoiding walks on the square lattice $\mathbb{Z}^2$. For large L, consider the set of all self-avoiding walks which start at the origin $(0, 0)$, end at (L, L), and are entirely contained in the square $[0, L] \times [0, L]$. Associate a fugacity x with each step of the walk. Whittington and Guttmann (1990) showed that when x is small the dominant walks have $O(L)$ steps, while when x is large the dominant walks have $O(L^2)$ steps. They showed that the transition occurred for x somewhere between μ^{-1} and μ_{H}^{-1}, where μ is the connective constant for (unconstrained) self-avoiding walks and μ_{H} is the connective constant for Hamiltonian walks in a square. They conjectured, on numerical grounds, that there was a single transition point at μ^{-1}. This conjecture was supported by a renormalization analysis (Prentis 1991) and by a correspondence with N-vector models (Burkhardt and Guim 1991).

In this paper we give a rigorous proof of the conjecture of Whittington and Guttmann (1990). We also discuss what can be said rigorously about two scaling exponents associated

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with this phase transition. This is compared with analogous results that have been obtained exactly (and rigorously) on the pre-Sierpinski gasket (Hattori *et al* 1990). We shall also describe some generalizations: to hypercubes in three or more dimensions, to walks with free endpoints that are constrained to lie in a hypercube (which may be a more natural model for the dilute-to-dense transition), and to analogous problems with lattice trees and lattice animals (modelling branched polymers in a good solvent). We also discuss the relation of the high-fugacity phase to systems of infinitely dense polymers.

2. Definitions and statement of results

We shall do all of our work in the d-dimensional hypercubic lattice $\mathbb{Z}^d$ with $d \geqslant 2$. If L is an integer, then we shall write $\mathbf{L} := (L, \dots, L) \in \mathbb{Z}^d$. In particular, $\mathbf{0}$ denotes the origin. We shall also write $[0, L]^d$ to denote the d-dimensional hypercube that has $\mathbf{0}$ and $\mathbf{L}$ as opposite corners.

For $n \geqslant 0$, let c_n be the number of n-step self-avoiding walks in $\mathbb{Z}^d$ which start at the origin (and end anywhere). Then there exists a *connective constant* μ with the property that

$$\lim_{n\to\infty} c_n^{1/n} = \mu \tag{1}$$

(Hammersley 1957). For $n, L \geqslant 1$, let $c_n(L)$ denote the number of n-step self-avoiding walks which start at $\mathbf{0}$, end at $\mathbf{L}$, and are entirely contained in $[0, L]^d$. For $x > 0$, we define the generating function

$$C_L(x) := \sum_n c_n(L)x^n \,. \tag{2}$$

Thus x is the step fugacity. We define the following limits, which exist by theorem 2.1 below (although they may be infinite for some values of x):

$$\lambda_1(x) := \lim_{L\to\infty} C_L(x)^{1/L} \tag{3}$$

$$\lambda_2(x) := \lim_{L\to\infty} C_L(x)^{1/L^d} \,. \tag{4}$$

Theorem 2.1.

(i) The limit (3) exists and is finite for $0 < x \leqslant \mu^{-1}$, and is infinite for $x > \mu^{-1}$. We have $0 < \lambda_1(x) < 1$ for $0 < x < \mu^{-1}$ and $\lambda_1(\mu^{-1}) = 1$.

(ii) The limit (4) exists and is finite for all $x > 0$. We have $\lambda_2(x) = 1$ for $0 < x \leqslant \mu^{-1}$ and $\lambda_2(x) > 1$ for all $x > \mu^{-1}$.

The existence of the limits follow from concatenation and subadditivity arguments (see lemma 4.1). Given the existence of the limit, it is easy to see that $\lambda_1(x)$ is strictly between 0 and 1 when $0 < x < \mu^{-1}$: Simply notice that the shortest walk from $\mathbf{0}$ to $\mathbf{L}$ contains exactly dL steps. Therefore $c_{dL}(L) \geqslant 1$ and $c_n(L) = 0$ for $n < dL$, and so

$$x^{dL} \leqslant C_L(x) \leqslant \sum_{n=dL}^{\infty} c_n x^n \,. \tag{5}$$

From equation (3) and (1), we can now see that

$$x^d \leqslant \lambda_1(x) \leqslant (\mu x)^d \qquad \text{for} \quad 0 < x < \mu^{-1} \,. \tag{6}$$

Every real $x > 0$ and integer $L \geqslant 1$ determine a probability measure $P_{x,L}$ on the set of self-avoiding walks in $[0, L]^d$ that start at $\mathbf{0}$ and end at $\mathbf{L}$: each such walk ω is assigned the probability $x^{|\omega|}/C_L(x)$, where $|\omega|$ is the length of ω (that is, the number of steps in ω). We shall use $\langle|\omega|\rangle_{x,L}$ to denote the expected length of a walk with respect to $P_{x,L}$. The critical value $x = \mu^{-1}$ denotes the transition from the expected length being proportional to L (so that an average walk is roughly like a straight line) to being proportional to L^d (so that an average walk fills space with some non-zero density). The behaviour at $x = \mu^{-1}$ is presumably in between (intuitively $L^{1/\nu}$), but we cannot prove much about this. The non-critical scaling is described in the following theorem. (We use the notation '$f(\cdot) \approx g(\cdot)$' to mean that there exist positive, finite constants C and C' such that $Cg(\cdot) \leqslant f(\cdot) \leqslant C'g(\cdot)$.)

Theorem 2.2. As $L \to \infty$, we have $\langle|\omega|\rangle_{x,L} \approx L$ for $0 < x < \mu^{-1}$ and we have $\langle|\omega|\rangle_{x,L} \approx L^d$ for $x > \mu^{-1}$.

We now recall the definition and some properties of the *mass* for the self-avoiding walk (see Madras and Slade 1993 for more details). For $0 < x < \mu^{-1}$ and $y \in \mathbb{Z}^d$, let $G_x(\mathbf{0}, y)$ be the generating function for the collection of all self-avoiding walks that start at $\mathbf{0}$ and end at y. We define the mass $m(x)$ to be the rate of decay of $G_x(\mathbf{0}, y)$ along a coordinate axis:

$$m(x) := \lim_{n\to\infty} \frac{-\log G_x(\mathbf{0}, (n, 0, \ldots, 0))}{n}\,. \tag{7}$$

It is known that this limit exists and is strictly positive whenever $0 < x < \mu^{-1}$, and that $m(x)$ tends to 0 as $x \nearrow \mu^{-1}$. It is generally believed that the mass tends to 0 as a power law

$$m(x) \sim \text{constant} \times (\mu^{-1} - x)^{\nu} \qquad \text{as } x \nearrow \mu^{-1} \tag{8}$$

where ν is the exponent which corresponds to the mean end-to-end distance of a self-avoiding walk. It is believed that ν equals $\frac{3}{4}$ in two dimensions, 0.588... in three dimensions, and $\frac{1}{2}$ (with logarithmic corrections) in four dimensions. In five or more dimensions, it is known rigorously (Hara and Slade 1992) that $\nu = \frac{1}{2}$, that (8) holds, and that the limit of (7) exists and equals 0 at $x = \mu^{-1}$.

Theorem 2.3. For $x > 0$, define

$$f_1(x) = \log\lambda_1(x) \qquad \text{and} \qquad f_2(x) = \log\lambda_2(x)\,.$$

(i) The function f_1 is a strictly increasing, negative-valued, convex function of $\log x$ for $0 < x \leqslant \mu^{-1}$, and $f_1(x) \approx -m(x)$ as $x \nearrow \mu^{-1}$.

(ii) For $x > \mu^{-1}$, the function f_2 is a strictly increasing, convex function of $\log x$, and satisfies $0 < f_2(x) \leqslant \log\mu + \log x < \mu(x - \mu^{-1})$.

An analogous model was studied rigorously on the discrete Sierpinski gasket by Hattori *et al* (1990). They defined a sequence of fractal-like graphs F_n, each consisting of $(3^{n+1} + 3)/2$ sites, and contained in a large triangle with 2^n sites on each side (see figure 1). Then they looked at the ensemble of self-avoiding walks on F_n that had its two endpoints at two specified corners of the large triangle, and gave each walk ω the weight $x^{|\omega|}$. They solved this model exactly, and found a transition point x_c such that the average length of a walk scaled as 2^n for $x < x_c$ and as 3^n for $x > x_c$. (Later, Hattori and Kusuoka (1992) proved that x_c equals the inverse of the connective constant for self-avoiding walks on the gasket.)

Hattori *et al* (1990) also proved direct analogues of theorems 2.1 and 2.3, with a stronger result in the analogue of theorem 2.3: they showed (i) that $f_1(x) \sim -\text{constant}\times(\mu^{-1} - x)^{\nu}$ as $x \nearrow \mu^{-1}$, where $\nu = \log 2/\log((7-\sqrt{5})/2)$ is the exponent for end-to-end distance of self-avoiding walks on the Sierpinski gasket (Rammal *et al* 1984, Klein and Seiz 1984, Hattori and Kusuoka 1992); and (ii) that $f_2(x) \sim \text{constant} \times (x - \mu^{-1})^{\overline{d}\nu}$ as $x \searrow \mu^{-1}$, where $\overline{d} = \log 3/\log 2$ is the Hausdorff dimension of the gasket. Our theorem 2.3 essentially

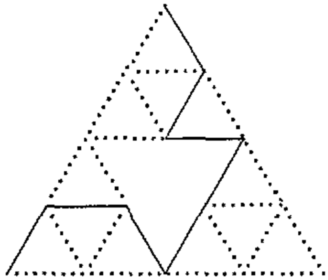

Figure 1. A typical self-avoiding walk (full line) on the finite gasket F_2 (dotted line), as studied by Hattori *et al* (1990). In that paper, all walks begin at the lower left vertex and end at the top vertex.

proves the analogue of (i), but we have no idea how to prove an analogue of (ii). However, it is believed that $f_2(x) \sim \text{constant} \times (x - \mu^{-1})^{d\nu}$ in Euclidean space (see equation (X.59) in de Gennes (1979), and equation (13) in Saleur (1987)). (Golowich and Imbrie (1993) prove this, with logarithmic corrections, for weakly self-avoiding walk on a four-dimensional hierarchical lattice.) All that we can say rigorously is that if $f_2(x) \approx (x - \mu^{-1})^q$ as $x \searrow \mu^{-1}$ for some exponent q, then $q \geqslant 1$ (by theorem 2.3(ii)). Since we believe $q = d\nu$, this corresponds to the assertion $\nu \geqslant 1/d$, which (sadly) is the most that one can say *rigorously* about ν in general d.

The scaling behaviour at the critical point x_c was also investigated by Hattori *et al* (1990). They showed that the average length scales as $2^{n\nu}$, and that their analogue of $C_L(\mu^{-1})$ converges to $(\sqrt{5} - 1)/2$ as $L \to \infty$. This last result is one place where we can prove a difference between the behaviours for the gasket and for $\mathbb{Z}^d$:

Theorem 2.4. $\lim_{L\to\infty} C_L(\mu^{-1}) = 0$.

3. Other models

In this section we consider analogues of the results of section 2 for some other models of polymers (lattice trees and lattice animals), as well as modifications that arise when the boundary conditions change.

A *lattice animal* is a finite connected subgraph of the lattice $\mathbb{Z}^d$ (in other papers, this is sometimes called a *bond animal*). A *lattice tree* is a lattice animal that contains no cycles. Let a_n (respectively, t_n) denote the number of lattice animals (respectively, trees) that contain exactly n bonds, and such that the origin is the smallest site of the animal (respectively, tree) with respect to lexicographic ordering of the sites of $\mathbb{Z}^d$. Then there are finite (d-dependent) growth constants μ_a and μ_t such that

$$\lim_{n\to\infty} (a_n)^{1/n} = \mu_a \qquad \text{and} \qquad \lim_{n\to\infty} (t_n)^{1/n} = \mu_t \tag{9}$$

(Klarner 1967, Klein 1981). Next, for $n, L \geqslant 1$, let $a_n(L)$ (respectively, $t_n(L)$) denote the number of animals (respectively, trees) with n sites that contain both $\mathbf{0}$ and $\boldsymbol{L}$ as sites and are entirely contained in $[0, L]^d$. For $x > 0$, define the analogues of $C_L(x)$:

$$A_L(x) := \sum_n a_n(L)x^n \qquad \text{and} \qquad T_L(x) := \sum_n t_n(L)x^n . \tag{10}$$

Here x is a bond fugacity (but we could do similar things if we counted animals by the number of sites instead). In either model, the methods of this paper can easily be adapted to show that there is a phase transition at the inverse of the growth constant:

Theorem 3.1.

(i) The limit

$$\lambda_1^a(x) := \lim_{L\to\infty} A_L(x)^{1/L} \tag{11}$$

exists and lies in the interval (0, 1) for $0 < x < \mu_a^{-1}$, and is infinite for $x > \mu_a^{-1}$. The limit

$$\lambda_2^a(x) := \lim_{L\to\infty} A_L(x)^{1/L^d} \tag{12}$$

exists and is finite for all $x > 0$. It equals 1 for $0 < x \leqslant \mu_a^{-1}$ and is strictly bigger than 1 for all $x > \mu_a^{-1}$.

(ii) The exact analogue of (i) holds for trees, with A_L and μ_a replaced by T_L and μ_t.

Corollary 3.2. The analogue of theorem 2.2 holds for both of the ensembles corresponding to the generating functions of (10).

The proofs of these results are very much the same as the proofs for self-avoiding walks (see section 4). In particular, the proof of the above corollary is omitted, since it is the same as the proof of theorem 2.2.

We now consider what happens when the boundary conditions are removed—that is, when we no longer require that the walk (or animal, or tree) join opposite corners of a large cube. There are several ways to define such models, but we shall proceed as follows. For $n, L \geqslant 1$, let $\tilde{c}_n(L)$ be the number of self-avoiding walks (respectively, lattice animals and lattice trees) that begin at the origin, end anywhere, and are entirely contained in the box $[-L, L]^d$. For $x > 0$, let

$$\tilde{C}_L(x) = \sum_n \tilde{c}_n(L)x^n. \tag{13}$$

Similarly, let $\tilde{a}_n(L)$ (respectively, $\tilde{t}_n(L)$) be the number of lattice animals (respectively, lattice trees) that contain the origin and are entirely contained in the box $[-L, L]^d$. Also define

$$\tilde{A}_L(x) = \sum_n \tilde{a}_n(L)x^n \quad \text{and} \quad \tilde{T}_L(x) = \sum_n \tilde{t}_n(L)x^n\,. \tag{14}$$

Now things are a little different:

Theorem 3.3.

(i) For $x > 0$, we have

$$\lim_{L\to\infty} \tilde{C}_L(x) = \sum_n c_n x^n \equiv \chi(x) \tag{15}$$

where $\chi(x) \equiv \sum_n c_n x^n$ is the *susceptibility* of self-avoiding walks (which is finite only when $x < \mu^{-1}$).

(ii) For $x > \mu^{-1}$, we have

$$1 < \lambda_2(x) \leqslant \liminf_{L\to\infty} \tilde{C}_L(x)^{1/(2L)^d} \leqslant \limsup_{L\to\infty} \tilde{C}_L(x)^{1/(2L)^d} \leqslant x\mu\,. \tag{16}$$

Proof. Equation (15) follows from the monotone convergence theorem, since $c_n(L)$ increases to c_n as $L \to \infty$. The leftmost inequality of (16) comes from theorem 2.1(ii), and the rightmost inequality is a consequence of the bound

$$\tilde{C}_L(x) \leqslant \sum_{n=0}^{(2L+1)^d} c_n x^n$$

and equation (1). The second inequality of (16) will be proven in section 4 (proposition 4.6). □

There is an obvious analogue of theorem 2.2 for this model. Again, the case $x < \mu^{-1}$ is different because now the mean length converges to a finite limit as $L \to \infty$. Analogues of the above results can be formulated and proven for lattice animals and trees in the obvious way.

We do not know how to prove that $\lim_{L\to\infty} \tilde{C}_L(x)^{1/(2L)^d}$ exists for $x > \mu^{-1}$ (observe that the concatenation idea (see lemma 4.1) does not seem to work here). But it is reasonable to expect that this limit exists and equals $\lambda_2(x)$. In fact, this is one place where we can say more about animals and trees than we can for walks.

Theorem 3.4. For $x > \mu_a^{-1}$,

$$\lim_{L\to\infty} \tilde{A}_L(x)^{1/(2L)^d} = \lambda_2^a(x). \tag{17}$$

4. Proofs

Lemma 4.1. For every $x > 0$, the limits of (3) and (4) exist in $(0, +\infty]$.

Proof. Let L and L' be positive integers. Any walk from $\mathbf{0}$ to $\boldsymbol{L}$ that lies in $[0, L]^d$ can be joined to the front of any walk from $\boldsymbol{L}$ to $\boldsymbol{L} + \boldsymbol{L}'$ that lies in $[L, L + L']^d$. The result is a walk from $\mathbf{0}$ to $\boldsymbol{L} + \boldsymbol{L}'$ that lies in $[0, L + L']^d$. Therefore $C_{L+L'}(x) \geqslant C_L(x)C_{L'}(x)$ for all $x > 0$. The existence of the limit of (3) is now a consequence of subadditivity.

The existence of the limit of (4) may be proven in the manner of Whittington and Guttmann (1990), who prove the result for $d = 2$. (We note that their proof contains a minor error: the term $2p(p-1)$ in their equation (3.4) should be multiplied by a term of order M. This means only that the $\log x$ term in their equation (3.8) should be divided by $M + 2$ instead of $(M+2)^2$. This does not affect the rest of their proof.) □

The next result is the key to proving that x_c cannot be greater than μ^{-1}. It will require some notational preparation and a couple of lemmas before we complete the proof.

Proposition 4.2. For any $x > \mu^{-1}$ we have $\lim_{L\to\infty} C_L(x)^{1/L^d} > 1$.

We recall some definitions and notation from Madras and Slade (1993). If ω is an n-step self-avoiding walk in $\mathbb{Z}^d$, then we shall write $\omega = (\omega(0), \ldots, \omega(n))$, where $\omega(i)$ is the ith site of the walk. We denote the coordinates of the site $\omega(i)$ by $\omega_j(i)$ $(j = 1, \ldots, d)$.

An *n-step bridge* is defined to be an n-step self-avoiding walk ω whose first coordinates satisfy the inequality

$$\omega_1(0) < \omega_1(i) \leqslant \omega_1(n) \qquad \text{for every} \quad i = 1, \ldots, n. \tag{18}$$

The number of n-step bridges starting at the origin is denoted by b_n. The *span* of the n-step bridge ω is defined to be $\omega_1(n) - \omega_1(0)$.

It will often be convenient to write $\mathbb{Z}^d$ as $\mathbb{Z} \times \mathbb{Z}^{d-1}$, grouping the last $d - 1$ coordinates together as a single vector. Thus if $l \in \mathbb{Z}$ and $y = (y_1, \ldots, y_{d-1}) \in \mathbb{Z}^{d-1}$, we write (l, y) to denote the point $(l, y_1, \ldots, y_{d-1})$ in $\mathbb{Z}^d$. In particular, we will write

$(l, \boldsymbol{L}) = (l, L, \dots, L) \in \mathbb{Z}^d$ (in this context, $\boldsymbol{L}$ is in $\mathbb{Z}^{d-1}$). The number of n-step bridges starting at the origin and ending at $(l, y) \in \mathbb{Z}^d$ is denoted $b_{n,l}(y)$.

Notice that a walk from $\mathbf{0}$ to $\boldsymbol{L}$ that is contained in $[0, L]^d$ need not be a bridge, since it may touch the set $\{0\} \times [0, L]^{d-1}$ more than once. However, if we add a single step from $(-1, \mathbf{0})$ to the origin, then we get a bridge of span $L + 1$. Therefore

$$c_n(L) \leqslant b_{n+1,L+1}(\boldsymbol{L}) \leqslant b_{n+1} \leqslant \mu^{n+1} \tag{19}$$

(the last inequality comes from equation (1.2.17) of Madras and Slade 1993).

Lemma 4.3. Let $d \geqslant 2$ and let $\epsilon > 0$. Then there exist odd integers s and M such that $b_{s,M}(\mathbf{0}) > (\mu - \epsilon)^s$.

Proof. Since $\lim_{n\to\infty}(b_n)^{1/n} = \mu$ (corollary 3.1.6 of Madras and Slade 1993), there exists an $n > 0$ such that

$$(2n+1)^{-d} b_n > (\mu - \epsilon)^{n+1}\,.$$

Therefore there exists $(l, y) \in ([1, n] \times [-n, n]^{d-1}) \cap \mathbb{Z}^d$ such that $b_{n,l}(y) > (\mu - \epsilon)^{n+1}$. Consider the concatenation of a bridge from the origin to (l, y), followed by a single step to $(l + 1, y)$, followed by a bridge from $(l + 1, y)$ to $(2l + 1, \mathbf{0})$. We then see that

$$b_{2n+1,2l+1}(\mathbf{0}) \geqslant b_{n,l}(y) b_{n,l}(-y) = b_{n,l}(y)^2 > (\mu - \epsilon)^{2n+2}\,.$$

Setting $s = 2n + 1$ and $M = 2l + 1$ implies the result. □

Lemma 4.4. Let $\epsilon > 0$, and choose s and M as in lemma 4.3. Let j and p be positive integers with p odd. Define $N = p^{d-1}js + (2s + 1)(p^{d-1} + d - 2) + 1$ and $L = 2ps + 1$. Then the number of N-step self-avoiding walks that start at the origin, end at $(jM + 1, \boldsymbol{L})$, and lie entirely in $[0, jM + 1] \times [0, L]^{d-1}$, is at least $(\mu - \epsilon)^{p^{d-1}js}$.

Proof. For positive integers n and l, let $\mathcal{B}^s_{n,l}$ denote the set of all n-step bridges ω of span l such that $\omega(0) = \mathbf{0}$, $\omega(n) = (l, \mathbf{0})$, and $\omega(i) \in (0, l] \times (-s, s)^{d-1}$ for every $i = 1, \dots, n$. Since every s-step bridge of span l is contained in the box $[0, l] \times (-s, s)^{d-1}$, we have $b_{s,l}(\mathbf{0}) = |\mathcal{B}^s_{s,l}|$ for every $l \geqslant 1$. Also, concatenation of bridges implies that for every $j \geqslant 1$,

$$|\mathcal{B}^s_{js,jM}| \geqslant |\mathcal{B}^s_{s,M}|^j = b_{s,M}(\mathbf{0})^j > (\mu - \epsilon)^{sj} \tag{20}$$

where we have used lemma 4.3 for the last inequality.

Let j and p be positive integers with p odd. Let $\mathcal{V}(p)$ be the following set of vectors in $\mathbb{Z}^d$:

$$\mathcal{V}(p) := \{(0, v_2, \dots, v_d) : 1 \leqslant v_i \leqslant 2p - 1 \text{ and } v_i \text{ is odd}, i = 2, \dots, d\}\,.$$

Thus $\mathcal{V}(p)$ contains p^{d-1} vectors. For each vector $\boldsymbol{v} \in \mathcal{V}$, define the (translated) box

$$T[\boldsymbol{v}] := \big([0, jM] \times (-s, s)^{d-1}\big) + s\boldsymbol{v}\,.$$

Observe that the boxes $T[\boldsymbol{v}]$ are pairwise disjoint and that each is contained in the large box $[0, jM] \times [0, 2ps]^{d-1}$.

The sites of $\mathcal{V}(p)$ form a $(d - 1)$-dimensional cube, and since p is odd it is possible to order them as $\boldsymbol{v}^{(1)}, \boldsymbol{v}^{(2)}, \dots, \boldsymbol{v}^{(p^{d-1})}$ so that $\boldsymbol{v}^{(1)} = (0, \mathbf{1})$, $\boldsymbol{v}^{(p^{d-1})} = (0, \overline{2p-1})$, and $\boldsymbol{v}^{(i)}$ and $\boldsymbol{v}^{(i-1)}$ are Euclidean distance 2 apart for each i. (This may be proven by induction on d, exactly as in lemma 7.2.4(a) of Madras and Slade 1993).

Let $\omega^{(i)}$, $i = 1, \dots, p^{d-1}$, be a collection of bridges (not necessarily distinct) in $\mathcal{B}^s_{js,jM}$. Let $\psi^{(i)} = \omega^{(i)} + s\boldsymbol{v}^{(i)}$; then $\psi^{(i)}$ is a bridge which lies in the box $T[\boldsymbol{v}^{(i)}]$. We now join up these bridges by adding some additional steps, as follows. Start with $(d-1)s$ steps from $\mathbf{0}$ to $sv^{(1)}$; then $\psi^{(1)}$; then take $2s+2$ steps from $(jM,\mathbf{0})+sv^{(1)}$ to $(jM+1,\mathbf{0})+sv^{(1)}$ to $(jM+1,\mathbf{0})+sv^{(2)}$ to $(jM,\mathbf{0})+sv^{(2)}$; then the steps of $\psi^{(2)}$ in *reverse* order, ending at $sv^{(2)}$; then $2s$ steps from $v^{(2)}$ to $v^{(3)}$, then $\psi^{(3)}$, and so on. For each even i, we use $\psi^{(i)}$ in reverse order; then we take $2s$ steps (in the $x_1=0$ hyperplane) to get from $sv^{(i)}$ to $sv^{(i+1)}$; then we use $\psi^{(i+1)}$ in forward order; then we take $2s+2$ steps to get from $(jM,\mathbf{0})+sv^{(i+1)}$ to $(jM,\mathbf{0})+sv^{(i+2)}$, with all intermediate sites in the $x_1=jM+1$ hyperplane (this is because the bridges ψ may have many sites in the hyperplane $x_1=jM$, in contrast to the fact that only their initial sites can lie in the hyperplane $x_1=0$, by (18)). Finally, after the last bridge $\psi^{(p^{d-1})}$ is used (in its forward order), we take $(s+1)(d-1)+1$ steps to go from from $(jM,\mathbf{0})+sv^{(p^{d-1})}=(jM,s(2p-1),\ldots,s(2p-1))$ to $(jM+1,2ps+1,\ldots,2ps+1)=(jM+1,\boldsymbol{L})$. The result is a self-avoiding walk that starts at the origin, ends at $(jM+1,\boldsymbol{L})$, and lies entirely in $[0,jM+1]\times[0,L]^{d-1}$. The number of steps in this walk is exactly $p^{d-1}(js)+s(d-1)+(2s+2)(p^{d-1}-1)/2+2s(p^{d-1}-1)/2+(s+1)(d-1)+1$, which equals N. Finally, the construction shows that there are at least $|\mathcal{B}^s_{js,jM}|^{p^{d-1}}$ such walks, and so the lemma follows from (20). □

Proof of proposition 4.2. Fix $x>\mu^{-1}$, and choose $\epsilon>0$ such that $x(\mu-\epsilon)>1$. Let s and M be as in lemma 4.3. For any odd positive integer t, let $j=j(t)=2st$ and $p=p(t)=Mt$. Then lemma 4.4 defines

$$N=N(t)=2M^{d-1}s^2t^d+(2s+1)\big(M^{d-1}t^{d-1}+d-2\big)+1$$

and

$$L=L(t)=2sMt+1\,.$$

Noting that $L(t)=j(t)M+1$, lemma 4.4 says that

$$c_{N(t)}(L(t))\geqslant(\mu-\epsilon)^{p(t)^{d-1}j(t)s}\,. \tag{21}$$

Now, for any odd t, we have

$$C_{L(t)}(x)\geqslant c_{N(t)}(L(t))x^{N(t)}\,. \tag{22}$$

Now, raise both sides of (22) to the $1/L(t)^d$ power, and let $t\to\infty$. Since

$$\lim_{t\to\infty}\frac{L(t)^d}{t^d}=(2sM)^d$$

we see that

$$\lim_{t\to\infty}\frac{p(t)^{d-1}j(t)s}{L(t)^d}=\frac{2s^2M^{d-1}}{(2sM)^d}=\frac{2^{1-d}s^{2-d}}{M}=\lim_{t\to\infty}\frac{N(t)}{L(t)^d}\,.$$

Using these observations and (21), we conclude that

$$\liminf_{t\to\infty}C_{L(t)}(x)^{1/L(t)^d}\geqslant[(\mu-\epsilon)x]^{2^{1-d}s^{2-d}/M}>1$$

where the last inequality holds because $(\mu-\epsilon)x>1$. The existence of the limit follows from lemma 4.1, and thus the proposition is proved. □

A mass for bridges can be defined as follows. First, for $x>0$ and $(l,y)\in\mathbb{Z}^d$ with $l\geqslant0$, define the generating function

$$B_x(l,y):=\sum_{n=0}^{\infty}b_{n,l}(y)x^n\,. \tag{23}$$

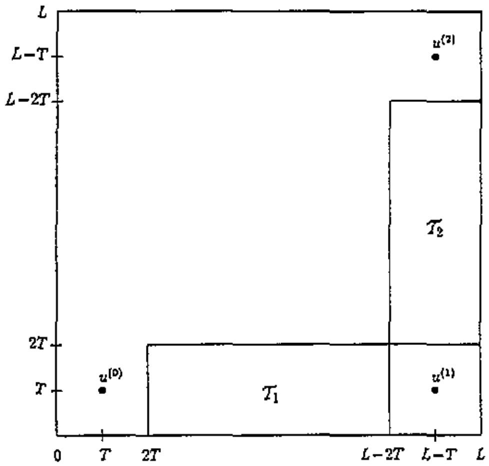

Figure 2. The rectangles $\mathcal{T}_1$ and $\mathcal{T}_2$ in the proof of proposition 4.5 ($d = 2$).

Then let

$$M(x) := \lim_{l\to\infty} \frac{-\log B_x(l, \mathbf{0})}{l}. \tag{24}$$

This limit always exists: it equals the usual mass $m(x)$ for $0 < x < \mu^{-1}$, is 0 for $x = \mu^{-1}$, and equals $-\infty$ for $x > \mu^{-1}$ (see Chayes and Chayes 1986 or section 4.1 of Madras and Slade 1993).

Proposition 4.5. For all $x > 0$, $-dM(x) \leqslant f_1(x) \leqslant -M(x)$. In particular, $f_1(\mu^{-1}) = 0$.

Proof. Equation (19) implies that $C_L(x) \leqslant x^{-1}B_x(l, \boldsymbol{L})$. Combining the second part of equation (4.1.12) with lemma 4.1.12 from Madras and Slade (1993), we see that $B_x(l, \boldsymbol{L}) \leqslant \mathrm{e}^{-LM(x)}$. It follows that $f_1(x) \leqslant -M(x)$ for all $x > 0$.

To prove the lower bound on $f_1(x)$, fix an integer $T > 0$ and let $L > 4T$. Define the sites $u^{(i)} \in \mathbb{Z}^d$, $i = 0, 1, \dots, d$, as follows. The first i coordinates of $u^{(i)}$ equal T and the remaining $d - i$ coordinates equal $L - T$. Let $e^{(i)}$, $i = 1, \dots, d$ denote the positive unit vectors of $\mathbb{Z}^d$ (i.e. the ith coordinate of $e^{(i)}$ is 1 and the other coordinates are all 0). Then $u^{(i+1)} = u^{(i)} + (L - 2T)e^{(i)}$ for every $i = 0, \dots, d - 1$. For $i = 1, \dots, d$, define the box $\mathcal{T}_i \subset [0, L]^d$ to be

$$\mathcal{T}_i := \{(y_1, \dots, y_d) \in \mathbb{Z}^d : 2T < y_i \leqslant L - 2T,\ \text{and } |y_j - u_j^{(i)}| < T \text{ for all } j \neq i\}.$$

(See figure 2 for the two-dimensional case.) Thus $\mathcal{T}_i$ is a 'square tube of radius T' and length $L - 4T$, centered along the line from $u^{(i-1)}$ to $u^{(i)}$. Also observe that the $\mathcal{T}_i$'s are pairwise disjoint.

Consider the set $\mathcal{W}_i$ of all self-avoiding walks that start at $u^{(i-1)}+Te^{(i)}$, end at $u^{(i)}-Te^{(i)}$ $(= u^{(i-1)} + (L - 3T)e^{(i)})$, and have all of their intermediate sites inside $\mathcal{T}_i$. The generating function of $\mathcal{W}_i$ is $B_x^{T-1}(L - 4T, \mathbf{0})$, using the notation of definition 4.1.10 of Madras and Slade (1993). If $\omega^{(i)}$ is a walk in $\mathcal{W}_i$ for each $i = 1, \dots, d$, then we can join these walks together as follows: for each $i = 1, \dots, d$, add T steps to go from $u^{(i-1)}$ to the beginning of $\omega^{(i)}$, and T more to go from the end of $\omega^{(i)}$ to $u^{(i)}$. Finally, add dT steps from $\mathbf{0}$ to $u^{(0)}$, and dT more steps from $u^{(d)}$ to $\boldsymbol{L}$. The result is a self-avoiding walk from $\mathbf{0}$ to $\boldsymbol{L}$ that is contained in $[0, L]^d$. Consideration of the generating function of walks that can be constructed in this way shows that

$$C_L(x) \geqslant \left[B_x^{T-1}(L - 4T, 0)\right]^d x^{4dt}$$

for all $L > 4T > 0$. Therefore

$$\frac{\log C_L(x)}{L} \geqslant \frac{L-4T}{L} \frac{d\log B_x^{T-1}(L-4T,\mathbf{0})}{L-4T} + \frac{4dT\log x}{L}. \tag{25}$$

Let $L \to \infty$ with T fixed. Then (4.1.17) of Madras and Slade (1993) yields $f_1(x) \geqslant -dM^{T-1}(x)$, where $M^{T-1}(x)$ is a 'truncated mass' for bridges restricted to a tube of radius T. Finally, lemma 4.1.11 of Madras and Slade (1993) says that $\lim_{T\to\infty} M^{T-1}(x) = M(x)$ for all $x > 0$, and so $f_1(x) \geqslant -dM(x)$. □

Proof of theorem 2.1. This all follows from lemma 4.1, proposition 4.2, and proposition 4.5. □

Proof of theorem 2.2. First consider a fixed x with $0 < x < \mu^{-1}$, and we shall prove that $\langle|\omega|\rangle_{x,L} \approx L$. Since $dL \leqslant |\omega| \leqslant L^d$ for every walk from $\mathbf{0}$ to $\boldsymbol{L}$, it suffices to show that $P_{x,L}\{|\omega| > AL\}$ decays exponentially as $L \to \infty$, for some finite A. Choose A large enough so that $(\mu x)^A < \lambda_1(x)$. Then, for any L,

$$\begin{aligned} P_{x,L}\{|\omega| \geqslant AL\} &= \sum_{n=AL}^{L^d} \frac{c_n(L)x^n}{C_L(x)} \\ &\leqslant \sum_{n=AL}^{L^d} \frac{\mu^{n+1}x^n}{C_L(x)} \qquad \text{(by equation (19))} \\ &\leqslant \frac{\mu(\mu x)^{AL}}{(1-\mu x)C_L(x)}. \end{aligned}$$

As $L \to \infty$, the $1/L$ power of the last expression tends to $(\mu x)^A/\lambda_1(x) < 1$. Thus we conclude that $\langle|\omega|\rangle_{x,L} \approx L$.

Now fix $x > \mu^{-1}$. To prove $\langle|\omega|\rangle_{x,L} \approx L^d$, it suffices to show that $P_{x,L}\{|\omega| \leqslant \delta L^d\}$ decays exponentially for some $\delta > 0$. To do this, choose δ small enough so that $(\mu x)^\delta < \lambda_2(x)$, and then argue analogously to the preceding paragraph. □

Proof of theorem 2.3. For any non-negative sequence $\{a_n : n \geqslant 0\}$, Hölder's inequality shows that $\log(\sum_n a_n e^{\beta n})$ is a convex function of β (lemma 4.1.2 of Madras and Slade 1993). Therefore $\log C_L(x)$ is a convex function of $\log x$ for every L. Since limits preserve convexity, we see that $f_1(x)$ and $f_2(x)$ are also convex functions of $\log x$. Proposition 4.5, together with the fact that $M(x) = m(x)$ for $0 < x < \mu^{-1}$, shows that $f_1(x) \approx m(x)$. The bounds $0 < f_2(x) \leqslant \log\mu + \log x$ for $x > \mu^{-1}$ follow from proposition 4.2 above and (3.15) of Whittington and Guttmann (1990).

Since $C_L(x)$ is non-decreasing in $x > 0$, so are $f_1(x)$ and $f_2(x)$. It only remains to show strict monotonicity on the appropriate intervals. Since $f_2(x)$ decreases to 0 as x decreases to μ^{-1} (by the bounds $0 < f_2(x) \leqslant \log\mu + \log x$), and since f_2 is a convex function of $\log x$, it follows that f_2 must be strictly increasing for $x > \mu^{-1}$. Similarly, $f_1(x)$ tends to $-\infty$ as x decreases to 0 (by the bound $f_1(x) \leqslant d\log(\mu x)$ from (6)). So the convexity of f_1 implies that it must be strictly decreasing. □

Proof of theorem 2.4. This proof uses the renewal theory structure of section 4.2 of Madras and Slade (1993). First, we recall that a bridge is *irreducible* if it may not be expressed as the concatenation of two smaller bridges. Let $\Lambda_x(l, y)$ denote the generating function of all irreducible bridges that start at $\mathbf{0}$ and end at $(l, y) \in \mathbb{Z}^d$. Then

$$\sum_{l=1}^{\infty} \sum_{y \in \mathbb{Z}^{d-1}} \Lambda_{\mu^{-1}}(l, y) = 1 \tag{26}$$

by (4.2.4) of Madras and Slade (1993). Let $X_1, X_2, \ldots$ be a sequence of independent $\mathbb{Z}^d$-valued random vectors with the common distribution

$$\Pr\{X_i = (l, y)\} = \Lambda_{\mu^{-1}}(l, y) \qquad \text{for every } i. \tag{27}$$

Then, arguing as for (4.2.28) of Madras and Slade (1993), we obtain

$$B_{\mu^{-1}}(l, y) = \Pr\{X_1 + \cdots + X_k = (l, y) \text{ for some } k \geqslant 1\}. \tag{28}$$

Now, the random walk $X_1 + \cdots + X_k$ is clearly transient (since the first coordinate of every X_i is strictly positive). Then proposition 25.3 of Spitzer (1976) tells us that $B_{\mu^{-1}}(l, y)$ tends to 0 as $|(l, y)|$ tends to infinity. In particular,

$$\lim_{L \to \infty} B_{\mu^{-1}}(L + 1, L) = 0. \tag{29}$$

Since $C_L(\mu^{-1}) \leqslant \mu B_{\mu^{-1}}(L + 1, L)$ (by the first inequality of (19)), equation (29) implies that $C_L(\mu^{-1})$ tends to 0 as $L \to \infty$. □

Proof of theorem 3.1. Existence of the limit follows as in lemma 4.1, and the proof that $0 < \lambda_1^a(x) < 1$ for $0 < x < \mu_a^{-1}$ is just like in (5) and (6). For $x > \mu_a^{-1}$, the proof that $\lambda_2^a(x) > 1$ also looks the same: for $n \geqslant 1$, $l \geqslant 1$, and $y \in \mathbb{Z}^{d-1}$, let $a_{n,l}(y)$ be the number of animals that contain the two sites $\mathbf{0}$ and (l, y), and are entirely contained in the set $\{x \in \mathbb{Z}^d : 0 < x_1 \leqslant l\}$. Then, as in lemma 4.3, for any $\epsilon > 0$ there exist odd positive integers s and M such that $a_{s,M}(\mathbf{0}) > (\mu - \epsilon)^s$. The proofs of lemma 4.4 and proposition 4.2 now proceed essentially unchanged. Finally, everything works for trees as well as for animals. □

We now present the final ingredient in the proof of theorem 3.3.

Proposition 4.6. For $x > \mu^{-1}$,

$$\liminf_{L \to \infty} \tilde{C}_L(x)^{1/(2L)^d} \geqslant \lambda_2(x). \tag{30}$$

Proof. We begin by proving the inequality

$$\tilde{C}_{L+2}(x) \geqslant x^{O(2^d L)} C_L(x)^{2^d} \tag{31}$$

for every L. Let $v^{[1]} \ldots, v^{[2^d]}$ be the corners of the cube $[-1, 1]^d$, listed so that $v^{[i]}$ and $v^{[i+1]}$ are distance 2 apart for each $i = 1, \ldots, 2^d - 1$. (This is possible; e.g. see lemma 7.2.4(a) of Madras and Slade (1993) with $b = 1$ in the proof.) For each $i = 1, \ldots, 2^d$, let ω_i be a self-avoiding walk from $v^{[i]}$ to $(L + 1)v^{[i]}$ which is contained in the cube of side L that has $v^{[i]}$ and $(L + 1)v^{[i]}$ as opposite corners. (So the ω_i's are disjoint and all lie in $[-L - 1, L + 1]^d$.) Notice that $(L + 1)v^{[i]}$ and $(L + 1)v^{[i+1]}$ differ in a single coordinate, and so the distance between them is exactly $2L + 2$.

Now we join up the ω_i's to make a big self-avoiding walk ξ that starts at the origin and is contained in the cube $[-L - 2, L + 2]^d$. The procedure is the following: join the origin to the first site of ω_1 (d steps); join the last site of ω_1 to the last site of ω_2 ($2L + 4$ steps: one step to get to a boundary face of $[-L - 2, L + 2]^d$, then $2L + 2$ steps in a straight line in that face, then one more step); join the first site of ω_2 to the first site of

ω_3 (two steps); and so on. The resulting walk ξ is made up of the ω_i's and an additional $d + 2^{d-1}(2L+4) + (2^{d-1}-1)2$ steps. The generating function of such animals is less than $C_{L+2}(x)$ and is greater than $x^{2^d(L+3)+d-2}C_L(x)^{2^d}$. This proves (31).

The result now follows from (31) and the definition of $\lambda_2(x)$ (equation (4)). □

Proof of theorem 3.4. We shall give the proof for animals; the same method applies to trees. First, we note that the proof of proposition 4.6 applies equally well to animals (or trees), and so

$$\liminf_{L\to\infty} \tilde{A}_L(x)^{1/(2L)^d} \geqslant \lambda_2^a(x)\,. \tag{32}$$

To prove the reverse inequality for the lim sup, we shall use the inequality

$$\tilde{a}_n(L) \leqslant \sum_{j=0}^{2dL} a_{n+j}(2L) \tag{33}$$

which is proven as follows. Let σ be an animal with n bonds that contains $\mathbf{0}$ and is contained in $[-L, L]^d$. Then it is possible to add at most $2dL$ bonds to σ and obtain an animal σ' that contains $-\boldsymbol{L}$ and $\boldsymbol{L}$, and is contained in $[-L, L]^d$. (In detail: fix a $2dL$-step self-avoiding walk ω that starts at $-\boldsymbol{L}$, ends at $\boldsymbol{L}$, and passes through $\mathbf{0}$. Let v_f (respectively, v_l) be the first (respectively, last) site of σ that occurs on ω. Let σ' be the union of σ, the part of ω between $-\boldsymbol{L}$ and v_f, and the part of ω between v_l and $\boldsymbol{L}$.) The inequality (33) follows from this. In terms of generating functions, (33) implies

$$\tilde{A}_L(x) \leqslant \sum_{j=0}^{2dL} A_{2L}(x)x^{-j} \leqslant (2dL+1)\max\{1, x^{2dL}\}A_{2L}(x)\,. \tag{34}$$

It is now evident that

$$\limsup_{L\to\infty} \tilde{A}_L(x)^{1/(2L)^d} \leqslant \lambda_2^a(x)\,. \tag{35}$$

Combining (32) and (35) proves the theorem. □

5. Discussion

We have proved that the ensemble of walks crossing a square (or more generally a d-dimensional hypercube) exhibits a transition from linear ($\langle|\omega|\rangle_{x,L} \approx L$) to dense ($\langle|\omega|\rangle_{x,L} \approx L^d$) behaviour at $x = \mu^{-1}$, where μ is the connective constant for self-avoiding walks in $\mathbb{Z}^d$. This confirms a conjecture of Whittington and Guttmann (1990) for the two-dimensional case, and it also rules out any intermediate transitions (such as a range of x over which $\langle|\omega|\rangle_{x,L} \approx L^2$ in $d = 3$). We also prove a corresponding result for walks with free endpoints in a cube, as well as similar results for lattice animals and lattice trees. We also investigated the scaling of the limiting free energy as x increases to μ^{-1}, concluding that $f_1(x) \approx (\mu^{-1} - x)^\nu$ (assuming that the exponent ν governs the decay of the mass of self-avoiding walks in $\mathbb{Z}^d$). Analogues of these results have previously been proved rigorously for the Sierpinski gasket by Hattori *et al* (1990).

The methods and results of the present paper also confirm part of the analysis of Živić, Milošević and Stanley (1993) concerning a certain fractal-to-Euclidean crossover. They considered a family of (discrete) fractals which consist of $b \times b$ blocks of $\mathbb{Z}^2$ which are joined to other blocks only at two opposite corners. Their generating function for the number of self-avoiding walks, $C_b^{\mathrm{ZMS}}(x)$, clearly lies between our $C_b(x)$ and the ordinary susceptibility $\chi(z)$ for $\mathbb{Z}^2$ (see equation (15)). So our theorem 2.1(ii) shows that the critical fugacity x_b^* of $C_b^{\mathrm{ZMS}}(x)$ converges to μ^{-1} as $b \to \infty$ (see table 2 and footnote [23] in Živić *et al* (1993)). (We remark that the squares in Živić *et al* (1993) are rotated by 45°, but that does not affect our methods.)

Two questions regarding the dense phase ($x > \mu^{-1}$) were left conspicuously unanswered in the present paper, namely, can we say anything rigorous about the belief that the limiting free energy f_2 behaves as $(x - \mu^{-1})^{d\nu}$ as x decreases to μ^{-1}? And can we prove the existence of the limiting free energy for dense walks with free endpoints? These appear to be hard questions which deal directly with detailed properties of dense walks.

There is one more intriguing question about the dense phase: can we prove the existence of a limiting *probability distribution* for any of the ensembles described in this paper, for any $x > \mu^{-1}$? This would give a natural measure on a class of *infinite, dense* polymers. We believe that this would be easier for animals or trees than for walks. For one very special case, this has actually been accomplished by Pemantle (1991): he considered uniformly distributed spanning trees of $[-L, L]^d$, corresponding to $x = +\infty$ in our tree models. Pemantle showed that these distributions have a weak limit as $L \to \infty$, but the limiting objects are trees only for $d \leqslant 4$; for $d \geqslant 5$, they are *disconnected*, so the limiting distribution is actually on spanning forests of $\mathbb{Z}^d$. We do not know whether this surprising fact has any analogue when $\mu^{-1} < x < +\infty$, or whether something similar happens for walks or animals.

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