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Contacts in self-avoiding walks and polygons

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Abstract

We prove several results concerning the numbers of n-edge self-avoiding polygons and walks in the lattice Z^d which had previously been conjectured on the basis of numerical results. If the number of n-edge self-avoiding polygons (walks) with k contacts is $p_n(k)$ $(c_n(k))$ then we prove that $\kappa_0 \equiv \lim_{n\to\infty} n^{-1} \log p_n(k) = \lim_{n\to\infty} n^{-1} \log c_n(k)$ exists for all fixed k and is independent of k. For polygons in Z^2, we prove that there exist two positive functions B_1 and B_2, independent of n but depending on k, such that $B_1 n^k p_n(0) \leqslant p_n(k) \leqslant B_2 n^k p_n(0)$ for fixed k and n large. Also, provided the limit exists, we prove that $0 < \lim_{n\to\infty} \langle k \rangle_n / n < 1$.

In addition, we consider the number of polygons with a density of contacts, i.e. $k = \alpha n$, and show that the corresponding connective constant, $\kappa(\alpha)$, exists and is a concave function of α. For $d = 2$, we prove that $\lim_{\alpha\to 0^+} \kappa(\alpha) = \kappa_0$ and the right derivative of $\kappa(\alpha)$ at $\alpha = 0$ is infinite.

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1. Introduction

Self-avoiding walks are the standard model for the configurational properties of polymers in good solvents [1]. Solvent quality can be modelled by incorporating a short-range vertex–vertex interaction into the self-avoiding walk model and this model has been used to study the collapse of linear polymers from an expanded open coil state to a compact state. Although there is a substantial amount of numerical work on this problem, including Monte Carlo methods, exact enumeration and series analysis, and transfer-matrix methods, there is no proof of the existence of a collapse transition in the model. That is, there is no proof that the limiting free energy has a singularity.

For a self-avoiding walk on a hypercubic lattice Z^d, label the vertices $i = 0, 1, 2, \ldots, n$ and write the coordinates of the ith vertex as r_i. Then if two vertices i and j, $|i - j| > 1$, are such that $|r_i - r_j| = 1$ then these vertices form a *contact*. Let $c_n(k)$ be the number of self-avoiding walks with n edges and k contacts, where two walks are considered the same if they can be superimposed by translation. Define the partition function

$$Z_n(\beta) = \sum_k c_n(k)\mathrm{e}^{\beta k}. \tag{1.1}$$

One expects that the limit

$$\lim_{n\to\infty} n^{-1} \log Z_n(\beta) \equiv \mathcal{F}(\beta) < \infty \tag{1.2}$$

will exist and $\mathcal{F}(\beta)$ will be singular at some $\beta = \beta_c$ corresponding to the location of the collapse transition. The existence of the limit has been proved only for $\beta \leqslant 0$ [2–4]. One possible route for proving that the limit in equation (1.2) exists for $\beta > 0$, and investigating the properties of $\mathcal{F}(\beta)$, might be to understand better the properties of $c_n(k)$.

Recently, Douglas and Ishinabe [5] and Douglas *et al* [6] have used a mixture of exact enumeration and Monte Carlo methods to investigate the properties of $c_n(k)$ on Z^d. Their evidence suggests that:

(a) the limits $\lim_{n\to\infty} n^{-1} \log c_n(k)$ exist for each fixed value of k, and they are equal to a real number $\kappa_0 > 0$, independent of k;
(b) $c_n(k) \sim A_k n^k c_n(0)$;
(c) there exists a constant $a > 0$ such that the average number of contacts for self-avoiding walks of length n is given by $\langle k\rangle_n \sim an$. Note that if this limit exists, $\lim_{n\to\infty} n^{-1} \frac{\partial \log Z_n(\beta)}{\partial\beta}\Big|_{\beta=0} = a$.

In this paper we prove some results relevant to items (a)–(c) above. In fact, most of our results will be for self-avoiding polygons with k contacts, though one would expect similar behaviour for walks and polygons. The advantage of focusing on self-avoiding polygons is that concatenation arguments have been used to prove that the limiting free energy analogous to equation (1.2)

$$\lim_{n\to\infty} n^{-1} \log Z_n^0(\beta) \equiv \mathcal{F}_0(\beta) < \infty \tag{1.3}$$

exists and is a convex function of β [2,3]. Here $Z_n^0(\beta)$ is the partition function for self-avoiding polygons, i.e.

$$Z_n^0(\beta) = \sum_k p_n(k)\mathrm{e}^{\beta k} \tag{1.4}$$

where $p_n(k)$ is the number of self-avoiding polygons with n edges and k contacts. In fact, it is known that $\mathcal{F}(\beta) = \mathcal{F}_0(\beta)$ for $\beta \leqslant 0$ [3] and this is believed [3, 4] to be true for all finite β though no proof exists for $\beta > 0$. In this paper, methods previously developed for studying $Z_n(\beta)$ and $Z_n^0(\beta)$ are modified for studying $c_n(0)$ and $p_n(0)$, the number of *neighbour-avoiding* walks and polygons, respectively. From these results, we prove pattern theorems for neighbour-avoiding walks and polygons for arbitrary dimensions and prove that $\lim_{n\to\infty} n^{-1} \log c_n(k) = \lim_{n\to\infty} n^{-1} \log p_n(k) = \kappa_0$ exists and is independent of k for fixed k, which is (a), above. For polygons on the square lattice ($d = 2$) we establish a bound of the form $p_n(k) \leqslant A_k \binom{\alpha n}{k} p_n(0)$ by developing an algorithm for removing contacts from a polygon. This, combined with the pattern theorem results, allows us to prove for $d = 2$ that

$$\lim_{n\to\infty} \frac{\log[p_n(k)/p_n(0)]}{\log n} = k \tag{1.5}$$

which establishes the n^k term in the analogue of (b). Related to (c), provided that $\mathcal{F}_0(\beta)$ is differentiable at $\beta = 0$ we show for $d = 2$ that $\langle k\rangle_n \sim an$ for polygons, with $0 < a < 1$.

If the derivative does not exist we prove a slightly weaker result. Other consequences of the $d = 2$ results are that $\lim_{\beta\to-\infty} \mathcal{F}_0(\beta) = \kappa_0$ and that for polygons with $k = \mathrm{o}(n)$ contacts $\lim_{n\to\infty;k=\mathrm{o}(n)} n^{-1} \log p_n(k) = \kappa_0$. The results related to (a) and (b) are presented in section 2, those related to (c) are presented in section 3, and in section 4 results about polygons with a fixed density of contacts are presented.

2. Walks and polygons with a fixed number of contacts

An n-step self-avoiding walk (or n-SAW) beginning at a lattice point r_0 consists of an $(n+1)$-tuple of distinct lattice points $(r_0, r_1, \ldots, r_n)$, where r_i and r_{i+1} are adjacent in the lattice, and n steps (directed edges) joining the ith to the $(i + 1)$th lattice points (vertices), $0 \leqslant i < n$. Let c_n be the number of distinct n-SAWs on Z^d where two n-SAWs are distinct if they cannot be superimposed by translation. An n-step self-avoiding circuit (n-SAC) is an $n - 1$ step self-avoiding walk (SAW) whose first and last vertices are unit distance apart, and are joined by a step going from the nth to the zeroth vertex. Any cyclic permutation of the vertices of an n-SAC is also an n-SAC. So too is the reverse permutation and all cyclic permutations of this reverse permutation. The resulting set of $2n$ n-SACs that originate from any given n-SAC can be regarded as a single geometrical entity, which we call an n-edge self-avoiding polygon (or n-SAP). Two n-SAPs are equivalent if one is a translate of the other. We write p_n for the number of inequivalent n-SAPs and $p_n(k)$ for the number of n-SAPs with k contacts. Hammersley [7] showed (see also [1]) that

$$0 < \lim_{n\to\infty} n^{-1} \log c_n = \lim_{n\to\infty} n^{-1} \log p_n \equiv \kappa < \log(2d - 1) \tag{2.1}$$

where the second limit is taken through even values of n, so that the numbers of walks and polygons increase exponentially with their length, at the same exponential rate.

A *neighbour-avoiding walk* is a self-avoiding walk with no contacts so that the number of n-step neighbour-avoiding walks is given by $C_n = c_n(0)$. Similarly, the number of neighbour-avoiding polygons is $P_n = p_n(0)$. We first prove a lemma about P_n and C_n which shows that the limit in (a) exists for $k = 0$. The arguments used are analogous to those used in [1] to prove equation (2.1). However, the concatenation needed must be modified to take into account the fact that no contacts can be formed.

Lemma 1. *There exists a positive constant κ_0 such that*

$$\lim_{n\to\infty} n^{-1} \log C_n = \lim_{n\to\infty} n^{-1} \log P_n \equiv \kappa_0 < \kappa. \tag{2.2}$$

Proof. First note that $C_n \geqslant \mathrm{d}^n$, which we obtain by considering walks which can only go in the positive coordinate directions. Then, since any neighbour-avoiding walk can be decomposed into a pair of neighbour-avoiding walks, we have the inequality

$$C_{n+m} \leqslant C_n C_m. \tag{2.3}$$

Similarly, a pair of neighbour-avoiding polygons can be concatenated to form a neighbour-avoiding polygon (the details of this concatenation are given below) so that

$$P_n P_m \leqslant P_{n+m+24}. \tag{2.4}$$

Standard subadditivity arguments [8–10] can be used to show that the required limits each exist and the arguments which lead to theorem 3.2.4 and corollary 3.2.5 of Madras and Slade [1] can be adapted to prove that the limits are equal. The final inequality in equation (2.2) follows from a pattern theorem argument for the class of all self-avoiding walks [11], since all except exponentially few sufficiently long self-avoiding walks contain the pattern $u_1u_2\bar{u}_1$ which contains a contact. Here u_i denotes the ith unit vector in Z^d and $\bar{u}_i = -u_i$. A sequence of unit vectors should be viewed as a sequence of steps in a self-avoiding walk.

The details of the concatenation of polygons needed for the above argument are given next. We suppose we have two neighbour-avoiding polygons, P_1 and P_2, and define the top vertex of P_1 to be v_t and the bottom vertex of P_2 to be v_b (the top and bottom vertex are defined, respectively, as the last and first vertex of the polygon in a lexicographic ordering of the polygon's vertices according to their coordinates). Let $V(P_1)$ and $V(P_2)$ represent the vertex sets of P_1 and P_2, respectively, and suppose $n = |V(P_1)|$ and $m = |V(P_2)|$. Fix the unique integer pair i_1, j_1 such that $1 \leqslant i_1 < j_1 \leqslant d$ and $v_t - u_{i_1}, v_t - u_{j_1} \in V(P_1)$ and the unique integer pair i_2, j_2 such that $1 \leqslant i_2 < j_2 \leqslant d$ and $v_b + u_{i_2}, v_b + u_{j_2} \in V(P_2)$.

If $d = 2$, then $i_1 = 1$, $j_1 = 2$, and $v_t - 2u_2 \in V(P_1)$ and similarly $i_2 = 1$, $j_2 = 2$, and $v_b + 2u_2 \in V(P_2)$. In this case, translate P_2 so that $v_b = v_t - 2u_2 + 2u_1$, add the two edges between v_t and $v_t + 2u_1$, and the two edges between $v_t - 2u_2$ and v_b, and then delete the two edges between v_t and $v_t - 2u_2$, and the two edges between v_b and $v_b + 2u_2$. The result is a new neighbour-avoiding polygon with $n + m$ edges. Hence for $d = 2$,

$$P_n P_m \leqslant P_{n+m}. \tag{2.5}$$

Note also that if instead we concatenate P_1 and P_2 by first translating P_2 so that $v_b = v_t - 2u_2 + (2 + k)u_1$, then adding the $(2 + k)$ edges between v_t and $v_t + (2 + k)u_1$, and the $(2 + k)$ edges between $v_t - 2u_2$ and v_b, and finally deleting the two edges between v_t and $v_t - 2u_2$, and the two edges between v_b and $v_b + 2u_2$, the result is a new neighbour-avoiding polygon with $n + m + 2k$ edges.

If $d > 2$, we convert, by a suitable concatenation argument, P_1 and P_2 into two new polygons $\tilde{P}_1$ and $\tilde{P}_2$ with no contacts such that for $\tilde{P}_1$, $i_1 = 1$, $j_1 = 2$, and $v_t - 2u_2 \in V(\tilde{P}_1)$, and for $\tilde{P}_2$, $i_2 = 1$, $j_2 = 2$, and $v_b + 2u_2 \in V(\tilde{P}_2)$. Then the concatenation just described for $d = 2$ can again be used to concatenate $\tilde{P}_1$ and $\tilde{P}_2$. The suitable concatenation argument needed to convert P_1 to $\tilde{P}_1$ is described next; the argument for converting P_2 to $\tilde{P}_2$ is essentially the same, except with v_t replaced by v_b, i_1, j_1 replaced by i_2, j_2 and with minus signs replaced by plus signs as appropriate.

The appropriate concatenation to convert P_1 to $\tilde{P}_1$ depends on the value of i_1. This results initially in three cases: $i_1 > 2$, $i_1 = 2$, $i_1 = 1$.

For $i_1 > 2$, add two edges from $v_t - u_{i_1}$ to $v_t - u_{i_1} + 2u_1$, one edge from $v_t - u_{i_1} + 2u_1$ to $v_t - u_{i_1} + 2u_1 - u_2$, one edge from $v_t - u_{i_1} + 2u_1 - u_2$ to $v_t + 2u_1 - u_2$, one edge from $v_t + 2u_1 - u_2$ to $v_t + 2u_1 - 2u_2$, and two edges from $v_t + 2u_1 - 2u_2$ to $v_t + 4u_1 - 2u_2$. Then add three edges from $v_t - u_{j_1}$ to $v_t - u_{j_1} + 3u_1$, one edge from $v_t - u_{j_1} + 3u_1$ to $v_t + 3u_1$, one edge from $v_t + 3u_1$ to $v_t + 4u_1$, and two edges from $v_t + 4u_1 - 2u_2$ to $v_t + 4u_1$. Delete one edge from v_t to $v_t - u_{i_1}$ and one edge from v_t to $v_t - u_{j_1}$. If P_1 had n edges to begin with then the resulting $\tilde{P}_1$ has $n + 12$ edges.

For $i_1 = 2$, add two edges from $v_t - u_2$ to $v_t - u_2 + 2u_1$, one edge from $v_t - u_2 + 2u_1$ to $v_t - 2u_2 + 2u_1$ and four edges from $v_t - 2u_2 + 2u_1$ to $v_t - 2u_2 + 6u_1$. Then add three edges from $v_t - u_{j_1}$ to $v_t - u_{j_1} + 3u_1$, one edge from $v_t - u_{j_1} + 3u_1$ to $v_t + 3u_1$, three edges from $v_t + 3u_1$ to $v_t + 6u_1$, and two edges from $v_t + 6u_1 - 2u_2$ to $v_t + 6u_1$. Delete one edge from v_t to $v_t - u_2$ and one edge from v_t to $v_t - u_{j_1}$. If P_1 had n edges to begin with then the resulting $\tilde{P}_1$ has $n + 12$ edges.

For $i_1 = 1$, there exists a unique $\delta \in \{-1, 1\}$ and unique $j \in \{1, 2, \ldots, d\}$ such that $v_t - u_{j_1} + \delta u_j \in V(P_1)$ with $\delta u_j \neq -u_{j_1}, u_1$ and if $\delta = 1$, $j > j_1$. Let $i_1' = \min\{j_1, j\}$. Here we obtain two subcases: $i_1' > 2$ and $i_1' = 2$.

For $i_1 = 1$ and $i_1' > 2$, add two edges from $v_t - u_{j_1} + \delta u_j$ to $v_t - u_{j_1} + \delta u_j + 2u_1$, two edges from $v_t - u_{j_1} + \delta u_j + 2u_1$ to $v_t - u_{j_1} + \delta u_j + 2u_1 - 2u_2$, one edge from $v_t - u_{j_1} + \delta u_j + 2u_1 - 2u_2$ to $v_t - u_{j_1} + 2u_1 - 2u_2$, one edge from $v_t - u_{j_1} + 2u_1 - 2u_2$ to $v_t - u_{j_1} + 3u_1 - 2u_2$, one edge from $v_t - u_{j_1} + 3u_1 - 2u_2$ to $v_t + 3u_1 - 2u_2$, and one edge from $v_t + 3u_1 - 2u_2$ to $v_t + 4u_1 - 2u_2$. Then add four edges from v_t to $v_t + 4u_1$ and two edges from $v_t + 4u_1 - 2u_2$ to $v_t + 4u_1$. Delete one edge from v_t to $v_t - u_{j_1}$ and one edge from $v_t - u_{j_1}$ to $v_t - u_{j_1} + \delta u_j$. If P_1 had n edges to begin with then the resulting $\tilde{P}_1$ has $n + 12$ edges.

For $i_1 = 1$ and $i_1' = 2$, then either $j = j_1 = 2$ or $j \neq j_1$. For $i_1 = 1$, $i_1' = 2$ and $j = j_1 = 2$, P_1 is already in the prescribed form. For $i_1 = 1$, $i_1' = 2$ and $j \neq j_1$, define j' and δ' such that $v_t - u_2 + \delta' u_{j'} = v_t - u_{j_1} + \delta u_j$. Add two edges from $v_t - u_2 + \delta' u_{j'}$ to $v_t - u_2 + \delta' u_{j'} + 2u_1$, one edge from $v_t - u_2 + \delta' u_{j'} + 2u_1$ to $v_t - 2u_2 + \delta' u_{j'} + 2u_1$, two edges from $v_t - 2u_2 + \delta' u_{j'} + 2u_1$ to $v_t - 2u_2 + \delta' u_{j'} + 4u_1$, one edge from $v_t - 2u_2 + \delta' u_{j'} + 4u_1$ to $v_t - 2u_2 + 4u_1$, and one edge from $v_t + 4u_1 - 2u_2$ to $v_t + 5u_1 - 2u_2$. Then add five edges from v_t to $v_t + 5u_1$ and two edges from $v_t + 5u_1 - 2u_2$ to $v_t + 5u_1$. Delete one edge from v_t to $v_t - u_{j_1}$ and one edge from $v_t - u_{j_1}$ to $v_t - u_{j_1} + \delta u_j$. If P_1 had n edges to begin with then the resulting $\tilde{P}_1$ has $n + 12$ edges.

In all the above cases the resulting $\tilde{P}_1$ has at most $n+12$ edges and similarly the resulting $\tilde{P}_2$ will have at most $m+12$ edges. Hence for all $d \geqslant 2$, we can always obtain a neighbour-avoiding polygon with $n + m + 24$ edges. □

Recall that any n-step walk in Z^d is represented by an n-tuple $(r_0, r_1, \ldots, r_n)$. For $i = 0, \ldots, n$, denote the coordinates of r_i by $(x_i, y_i, \ldots, z_i)$. We say that an n-edge neighbour-avoiding walk is *x-unfolded* if $x_0 < x_i < x_n$ for all $i \neq 0, n$. We write B_n for the number of n-edge x-unfolded neighbour-avoiding walks. Since every x-unfolded neighbour-avoiding walk is a neighbour-avoiding walk we have $B_n \leqslant C_n$. Every neighbour-avoiding walk can be converted into an x-unfolded neighbour-avoiding walk by successive reflections of subwalks in left-most and right-most planes (see Hammersley and Welsh [12] for details). This operation does not define a bijection but an argument similar to that given by Hammersley and Welsh [12] establishes that

$$C_n \leqslant B_n \mathrm{e}^{\mathrm{O}(\sqrt{n})}. \tag{2.6}$$

These two inequalities show that

$$\lim_{n\to\infty} n^{-1} \log B_n = \kappa_0. \tag{2.7}$$

The importance of this result is that the numbers of walks and unfolded walks are the same to exponential order, and it is easier to work with these unfolded walks. Define the generating function $\mathcal{B}(z) = \sum_{n>0} B_n z^n$. Equation (2.7) shows that $\mathcal{B}(z)$ converges when $z < z_0 = \mathrm{e}^{-\kappa_0}$ and diverges when $z > z_0$. An argument similar to that used by Kesten [11] in the proof of his theorem 5 shows that $\mathcal{B}(z)$ also diverges at $z = z_0$.

An x-unfolded walk has a *cutting plane* $x = a$, $a \in Z$, if exactly one vertex of the walk is in the plane $x = a$ and if subdividing the walk at this vertex yields two x-unfolded subwalks. An x-unfolded walk is *prime* if it does not contain a cutting plane.

We next prove a pattern theorem for neighbour-avoiding walks. Let W be a *prime pattern*, i.e. a fixed x-unfolded neighbour-avoiding walk which is prime. Let $C_n(\bar{W})$ be the number of n-step neighbour-avoiding walks in which a translate of W never occurs as a subwalk. The existence of the limit $\lim_{n\to\infty} n^{-1} \log C_n(\bar{W})$ follows by a standard concatenation argument upon noticing that subdividing any walk not containing W cannot create W in either of the subwalks.

Theorem 1. *For W a prime pattern, $C_n(\bar{W})$ satisfies the inequality*

$$\lim_{n\to\infty} n^{-1}\log C_n(\bar{W}) < \kappa_0. \tag{2.8}$$

Proof. The method of proof used here is based on an unpublished proof of the pattern theorem for self-avoiding walks due to Hammersley [13].

We write Q_n for the number of n-edge prime walks. An x-unfolded walk can be decomposed into its *prime components* by successive cuts at the cutting planes $x = a_1$, $x = a_2, \ldots$ with $a_1 < a_2 < \cdots$. By cutting at the first possible cutting plane we obtain the generalized renewal equation

$$B_n = Q_n + \sum_k B_k Q_{n-k}. \tag{2.9}$$

Defining the generating function

$$\mathcal{Q}(z) = \sum_{n>0} Q_n z^n \tag{2.10}$$

we can obtain an equation connecting $\mathcal{Q}(z)$ and $\mathcal{B}(z)$ by multiplying both sides of (2.9) by z^n and summing over n. This gives

$$\mathcal{B}(z) = \frac{\mathcal{Q}(z)}{1-\mathcal{Q}(z)}. \tag{2.11}$$

Consequently, the point $z = z_0$ is determined by the solution (on the positive real axis, closest to the origin) of the equation

$$\mathcal{Q}(z) = 1. \tag{2.12}$$

We define the numbers of x-unfolded neighbour-avoiding n-edge walks, and prime n-edge walks, which do not contain a translate of the prime pattern W, to be $B_n(\bar{W})$ and $Q_n(\bar{W})$ respectively, and their generating functions as

$$\mathcal{B}(z,\bar{W}) = \sum_n B_n(\bar{W}) z^n \tag{2.13}$$

and

$$\mathcal{Q}(z,\bar{W}) = \sum_n Q_n(\bar{W}) z^n. \tag{2.14}$$

For any prime pattern W such that $B_n(\bar{W}) > 0$ for some $n > 0$, concatenating the end of an m-step x-unfolded walk which does not contain W to the start of an n-step x-unfolded walk which does not contain W does not create any occurrences of W (since it is prime) and hence creates an $(n+m)$-step x-unfolded walk which does not contain W. This concatenation argument thus leads to the existence of the limit

$$\lim_{n\to\infty} n^{-1}\log B_n(\bar{W}) = \kappa_0(\bar{W}) \tag{2.15}$$

and the inequality $\kappa_0(\bar{W}) \leqslant \kappa_0$ follows by inclusion. $\mathcal{B}(z,\bar{W})$ converges when $z < z_0(\bar{W}) = \mathrm{e}^{-\kappa_0(\bar{W})}$ and diverges when $z > z_0(\bar{W})$. Clearly, $z_0(\bar{W}) \geqslant z_0$. An argument similar to that of Kesten [11], see also Janse van Rensburg *et al* [14], shows that $\mathcal{B}(z,\bar{W})$ also diverges at $z_0(\bar{W})$. We can derive a generalized renewal equation relating $\mathcal{B}(z,\bar{W})$ and $\mathcal{Q}(z,\bar{W})$, giving

$$\mathcal{B}(z,\bar{W}) = \frac{\mathcal{Q}(z,\bar{W})}{1-\mathcal{Q}(z,\bar{W})}. \tag{2.16}$$

$z_0(\bar{W})$ is the solution of the equation $\mathcal{Q}(z, \bar{W}) = 1$. Since there is at least one prime walk which contains the prime pattern W (e.g. the pattern W itself), we have the inequality $\mathcal{Q}(z, \bar{W}) < \mathcal{Q}(z)$ for $z > 0$ and therefore $\mathcal{Q}(z_0) < 1$ which shows that $z_0 < z_0(\bar{W})$. Therefore, $\kappa_0(\bar{W}) < \kappa_0$. Again, using arguments similar to those of Kesten [11] in the proof of his theorem 5, one can show that

$$\mathcal{B}(z, \bar{W}) \leqslant \mathcal{C}(z, \bar{W}) \leqslant \frac{e^{2\mathcal{B}(z,\bar{W})}}{z} \tag{2.17}$$

where

$$\mathcal{C}(z, \bar{W}) = \sum_n C_n(\bar{W}) z^n. \tag{2.18}$$

This shows that $\mathcal{C}(z, \bar{W})$ diverges at the same point as $\mathcal{B}(z, \bar{W})$, i.e. at $z = e^{\kappa_0(\bar{W})}$, which completes the proof. □

Define W to be a K*-pattern* if W is a finite neighbour-avoiding walk which can appear at least three times on at least one sufficiently long neighbour-avoiding walk.

Theorem 2. *Let W be a K-pattern and $C_n(\bar{W})$ be the number of n-edge neighbour-avoiding walks in which a translate of W never occurs. Then $C_n(\bar{W})$ satisfies the inequality*

$$\lim_{n\to\infty} n^{-1} \log C_n(\bar{W}) < \kappa_0. \tag{2.19}$$

Proof. By adding edges any K-pattern can be converted into a prime pattern, so that to each K-pattern W there exists a prime pattern $W^{\dagger}$ which contains W as a subwalk. Thus $C_n(\bar{W}) \leqslant C_n(\bar{W}^{\dagger})$ and the theorem follows as a corollary to theorem 1. □

Let $\tilde{W}$ be the undirected neighbour-avoiding walk associated with K-pattern W. Let $P_n(\bar{W})$ be the number of n-step neighbour-avoiding polygons in which a translate of $\tilde{W}$ never occurs.

Theorem 3. *$P_n(\bar{W})$ satisfies the inequality*

$$\limsup_{n\to\infty} n^{-1} \log P_n(\bar{W}) < \kappa_0. \tag{2.20}$$

Proof. Deleting two consecutive edges and orienting the remaining edges converts an n edge neighbour-avoiding polygon into an $(n-2)$-step neighbour-avoiding walk. Since deleting an edge from a polygon which does not contain a translate of $\tilde{W}$ cannot create the K-pattern W in the resulting walk, we have the inequality

$$P_n(\bar{W}) \leqslant C_{n-2}(\bar{W}). \tag{2.21}$$

Equation (2.20) follows from equations (2.19) and (2.21). □

Let $C_n(\epsilon, W)$ be the number of n-step neighbour-avoiding walks in which at most $\lfloor \epsilon n \rfloor$ translates of W occur. Let $P_n(\epsilon, W)$ be the number of n-step neighbour-avoiding polygons in which at most $\lfloor \epsilon n \rfloor$ translates of $\tilde{W}$ occur.

Theorem 4. *For every K-pattern W there exists $\epsilon > 0$ such that*

$$\limsup_{n\to\infty} n^{-1} \log C_n(\epsilon, W) < \kappa_0 \tag{2.22}$$

and

$$\limsup_{n\to\infty} n^{-1} \log P_n(\epsilon, W) < \kappa_0. \tag{2.23}$$

Proof. Equation (2.22) follows from an argument similar to that of lemma 7.2.5 in Madras and Slade [1], and equation (2.8). Equation (2.23) follows immediately from equation (2.22) and the fact that

$$P_n(\epsilon, W) \leqslant C_{n-2}(\epsilon, W) \tag{2.24}$$

by an argument similar to that leading to equation (2.21). □

Corollary 1. *There exists a K-pattern W and a positive number ϵ such that the number of self-avoiding walks (polygons) with k contacts is related to the number of neighbour-avoiding walks (polygons) by the inequalities*

$$\binom{\lfloor \epsilon n \rfloor}{k}[C_n - C_n(\epsilon, W)] \leqslant c_n(k) \tag{2.25}$$

$$\binom{\lfloor \epsilon n \rfloor}{k}[P_n - P_n(\epsilon, W)] \leqslant p_n(k). \tag{2.26}$$

Proof. Consider the K-pattern $W = u_1\bar{u}_2\bar{u}_2u_1u_1u_2$ in Z^2. This pattern occurs with positive density on all except exponentially few neighbour-avoiding walks and polygons. W can be converted to $u_1\bar{u}_2u_1\bar{u}_2u_1u_2$ by an edge permutation so that each walk containing more than $\lfloor \epsilon n \rfloor$ translates of W can be converted into a walk with k contacts in at least $\binom{\lfloor \epsilon n \rfloor}{k}$ ways. A similar argument works for polygons and a similar pattern can be constructed in any dimension greater than or equal to two. The details of this construction are given next.

For each $d > 2$ the pattern begins as follows $W_1 = u_1\bar{u}_2\bar{u}_2u_1u_1u_2u_3u_3\bar{u}_1$. For $k \geqslant 2$, we define $W_k = u_{2k}u_{2k}\bar{u}_{2k-1}\bar{u}_{2k-1}\bar{u}_{2k-1}\bar{u}_{2k-1}\bar{u}_{2k}\bar{u}_{2k}\bar{u}_{2k}\bar{u}_{2k}u_{2k-1}u_{2k-1}$. Then for $d = 2k$, $k \geqslant 2$, the pattern is taken to be $W = W_1W_2\ldots W_k$. For $d = 2k+1$, $k \geqslant 2$, the pattern is taken to be $W = W_1W_2\ldots W_ku_du_du_{d-1}u_{d-1}u_2u_2\bar{u}_d\bar{u}_d\bar{u}_d\bar{u}_d\bar{u}_2\bar{u}_2$. For $d = 3$, the pattern is $W = W_1u_2u_2u_1\bar{u}_3\bar{u}_3\bar{u}_1\bar{u}_3\bar{u}_3\bar{u}_2\bar{u}_2$. In all cases, the pattern W is constructed so that if the start of the pattern is at vertex v then vertex $v_0 = v + 2u_1 - u_2$ cannot be part of the walk or polygon, the vertices $v_0 \pm u_i$ for $i \geqslant 3$ cannot be part of the walk or polygon, and $v_0 + u_2$ cannot be part of the walk or polygon. W can then be converted to W' by changing W_1 in W to $u_1\bar{u}_2u_1\bar{u}_2u_1u_2u_3u_3\bar{u}_1$. Thus exactly one new contact is created. □

Corollary 2. *Given any integer $k \geqslant 0$, the following limits exist and are independent of k:*

$$\lim_{n\to\infty} n^{-1}\log c_n(k) = \lim_{n\to\infty} n^{-1}\log p_n(k) = \kappa_0. \tag{2.27}$$

Proof. The case $k = 0$ was proved in lemma 1. For $k > 0$, consider any walk (polygon), ω, in Z^d with k contacts. Each contact has two endpoints which are vertices in ω. Breaking ω at every endpoint of a contact, results in at most a $(2k+1)$-tuple ($(2k)$-tuple) of walks which are either neighbour-avoiding or have exactly one contact and that contact's endpoints are the first and last vertices of the walk. A walk of the second kind can be transformed into a neighbour-avoiding walk by removing the last step of the walk. Thus

$$c_n(k) \leqslant (2d-1)^{2k+1} \sum_{\{m_i \mid n-2k-1 \leqslant \sum_{i=1}^{2k+1} m_i \leqslant n\}} \prod_{i=1}^{2k+1} C_{m_i} \tag{2.28}$$

and

$$p_n(k) \leqslant (2d-1)^{2k} \sum_{\{m_i \mid n-2k \leqslant \sum_{i=1}^{2k} m_i \leqslant n\}} \prod_{i=1}^{2k} C_{m_i}. \tag{2.29}$$

Next, using the facts that $C_n \leqslant B_n e^{O(\sqrt{n})}$ and $B_n B_m \leqslant B_{n+m}$ (which follows from a concatenation argument), equations (2.28) and (2.29) establish the inequalities

$$c_n(k) \leqslant (2k+1)\binom{n+2k}{2k} B_n e^{O(\sqrt{n})} \tag{2.30}$$

and

$$p_n(k) \leqslant (2k)\binom{n+2k-1}{2k-1} B_n e^{O(\sqrt{n})}. \tag{2.31}$$

Taking logarithms, dividing by n, and then letting n go to infinity in equations (2.25), (2.30), (2.26), (2.31) and then using lemma 1 and equation (2.7) gives the required result. □

The above result establishes (a), however, the upper bounds obtained in equations (2.30) and (2.31) are too weak for establishing results related to (b). We next prove an improved upper bound for $p_n(k)$ in terms of $p_n(0)$ for $d = 2$. The basic idea is to start with an arbitrary polygon with n edges and $k \geqslant 1$ contacts and then, by an appropriate contact removal process, construct from it a sequence of one or more neighbour-avoiding polygons with a total of $m \leqslant n$ edges distributed between them. For our purposes, an appropriate contact removal process would have the property that the number of distinct k-contact n-edge polygons which reduce (via the contact removal process) to the same sequence of neighbour-avoiding polygons is bounded above by $C^k\binom{an}{k}$ for some numbers $C, a \geqslant 0$ which are independent of n and k. The contact removal process employed here is divided into a number of stages. Given a polygon ω with n edges and $k \geqslant 1$ contacts, these stages can be roughly described as follows:

(1) First perform a *U-turn reduction* on ω. This term will be clarified in section 2.1 but the basic idea is to perform a transformation such as that indicated in figure 1(a). In figure 1(a), the polygon on the left is converted to the polygon on the right by deleting a sequence of *U-turns* associated with the portion of the polygon that has vertices explicitly shown as full circles.

(2) Next perform a *tunnel reduction* on the U-turn reduced polygon. This process will be clarified in section 2.2 but the basic idea is to perform a transformation such as that indicated in figure 2(a). The *tunnel* in figure 2(a) is the section of the polygon that has vertices explicitly shown as full circles.

(3) Finally, since the contacts which remain in a tunnel-reduced polygon are relatively isolated, another construction which removes contacts by making local changes in the polygon in well defined regions around the contacts is used. The basic approach for this final stage is similar to one used for removing a vertex of degree four from a figure-eight graph (James and Soteros [15]) and is explained in section 2.3.

In this process we take advantage of the planarity of Z^2 and as a result the procedure does not easily extend to dimensions higher than two. The details of the process are presented next as a sequence of lemmas leading to a theorem which combines the lower bound of corollary 1 with the upper bound obtained from the sequence of lemmas.

We say that an event occurs *within a distance r of a vertex v* if the event occurs in the subgraph of the square lattice defined by the vertex set $\{v + \alpha_1 u_1 + \alpha_2 u_2 | -r \leqslant \alpha_1 \leqslant r, -r \leqslant \alpha_2 \leqslant r\}$, this subgraph is referred to as the $(2r) \times (2r)$ box centred at v.

2.1. U-turn reduction

A *U-turn* is defined to be any subwalk of a self-avoiding walk or polygon in Z^2 consisting of a sequence of three steps in the form $\delta_1 u_i, \delta_2 u_{i'}, (-\delta_1)u_i$ where $\delta_1, \delta_2 \in \{-1, 1\}$ and $i, i' \in \{1, 2\}$

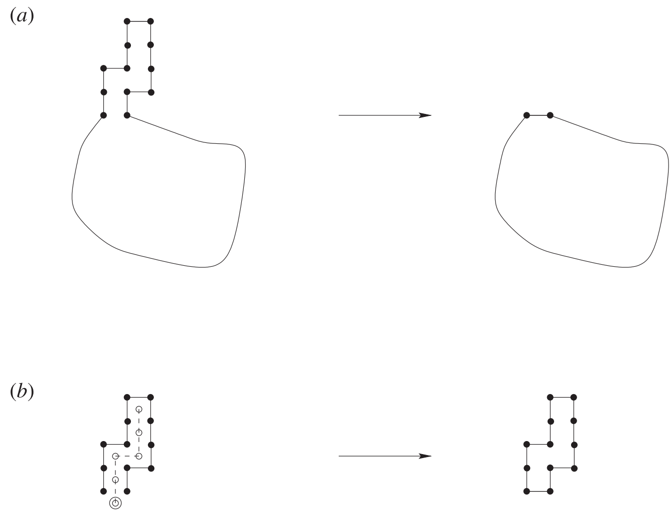


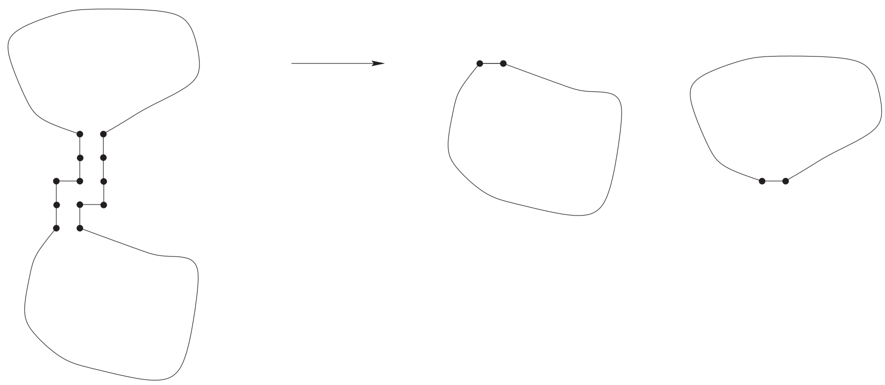
Figure 1. (*a*) An example of a U-turn reduction. The polygon on the left, ω, is converted into the polygon on the right by deleting a sequence of U-turns associated with the portion of the polygon that has vertices explicitly shown as full circles. (*b*) An example of a 5-cul-de-sac, $\mathcal{T}$, and its associated cul-de-sac polygon. $\mathcal{T}$ is shown on the left as a planted tree in $\mathcal{Z}^2$ (vertices in $\mathcal{Z}^2$ are denoted by open circles and edges are denoted by broken lines) with its plant vertex circled. In this case, $\mathcal{T}$ is associated with the indicated set of five contacts of ω. The cul-de-sac polygon associated with $\mathcal{T}$ is shown on the right.

such that $i \neq i'$. Note that the first and last vertex in a U-turn are necessarily the endpoints of a contact edge of the self-avoiding walk or polygon (provided the polygon has greater than four edges) and such a contact edge will be referred to as a *U-turn contact*.

Let $\mathcal{Z}^2$ be the square lattice dual to Z^2 such that vertices in $\mathcal{Z}^2$ are dual to a unit square in R^2 whose boundary is in Z^2. A vertex in $\mathcal{Z}^2$ is said to be *dual to a U-turn* of a walk or polygon in Z^2 if the boundary of its dual square consists of a U-turn and a U-turn contact. Let $\tilde{G}$ be a subset of R^2 which is formed from the union of unit squares whose boundaries are in Z^2. A subgraph G of $\mathcal{Z}^2$ is said to be dual to $\tilde{G}$ if G consists of the vertices of $\mathcal{Z}^2$ dual to the unit squares of $\tilde{G}$ and contains all the edges of $\mathcal{Z}^2$ which join vertices dual to unit squares in $\tilde{G}$ which share a common edge. Let $\mathcal{T}$ be a tree with e edges and s vertices of degree one in $\mathcal{Z}^2$ which is dual to a disc $D = D(\mathcal{T})$ in R^2 whose boundary is in Z^2; note that such a tree is necessarily a neighbour-avoiding tree. If $\mathcal{T}$ is a planted tree, form $\mathcal{T}''$ by removing the plant vertex and edge from $\mathcal{T}$. $\mathcal{T}''$ is dual to a disc D'' in R^2. We define the *cul-de-sac polygon* of $\mathcal{T}$ to be the boundary polygon of D'', i.e. $\partial D''$, and note that it has $2e + 2$ edges in Z^2 (see, for example, figure 1(*b*)). For $e \geqslant 2$, let $\mathcal{T}'$ be obtained from $\mathcal{T}$ by removing all vertices of degree one and their incident edges from $\mathcal{T}$. $\mathcal{T}'$ is dual to a disc D' in R^2. We define the *tunnel polygon* of $\mathcal{T}$, $T = T(\mathcal{T})$, to be the boundary polygon of D', i.e. $T = \partial D'$, and note that it has $2(e - s) + 4$ edges in Z^2 (see, for example, figure 2(*b*)).

Given two vertices, v_1 and v_2, in Z^2 if v_2 comes later than v_1 in a lexicographic ordering of the vertices of Z^2 according to their coordinates then this is denoted by $v_1 < v_2$. Given two edges, e_1 and e_2, in Z^2 let v_1 (v_2) represent the coordinates of the midpoint of e_1 (e_2). If v_2 comes later than v_1 in a lexicographic ordering of all the edge midpoints according to their coordinates then this is denoted by $e_1 < e_2$.

(*a*)



(*b*)

Figure 2. (*a*) An example of a tunnel reduction. The polygon on the left, ω, is converted into the two polygons on the right by deleting the portion of the polygon that has vertices explicitly shown as full circles. (*b*) An example of a 6-tunnel, $\mathcal{T}$, and its associated tunnel polygon. $\mathcal{T}$ is shown on the left as a planted tree in $\mathcal{Z}^2$ (vertices in $\mathcal{Z}^2$ are denoted by open circles and edges are denoted by broken lines) with its plant vertex circled. In this case, $\mathcal{T}$ is associated with the indicated set of six contacts of ω. The tunnel polygon associated with $\mathcal{T}$ is shown on the right.

Lemma 2. *Given a polygon ω with n edges and k contacts, there exist non-negative integers m, k', r, with $k' + (n-m)/2 \leqslant k$ and an algorithm for constructing from ω a unique 3-tuple $(\tilde{\omega}, F, \mathcal{E})$ where: $\tilde{\omega}$ is a polygon with m edges, r of which are distinguished, and k' contacts; F is an r-tuple of planted lattice trees each of which has one or more edges and is dual to a disc in R^2; $\mathcal{E}$ is an r-tuple of distinct edges, $\mathcal{E}_1 > \mathcal{E}_2 > \cdots > \mathcal{E}_r$ from the square lattice. Furthermore, $(\tilde{\omega}, F, \mathcal{E})$ satisfies the following.*

(a) Each edge in $\mathcal{E}$ is a contact edge of ω.
(b) $\tilde{\omega}$ does not contain any U-turns.
(c) Construct a subgraph, Ω, of Z^2 as follows. The lexicographically first distinguished edge of $\tilde{\omega}$ is translated to coincide with the first edge in $\mathcal{E}$ and $\tilde{\omega}$ is added to Ω. For each component of F, translate the plant edge in the jth component of F to be dual to the jth edge in $\mathcal{E}$ and add to Ω the cul-de-sac polygons associated with the component trees of F. Delete from Ω both edges of every pair of double edges formed in this process. The resulting graph is Ω and $\Omega = \omega$.

Proof. Consider a polygon ω with n edges and k contacts. If $k = 0$, then set $\tilde{\omega} = \omega$, $m = n$, $k' = k = 0$, $r = 0$, $F = \mathcal{E} = \phi$.

For $k \geqslant 1$, construct a subgraph $G(\omega)$ of $\mathcal{Z}^2$ as follows: for each contact edge $\mathcal{K}$ in ω add its dual edge in $\mathcal{Z}^2$ to $G(\omega)$. Since ω is a polygon in Z^2, $G(\omega)$ is a forest in $\mathcal{Z}^2$ with

k edges. A *branch point* in a tree is defined to be any vertex with degree greater than two; a *leaf* or *end point* is defined to be any vertex of degree one. A *branch* of a tree is defined to be any path between two branch points or a branch and an end point or two end points of the tree such that all but the first and last vertices of the path are vertices of degree two in the tree.

Let $G'(\omega)$ be the subforest of $G(\omega)$ formed as follows: first add each component of $G(\omega)$ for which at most one vertex of degree one is not dual to a U-turn in ω; next, for each component, $\mathcal{T}$, of $G(\omega)$ with more than one vertex of degree one not dual to a U-turn and for each branch point of $\mathcal{T}$, if all but one of the branches connected to it contain an end point dual to a U-turn then add all the branches connected to it to $G'(\omega)$ otherwise add to $G'(\omega)$ only the branches which contain an end point dual to a U-turn. In this way, each component of $G'(\omega)$ has at most one unit degree vertex which is not dual to a U-turn. A vertex v of $G'(\omega)$ is said to be a *type one* vertex if it has unit degree and is not dual to a U-turn of ω; a *type two* vertex if it has degree two, is incident on two perpendicular edges of $G'(\omega)$, and has exactly three of its four nearest neighbours from Z^2 being vertices in ω; or a *type three* vertex if it has degree two and corresponds to a vertex of degree four in a component of $G(\omega)$. Using $G'(\omega)$, we next form a forest, $G''(\omega)$, consisting of one or more planted lattice trees.

Given a component of $G'(\omega)$, if it has one type one vertex and no vertices of type two or three we plant the component at that unit degree vertex and add the planted tree to $G''(\omega)$. Otherwise, either the component has no type one, two or three vertices and hence is dual to ω, or it has at least one vertex, v, of type two or three. In the first case, plant the tree at the vertex of degree one which is lexicographically first in an ordering of the vertices of degree one of the component and add the planted tree to $G''(\omega)$. In the second case, if the component contains no type one vertex and only one vertex v of either type two or three, then create two planted trees (both planted at v) by dividing the component into two parts at v and repeating the vertex v; add both trees to $G''(\omega)$. Otherwise there are vertices $v_1, \ldots, v_l$ $l > 1$ such that v_i is either type one, two, or three (note that there is at most one type one and at most one type three vertex in the list), in this case for each $i \neq j$ remove all the edges in the component that are part of the path between v_i and v_j and remove any isolated vertices that result from this operation. After this edge and vertex deletion process, the result is a forest in which each component has exactly one vertex v either of type one, two or three; a planted tree for each component can thus be obtained as discussed previously. Add the resulting planted trees to $G''(\omega)$.

Any component of $G''(\omega)$ consisting of $r' \geqslant 1$ edges is called an *r'-cul-de-sac* of ω. If $G''(\omega) = \phi$, then ω has no U-turns and thus set $\tilde{\omega} = \omega$, $m = n$, $k' = k$, $r = 0$, $F = \mathcal{E} = \phi$. Otherwise, every plant edge in $G''(\omega)$ is dual to a contact edge in ω. Let $\mathcal{L}_1$ be the top (i.e. last) plant edge of $G''(\omega)$ in a lexicographic ordering of the plant edge midpoint coordinates, and let K_1 be the contact edge in Z^2 dual to $\mathcal{L}_1$. The edge K_1 of Z^2 and the edges of ω divide R^2 into three regions. Let ω_1 be the polygon which forms the boundary of the region in R^2 containing the plant vertex incident on $\mathcal{L}_1$, distinguish the edge K_1 in ω_1 and add K_1 to $\mathcal{E}$. The component of $G''(\omega)$ which contains $\mathcal{L}_1$ becomes the first component, t_1, of F. Let $\mathcal{L}_2$ be the top plant edge among the plant edges of $G''(\omega_1)$. Let K_2 be the contact edge dual to $\mathcal{L}_2$. The edge K_2 of Z^2 and the edges of ω_1 divide R^2 into three regions. Let ω_2 be the boundary polygon of the region containing the plant vertex incident on $\mathcal{L}_2$ and distinguish the edge K_2 in ω_2. Let K_2 be the next edge in $\mathcal{E}$. The component of $G''(\omega_1)$ which contains $\mathcal{L}_2$ is the next component, t_2, of F. The process is continued until $G''(\omega_r)$ is empty. $\tilde{\omega}$ is ω_r and the edges in $\mathcal{E}$ along with the associated components of F are reordered so that the edges in $\mathcal{E}$ are in reverse lexicographic order.

The process just described for forming $\tilde{\omega}$ (a polygon with $m \geqslant 4$ edges and k' contacts and no U-turns) can be viewed as the following process. Start with ω. Next, U-turns (and any new U-turns that are formed) associated with edges in the components of F are successively deleted. The deletion of a U-turn with polygon edges $\{v_1, v_2\}$, $\{v_2, v_3\}$, $\{v_3, v_4\}$ is accomplished by deleting from the polygon the three edges of the U-turn and then adding to the polygon the edge $\{v_1, v_4\}$; the resulting polygon therefore has two fewer edges. Since each U-turn removed in this process corresponds to an edge of a component of F, the total number of edges in F is thus $(n - m)/2$. Note also that it is possible that some components of $G''(\omega)$ may not be components of F. Therefore, the total number of edges in F may be less than the total number of edges in $G''(\omega)$ which is $k - k'$. □

The resulting polygon, $\tilde{\omega}$, is called a *U-turn reduced* polygon. Let $\hat{p}_n(k)$ denote the number (up to translation) of n-edge k-contact U-turn reduced polygons. Note that for any n and k such that $p_n(k) > 0$, $n \geqslant 4$ and must be even and $k \leqslant (d-1)n$. Furthermore, for $d = 2$, since there must be at least four vertices in the polygon which are not part of a contact,

$$0 \leqslant k \leqslant n - 4. \tag{2.32}$$

Lemma 3. *Given any n and k, there exists $B > 0$ such that*

$$p_n(k) \leqslant B^k \sum_{k'=0}^{k} \binom{2n}{k-k'} \hat{p}_n(k'). \tag{2.33}$$

Proof. By lemma 2, there is a one-to-one correspondence between n-edge, k-contact polygons and 3-tuples $(\tilde{\omega}, F, \mathcal{E})$ satisfying the conditions of lemma 2. Note that $\tilde{\omega}$ is an m-edge, k'-contact, U-turn reduced polygon with r distinguished edges. Hence $p_n(k)$ is equal to the sum over m, k', r, and the associated possible choices of 3-tuples $(\tilde{\omega}, F, \mathcal{E})$ which satisfy the conditions (1)–(3) of lemma 2. Given a 3-tuple $(\tilde{\omega}, F, \mathcal{E})$ which satisfies conditions (1)–(3) of lemma 2, let e_j be the total number of edges and s_j be the total number of vertices of degree one in the jth component of F so that $\sum_{j=1}^{r} e_j = (n-m)/2 \leqslant k-k'$ and $2 \leqslant s_j \leqslant (2e_j+4)/3$ (this upper bound is clear from the fact that for each vertex of degree one in a tree in F there must be three edges in its dual polygon in Z^2).

With the variables $m, k', r, e_1, \ldots, e_r, s_1, \ldots, s_r$ fixed, an upper bound will be determined on the number of ways to construct $\tilde{\omega}$ and F and then connect the components of F to $\tilde{\omega}$ (i.e. form $\mathcal{E}$) in order to construct a polygon. Then, by summing appropriately over the variables $m, k', r, e_1, \ldots, e_r, s_1, \ldots, s_r$, an upper bound on $p_n(k)$ is obtained.

The number of ways to construct $\tilde{\omega}$ is $\hat{p}_m(k')$ for $m \geqslant 4$. The number of ways to construct a forest F which is an r-tuple of planted lattice trees is $\prod_{i=1}^{r} s_i t_{e_i}(s_i)$, where $t_{e_i}(s_i)$ is the number of lattice trees (up to translation) on $\mathcal{Z}^2$ with e_i edges and s_i vertices of degree one and this is multiplied by s_i, the number of ways to select a plant edge. The number of ways to reconstruct a polygon from $\tilde{\omega}$ and F (i.e. the number of ways to form $\mathcal{E}$) is bounded above by the number of ways to distinguish r edges in $\tilde{\omega}$, i.e. $\binom{m}{r}$. This results in the following bound:

$$p_n(k) \leqslant \sum_{k'=0}^{k} \sum_{m=n-2(k-k')}^{n} \sum_{r=0}^{\min\{m,k-k'\}} \hat{p}_m(k') \binom{m}{r} \sum_{\{e_i\}} \sum_{\{s_i\}} \prod_{i=1}^{r} s_i t_{e_i}(s_i) \tag{2.34}$$

where the sum over $\{e_i\}$ is the sum over $\{e_i \geqslant 1 | i = 1, \ldots, r, r \leqslant \sum_i e_i = (n-m)/2 \leqslant k-k'\}$ and the sum over $\{s_i\}$ is over $\{s_i \geqslant 2 | i = 1, \ldots, r; s_i \leqslant (2e_i + 4)/3\}$. Let $t_e = \sum_{s \geqslant 2} t_e(s)$, then (see, for example, [16])

$$\log \lambda \equiv \lim_{e \to \infty} e^{-1} \log t_e = \sup_{e \geqslant 1} e^{-1} \log t_e \leqslant 3 \log 2 \tag{2.35}$$

and hence for any choice of e, $t_e \leqslant \lambda^e$. Using this fact and that $s_i \leqslant (2e_i + 4)/3 \leqslant 2e_i$ and that for any $b \leqslant A$, $\binom{A}{b} \leqslant 2^A$,

$$\begin{aligned}
\sum_{\{e_i\}} \sum_{\{s_i\}} \prod_{i=1}^{r} s_i t_{e_i}(s_i) &\leqslant \sum_{\{e_i\}} 2^r \left(\prod_{i=1}^{r} e_i \right) \sum_{\{s_i\}} \left(\prod_{i=1}^{r} t_{e_i}(s_i) \right) \\
&= 2^r \sum_{\{e_i\}} \prod_{i=1}^{r} \binom{e_i}{1} \prod_{i=1}^{r} \left[\sum_{s_i \geqslant 2} t_{e_i}(s_i) \right] = 2^r \sum_{\{e_i\}} \prod_{i=1}^{r} \binom{e_i}{1} \prod_{i=1}^{r} t_{e_i} \\
&\leqslant 2^r (2\lambda)^{(n-m)/2} \sum_{\{e_i\}} 1 = 2^r (2\lambda)^{(n-m)/2} \binom{(n-m)/2 - 1}{r-1} \\
&\leqslant 2^r (4\lambda)^{(n-m)/2} \leqslant (8\lambda)^{k-k'}
\end{aligned} \tag{2.36}$$

where the fact that $r \leqslant (n-m)/2 \leqslant k - k'$ was used to obtain the last inequality. Therefore, equations (2.34) and (2.36) lead to

$$p_n(k) \leqslant \sum_{k'=0}^{k} (8\lambda)^{k-k'} \sum_{m=n-2(k-k')}^{n} \sum_{r=0}^{\min\{m,k-k'\}} \hat{p}_m(k') \binom{m}{r} \tag{2.37}$$

$$\leqslant \sum_{k'} \hat{p}_n(k')(8\lambda)^{k-k'} \sum_{m=n-2(k-k')}^{n} \sum_{r=0}^{k-k'} \binom{2n}{r} \tag{2.38}$$

$$\leqslant \sum_{k'} \hat{p}_n(k')(8\lambda)^{k-k'} [2(k-k')+1] \sum_{r=0}^{k-k'} \binom{2n}{r} \tag{2.39}$$

$$\leqslant \sum_{k'} \hat{p}_n(k')(8\lambda)^{k-k'} [2(k-k')+1](k-k'+1) \binom{2n}{k-k'} \tag{2.40}$$

$$\leqslant \sum_{k'=0}^{k} \hat{p}_n(k')(64\lambda)^{k-k'} \binom{2n}{k-k'} \tag{2.41}$$

where the facts that $j + 1 \leqslant 2^j$ for all $j \geqslant 1$ and that $n \geqslant k$ have been used several times. Taking $B = 64\lambda$ gives the required result. □

2.2. Tunnel reduction

Lemma 4. *Given an integer $g \geqslant 2$ and a U-turn reduced polygon ω with n edges and k contacts, there exist non-negative integers m, k', b, $m_1, \ldots, m_b$, $k_1, \ldots, k_b$ and $r_1, \ldots, r_b$ with $1 \leqslant b \leqslant (k-k')/2 + 1 - (n-m)/4$, $\sum_{i=1}^{b} m_i = m$, and $\sum_{i=1}^{b} k_i = k'$, and an algorithm for constructing from ω a unique b-tuple $((\omega_1, F_1, \mathcal{E}_1), \ldots, (\omega_b, F_b, \mathcal{E}_b))$ where: ω_1 is a polygon with m_1 edges, r_1 of which are distinguished and k_1 contacts; for $i > 1$, ω_i is an edge-rooted polygon with m_i edges, with $r_i - 1 \geqslant 0$ non-root distinguished edges, and k_i contacts; F_1 (F_i, $i > 1$) is an r_1-tuple ($(r_i - 1)$-tuple) of planted lattice trees, each of which has g or more edges and is dual to a disc in R^2; and $\mathcal{E}_i$ is an r_i-tuple of distinct edges, $\mathcal{E}_{i1}, \ldots, \mathcal{E}_{ir_i}$, from the square lattice with $\mathcal{E}_{i2} > \mathcal{E}_{i3} > \cdots > \mathcal{E}_{ir_i}$ (for $i = 1$, $\mathcal{E}_{i1} > \mathcal{E}_{i2}$ as well). Furthermore, the $(\omega_i, F_i, \mathcal{E}_i)$ satisfy the following:*

(1) Each edge in $\mathcal{E}_i$ is a contact edge of ω.

(2) *Construct a graph Ω as follows. For all $i > 1$, the root edge of ω_i is translated to coincide with the first edge in $\mathcal{E}_i$ and ω_i is added to Ω. The top distinguished edge of ω_1 is translated to coincide with the first edge in $\mathcal{E}_1$ and ω_1 is added to Ω. For each component of F_1, translate the plant edge in the jth component of F_1 to be dual to the jth edge in $\mathcal{E}_1$ and add to Ω the tunnel polygons associated with the component trees of F_1. For each $i > 1$ and each component of F_i, translate the plant edge in the jth component of F_i to be dual to the $(j+1)$th edge in $\mathcal{E}_i$ and add to Ω the tunnel polygons associated with the component trees of F_i. Delete from Ω both edges of every pair of double edges formed in this process. The resulting graph is Ω and $\Omega = \omega$. Hence the total number of edges in the F_is is $(n-m)/2 + 2(b-1)$.*

(3) *Let $r \equiv \sum_{i=1}^{b} r_i$. Then the total number of component trees is $r_1 + \sum_{i=2}^{b}(r_i - 1) = r - b + 1$ with $0 \leqslant b - 1 \leqslant r \leqslant k - k'$ and for $b > 1$, $2 \leqslant b \leqslant r$. If $g \geqslant 3$, then $r + b - 1 + k' \leqslant k$.*

Proof. Given $g \geqslant 2$, consider a U-turn reduced polygon ω with n edges and k contacts. If $k = 0$, then set $b = 1$, $\tilde{\omega}_1 = \omega$, $m_1 = n$, $k' = k_1 = k = 0$, $r = r_1 = 0$ and $F_1 = \mathcal{E}_1 = \phi$.

For $k \geqslant 1$, construct a subgraph $G(\omega)$ of $\mathcal{Z}^2$ as follows: for each contact edge $\mathcal{K}$ in ω add its dual edge in $\mathcal{Z}^2$ to $G(\omega)$. Since ω is a polygon in Z^2, $G(\omega)$ is a forest in $\mathcal{Z}^2$ with k edges. For each vertex v of degree two in $G(\omega)$ which is incident on two perpendicular edges of $G(\omega)$ and with exactly three of its four nearest neighbours from Z^2 being vertices in ω, create two trees (both containing v) by dividing the component into two parts at v and repeating the vertex v. Thus we obtain a forest, $G'(\omega)$, consisting of one or more lattice trees. Any component of $G'(\omega)$ consisting of r' edges is called an *r'-tunnel* of ω. Let $F^g(\omega)$ be the subforest of $G'(\omega)$ consisting of the components of $G'(\omega)$ with at least g edges, i.e. all r'-tunnels for which $r' \geqslant g$.

If $F^g(\omega) = \phi$, then set $b = 1$, $\tilde{\omega}_1 = \omega$, $m_1 = n$, $k' = k_1 = k$, $r = r_1 = 0$, and $F_1 = \mathcal{E}_1 = \phi$. Otherwise, every leaf in $F^g(\omega)$ is dual to a contact edge in ω. Let $\mathcal{L}_1$ be the top leaf of $F^g(\omega)$ in a lexicographic ordering of the coordinates of the leaf midpoints, and let K_1 be the contact edge in Z^2 dual to $\mathcal{L}_1$. The edge K_1 of Z^2 and the edges of ω divide R^2 into three regions. Let ω_1^1 be the polygon which forms the boundary of the region in R^2 containing the vertex of degree one incident on $\mathcal{L}_1$, distinguish the edge K_1 in ω_1^1 and add K_1 to $\mathcal{E}_1$. The component of $F^g(\omega)$ which contains $\mathcal{L}_1$ is considered planted at $\mathcal{L}_1$ and becomes the first component, t_1, of F_1. Let $\mathcal{L}_2$ be the top leaf of the set of leaves of $F^g(\omega)$ which are dual to a contact of ω_1^1. Let $\mathcal{T}$ the component of $F^g(\omega)$ which contains $\mathcal{L}_2$. The edges of ω_1^1 along with the edges of Z^2 which are dual to a leaf of $\mathcal{T}$ divide R^2 into a number of regions each bounded by a polygon. Let ω_1^2 be the boundary polygon that contains K_1 and define K_2 to be the edge of Z^2 contained in ω_1^2 which is dual to a leaf of $\mathcal{T}$. Distinguish the edge K_2 in ω_1^2 and define $\mathcal{L}_2$ to be the leaf of $\mathcal{T}$ which is dual to K_2. Let K_2 be the next edge in $\mathcal{E}_1$. $\mathcal{T}$ is planted at $\mathcal{L}_2$ and is the next component, t_2, of F_1. The process is continued until $\omega_1^{r_1}$ has no contact edges dual to leaves of $F^g(\omega)$. ω_1 is defined to be $\omega_1^{r_1}$ and the edges of $\mathcal{E}_1$ along with their associated components in F_1 are reordered so that the edges of $\mathcal{E}_1$ are in reverse lexicographic order.

Next consider $\omega - \omega_1$ (that is the graph obtained from ω by removing any edges of ω_1 contained in it). Consider the top leaf of t_1, other than $\mathcal{L}_1$. When the edge of Z^2 dual to this top leaf is added to $\omega - \omega_1$, R^2 is divided into three regions. Let ω_2^1 be the boundary of the region containing the vertex of degree one incident on a leaf of t_1. ω_2, F_2, and $\mathcal{E}_2$ are then formed from ω_2^1 by performing the same procedure that was used to form ω_1 from ω_1^1. The process continues through the leaves of $t_1, t_2, \ldots$ in a breadth first fashion to result in b 3-tuples satisfying conditions (1) and (2).

To show that condition (3) is satisfied, consider $g \geqslant 3$ and let t be the jth component of F_i. Suppose t has $e_i^{(j)} \geqslant 3$ edges and $s_i^{(j)} \geqslant 2$ vertices of degree one. It is first shown that

$e_i^{(j)} \geqslant 2s_i^{(j)} - 1$. Let v_3 and v_4 be respectively the number of vertices of degree three and four in t. Then $s_i^{(j)} = 2 + v_3 + 2v_4$. If $v_3 = v_4 = 0$, then $s_i^{(j)} = 2$ and $e_i^{(j)} \geqslant 3 = 2s_i^{(j)} - 1$. Otherwise either $v_3 \neq 0$ or $v_4 \neq 0$. Since ω contains no U-turns, for each vertex of degree three in t there must be at least three non-leaf edges, and for each vertex of degree 4 in t there must be at least eight such edges. Hence $e_i^{(j)} \geqslant s_i^{(j)} + 3v_3 + 8v_4 = 2s_i^{(j)} + 2v_3 + 6v_4 - 2 \geqslant 2s_i^{(j)}$. Thus the total number of edges in the F_is, e', satisfies

$$\begin{aligned} &\sum_{i=1}^{b}\sum_{j=1}^{r_i'}(2s_i^{(j)} - 1) \leqslant e' \leqslant k - k' \\ &r + b - 1 = 2r - (r - b + 1) \leqslant e' \leqslant k - k' \end{aligned} \tag{2.42}$$

where $r_1' = r_1$ and $r_i' = r_i - 1$ for $i > 1$. □

Define $\tilde{p}_n(k)$ to be the number (up to translation) of n-edge k-contact U-turn reduced polygons ω such that if $g = 3$ in the above lemma then $F^3(\omega)$ is empty and $m = n$, $k = k'$, $b = 1$, and $\omega_1 = \omega$ (i.e. the number of polygons such that $G'(\omega)$ contains no connected components with three or more edges). Polygons counted in $\tilde{p}_n(k)$ are denoted *tunnel-reduced polygons*.

Lemma 5. *Given any n and k, there exists $D > 0$ such that*

$$\hat{p}_n(k) \leqslant D^k \sum_{k'=0}^{k} \binom{2n}{k - k'} \tilde{p}_n(k'). \tag{2.43}$$

Proof. Let P be an m-edge, l-contact, tunnel-reduced polygon in Z^2 and let Q be an n-edge, k-contact, tunnel-reduced polygon in Z^2. Since P and Q do not contain any U-turns, the concatenation argument of lemma 1 that leads to equation (2.5) can be applied to concatenate P and Q and create an $(m+n)$-edge, $(l+k)$-contact, tunnel-reduced polygon. Hence

$$\tilde{p}_m(l)\tilde{p}_n(k) \leqslant \tilde{p}_{m+n}(l+k). \tag{2.44}$$

Let ω be a U-turn reduced polygon in Z^2 with n edges and k contacts. By the proof of lemma 4, there exists a forest $G'(\omega)$. If no component of $G'(\omega)$ consists of three or more edges, i.e. $F^3(\omega)$ is empty, then ω is itself a tunnel-reduced polygon. Otherwise the proof will rely on removing tunnel polygons associated with $F^3(\omega)$ from ω to remove some of the contacts in ω and create a tunnel-reduced polygon.

By lemma 4, $\hat{p}_n(k)$ is equal to the sum over m, k', b, and the associated possible choices of b-tuples $((\omega_1, F_1, \mathcal{E}_1), \ldots, (\omega_b, F_b, \mathcal{E}_b))$ which satisfy the conditions (1)–(3) of lemma 4. Let $\mathcal{F}$ represent the l-tuple, $l = r - b + 1$, formed from the component trees of the F_is in the order prescribed by $F_1, F_2, \ldots, F_b$. Note that $\omega_1, \ldots, \omega_b$ are tunnel-reduced polygons. Given a b-tuple, let m_i be the total number of edges, r_i be the number of roots and distinguished edges, and k_i the total number of contacts in ω_i such that $m = \sum_{i=1}^{b} m_i$, $k' = \sum_{i=1}^{b} k_i$ and $r = \sum_{i=1}^{b} r_i$. Hence $k - k'$ is an upper bound on the total number of edges and r is the total number of vertices of degree one in $\mathcal{F}$. Let e_j be the number of edges in the jth component tree so that $\sum_{j=1}^{l} e_j = e' = (n-m)/2 + 2(b-1) \leqslant k - k'$. Note also that $n = m + 2e' + 4l - 4r$. With the variables $m, k', b, r, m_1, \ldots, m_b, k_1, \ldots, k_b$ fixed we determine an upper bound on the number of ways to construct the b polygons, the forest $\mathcal{F}$, and the ways to connect these to form a polygon (i.e. the number of ways to form the $\mathcal{E}_i$s), and then summing appropriately over the variables $m, k', b, r, m_1, \ldots, m_b, k_1, \ldots, k_b$ we obtain an upper bound on $\hat{p}_n(k)$.

The number of ways to construct the b polygons is $U_1 = \prod_{i=1}^{b} \tilde{p}_{m_i}(k_i)$ and using equation (2.44) this is bounded from above by $\tilde{p}_m(k')$. In analogy with equation (2.36), the number of ways, U_2, to construct the forest and an associated upper bound are given by

$$\begin{aligned} U_2 &= \sum_{\{e_i\}} \sum_{\{s_i\}} \prod_{i=1}^{l} s_i t_{e_i}(s_i) \leqslant 2^r \sum_{\{e_i\}} \sum_{\{s_i\}} \prod_{i=1}^{l} t_{e_i}(s_i) \\ &\leqslant 2^r (\lambda)^{(n-m)/2+2(b-1)} \binom{(n-m)/2+2(b-1)-1}{r-b} \\ &\leqslant 2^r (2\lambda)^{(n-m)/2+2(b-1)} \leqslant (4\lambda)^{k-k'} \end{aligned} \tag{2.45}$$

where the sum over $\{e_i\}$ is the sum over $\{e_i \geqslant 1, i = 1, \ldots, l | r \leqslant \sum_i e_i = (n-m)/2 + 2(b-1) \leqslant k - k'\}$ and the sum over $\{s_i\}$ is over $\{s_i \geqslant 2, i = 1, \ldots, l | \sum_{i=1}^{l} s_i = r\}$. The number of ways to reconstruct the polygon from the b polygons and forest $\mathcal{F}$ is bounded above by the number of ways to root and distinguish r edges in the b polygons, U_3. This number and an associated bound is given by

$$U_3 = \sum_{\{r_i\}} \left[\prod_{i=1}^{b} \binom{m_i}{r_i} \right] \left[\prod_{i=2}^{b} \binom{r_i}{1} \right] \leqslant 2^r \sum_{\{r_i\}} \left[\prod_{i=1}^{b} \binom{m_i}{r_i} \right] \leqslant 2^r \binom{m}{r} \tag{2.46}$$

where the sum over $\{r_i\}$ is over $\{r_i, i = 1, \ldots, b | r_1 \geqslant 0, r_i \geqslant 1 \text{ for } i \geqslant 2, \sum_{i=1}^{b} r_i = r\}$ and where for the last inequality the following combinatorial identity has been used:

$$\binom{a}{b} = \sum_{b_i} \prod_{i=1}^{s} \binom{a_i}{b_i} \tag{2.47}$$

where $\sum_{i=1}^{s} a_i = a$ and the sum is over all choices of $\{b_i | \sum_{i=1}^{s} b_i = b\}$. Combining these bounds and using the fact that $r + b - 1 \leqslant k - k'$ results in the following bound with $r_{max} = \min\{m, k - k' - b + 1\}$:

$$\begin{aligned} \hat{p}_n(k) &\leqslant \sum_{k'=0}^{k} \sum_{m=n-2(k-k')}^{n} \sum_{b=1}^{1+(k-k')/2-(n-m)/4} \sum_{r=0}^{r_{max}} \sum_{\{m_i\}} \sum_{\{k_i\}} U_1 U_2 U_3 \\ &\leqslant \sum_{k'=0}^{k} (4\lambda)^{k-k'} \sum_{m=n-2(k-k')}^{n} \tilde{p}_m(k') \sum_{b=1}^{1+(k-k')/2} \sum_{r=0}^{r_{max}} 2^r \binom{m}{r} \sum_{\{m_i\}} \sum_{\{k_i\}} 1 \\ &\leqslant \sum_{k'=0}^{k} (4\lambda)^{k-k'} \tilde{p}_n(k') \sum_{m=n-2(k-k')}^{n} \sum_{b=1}^{1+(k-k')/2} \sum_{r=0}^{r_{max}} 2^r \binom{m}{r} \binom{m-1}{b-1} \binom{k'+b-1}{k'} \\ &\leqslant 2^k \sum_{k'=0}^{k} (4\lambda)^{k-k'} \tilde{p}_n(k') \sum_{m=n-2(k-k')}^{n} \sum_{b=1}^{1+(k-k')/2} \sum_{r=0}^{r_{max}} 2^r \binom{m}{r} \binom{m-1}{b-1} \\ &\leqslant 2^k \sum_{k'=0}^{k} (8\lambda)^{k-k'} \tilde{p}_n(k') \sum_{m=n-2(k-k')}^{n} \sum_{b=1}^{1+(k-k')/2} \sum_{r=0}^{r_{max}} \binom{2m-1}{r+b-1} \\ &\leqslant 2^k \sum_{k'=0}^{k} (8\lambda)^{k-k'} \tilde{p}_n(k') \sum_{m=n-2(k-k')}^{n} \sum_{b=1}^{1+(k-k')/2} \sum_{r=0}^{k-k'-b+1} \binom{2n-1}{r+b-1} \\ &\leqslant 2^k \sum_{k'=0}^{k} (8\lambda)^{k-k'} \tilde{p}_n(k') \sum_{m=n-2(k-k')}^{n} \sum_{b=1}^{1+(k-k')/2} \sum_{s=0}^{k-k'} \binom{2n-1}{s} \end{aligned}$$

$$\leqslant 2^k \sum_{k'=0}^{k} (8\lambda)^{k-k'} \tilde{p}_n(k') \sum_{m=n-2(k-k')}^{n} (1 + (k-k')/2)(k-k'+1) \binom{2n-1}{k-k'}$$

$$\leqslant 2^k \sum_{k'=0}^{k} (8\lambda)^{k-k'} \tilde{p}_n(k')[2(k-k')+1](1+(k-k')/2)(k-k'+1) \binom{2n-1}{k-k'}$$

$$\leqslant 2^k \sum_{k'} (128\lambda)^{k-k'} \tilde{p}_n(k') \binom{2n-1}{k-k'} \tag{2.48}$$

where the fact that $A+1 \leqslant 2^A$ for all $A \geqslant 1$ has been used for the last inequality. Thus setting $D = 256\lambda$ gives the required result. □

2.3. Final stage

Lemma 6. *Given the box* $R = \{(x, y) \in Z^2 | -8 \leqslant x \leqslant 8, -8 \leqslant y \leqslant 8\}$ *and any polygon* ω *with* n *edges and* $k \geqslant 1$ *contacts in* Z^2*, suppose* $\{(x_0, y_0), (x_1, y_1)\}$ *is a contact of* ω *with* $x_1 \geqslant x_0$, $y_1 \geqslant y_0$. *If there are no other contacts in the box* $(x_0, y_0) + R$*, then it is possible, by only altering edges and vertices within the box, to construct a new* m*-edge,* k'*-contact polygon* ω' *with* $n - 8 \leqslant m \leqslant n$, $k' \leqslant k - 1$*, no contacts within the box, and such that* $\omega' = \omega$ *outside the box.*

Proof. Let ω be a polygon in Z^2 and suppose $\{(x_0, y_0), (x_1, y_1)\}$ is a contact of ω with $x_1 \geqslant x_0$, $y_1 \geqslant y_0$ and such that there are no other contacts within a distance 8 from (x_0, y_0). There are two possibilities:

(i) $x_1 = x_0 + 1$;
(ii) $y_1 = y_0 + 1$.

If ω satisfies case (ii), then we can rotate ω 90° about (x_0, y_0) in a clockwise direction and obtain a polygon satisfying case (i). Hence, without loss of generality, we assume that ω satisfies case (i). Let $v = (x_0, y_0)$.

In the remainder of the proof we shall frequently take advantage of the fact that each vertex in the polygon has degree two and also the fact that if two adjacent vertices in the box $v + R$, other than those making the contact, are in the polygon then the edges joining them must also be in the polygon.

Since there are no other contacts in the box $v + R$, ω has one of four forms near v:

(I) $(x_0, y_0), (x_0, y_0 + 1), (x_0 + 1, y_0 + 1), (x_1, y_1) \in \omega$; or
(II) $(x_0, y_0), (x_0, y_0 - 1), (x_0 + 1, y_0 - 1), (x_1, y_1) \in \omega$; or
(III) $(x_0, y_0), (x_0, y_0+1), (x_0, y_0+2), (x_0-1, y_0), (x_0+1, y_0), (x_0+1, y_0-1), (x_0+1, y_0-2), (x_0+2, y_0) \in \omega$ and $(x_0-1, y_0+1), (x_0+1, y_0+1), (x_0, y_0-1), (x_0+2, y_0-1) \notin \omega$; or
(IV) $(x_0, y_0), (x_0, y_0-1), (x_0, y_0-2), (x_0-1, y_0), (x_0+1, y_0), (x_0+1, y_0+1), (x_0+1, y_0+2), (x_0+2, y_0) \in \omega$ and $(x_0-1, y_0-1), (x_0+1, y_0-1), (x_0, y_0+1), (x_0+2, y_0+1) \notin \omega$.

If case (I) or (II) applies, the contact is a U-turn contact. For case (I) the contact can be removed by deleting the vertices $(x_0, y_0 + 1)$ and $(x_0 + 1, y_0 + 1)$ and the three incident edges, and joining (x_0, y_0) and (x_1, y_1) by an edge. Case (II) can be handled similarly. If case (IV) applies to ω, then we can reflect ω through the line $x = x_0$ to obtain a polygon satisfying case (III). Henceforth we assume ω satisfies case (III) (see the top of figure 3).

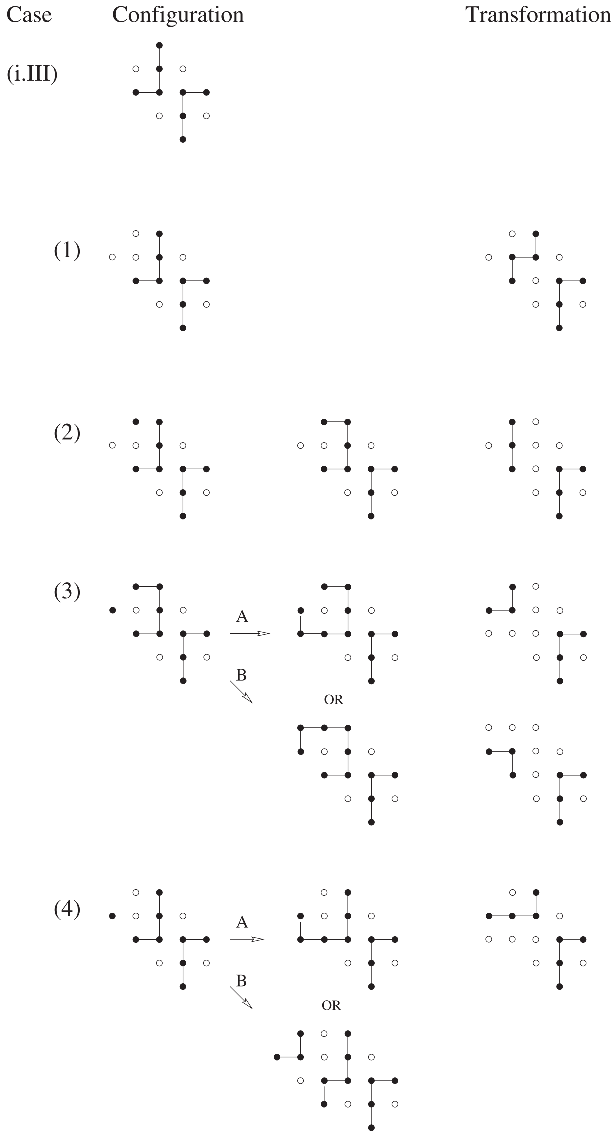


Figure 3. A type (i.III) contact configuration and the cases (1), (2), (3A), (3B), (4A), (4B) with appropriate transformations for cases (1), (2), (3A), (3B), (4A). Polygon edges are depicted by lines; polygon vertices are depicted by full circles; empty vertices are depicted by open circles.

We next consider the following four cases:

(1) $(x_0 - 1, y_0 + 2), (x_0 - 2, y_0 + 1) \notin \omega$
(2) $(x_0 - 1, y_0 + 2) \in \omega$ and $(x_0 - 2, y_0 + 1) \notin \omega$
(3) $(x_0 - 1, y_0 + 2), (x_0 - 2, y_0 + 1) \in \omega$
(4) $(x_0 - 1, y_0 + 2) \notin \omega$ and $(x_0 - 2, y_0 + 1) \in \omega$.

The first two columns of figure 3 show the polygon edges (lines) and vertices (full circles) and the empty sites (open circles) induced by these four cases. Note that in each of the

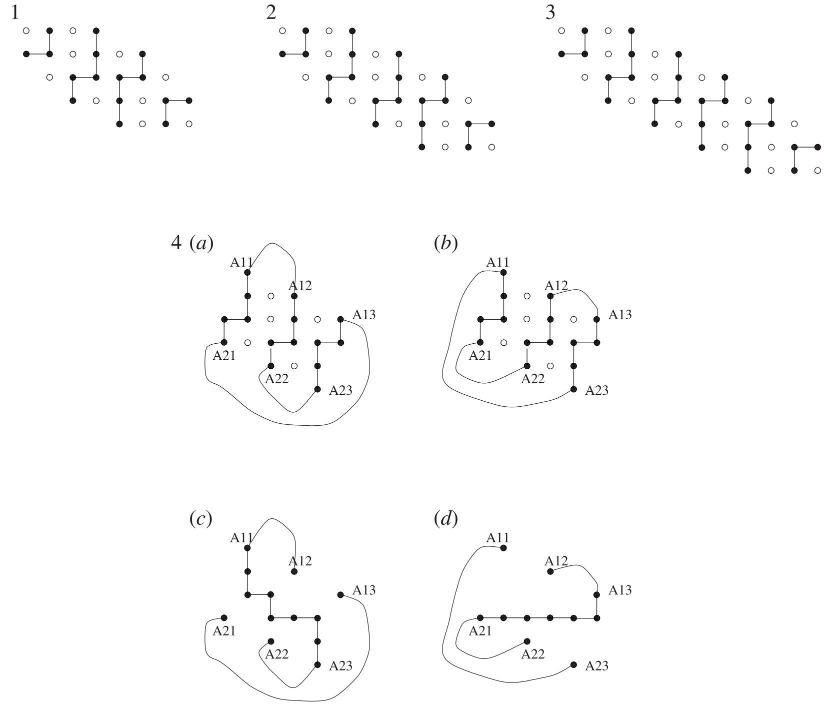


Figure 4. The polygon configurations relevant to case (i.III.4B).

cases (3) and (4) there are two possible subcases induced: (3A), (3B) and (4A), (4B). The last column of figure 3 indicates for each of the cases (1), (2), (3A), (3B) and (4A) the required rearrangement needed to convert ω into a polygon with one less contact (these changes can be done within a distance of 3 from (x_0, y_0)). The case (4B) will be treated separately next.

Assume now that ω satisfies case (4B). Rotate ω 180° around the point (x_0, y_0) to obtain ω_π. Because ω satisfies case (4B), ω_π falls into cases (i) and (III) above with a new (x_0, y_0) defined appropriately. Hence if ω_π falls into one of the cases (1), (2), (3A), (3B) and (4A) above it can be converted into a polygon with no contacts in the box as shown in figure 3 (within a distance 4 from the original (x_0, y_0)). If ω_π falls into case (4B) then ω must have the form depicted in figure 4.1.

Now assume that ω satisfies case (4B) and has the form depicted in figure 4.1. If the vertex (x_0, y_0) in ω is removed and the vertex $(x_0 - 1, y_0 + 1)$ is added a new polygon ω_1 is obtained by joining $(x_0 - 1, y_0 + 1)$ to $(x_0 - 1, y_0)$ by an edge and $(x_0 - 1, y_0 + 1)$ to $(x_0, y_0 + 1)$ by an edge. ω_1 is now a polygon which falls into cases (i) and (III) above with a new (x_0, y_0) (within a distance 2 of the original (x_0, y_0)) defined appropriately. Hence if ω_1 falls into one of the cases (1), (2), (3A), (3B), and (4A) above it can be converted into a polygon with no contacts in the box as shown in figure 3. If ω_1 falls into case (4B) then ω must have the form depicted in figure 4.2.

Now assume that ω satisfies case (4B) and has the form depicted in figure 4.2. If the vertex $(x_0 + 1, y_0)$ in ω is removed and the vertex $(x_0 + 2, y_0 - 1)$ is added a new polygon ω_2 is obtained by joining $(x_0 + 2, y_0 - 1)$ to $(x_0 + 2, y_0)$ by an edge and $(x_0 + 2, y_0 - 1)$ to $(x_0 + 1, y_0 - 1)$ by an edge. ω_2 is now a polygon which falls into cases (i) and (III) above with a new (x_0, y_0) defined appropriately. Hence if ω_2 falls into one of the cases (1), (2), (3A), (3B) and (4A) above it can be converted into a polygon with no contacts in the box as shown in figure 3. If ω_2 falls into case (4B) then either the contact can be removed as described above or ω must have the form depicted in figure 4.3.

Now assume that ω satisfies case (4B) and has the form depicted in figure 4.3. Note that figure 4.3 is invariant under rotation by 180° and that the configuration shown in figure 4.3 is contained in $v + R$. Figures 4.4(*a*) and (*b*) show three paths from figure 4.3 and the two possible ways in which they could be connected within the polygon ω (i.e. it is assumed that all the edges of ω are included in the polygon depicted in figures 4.4(*a*) or (*b*)). Let P_i represent the path from figure 4.3 that joins $A_{1,i}$ to $A_{2,i}$ in figure 4.4(*a*) and (*b*). If in the case depicted in figure 4.4(*a*) $A_{1,1}$ is joined to $A_{1,2}$ by a path, P', which is completely contained in $v + R$, then a polygon ω' can be obtained with no contacts in $v + R$ by performing the following transformation within $v + R$: delete P', the path from $A_{1,1}$ to $A_{1,1} - 2u_2$, and the path from $A_{1,2}$ to $A_{1,2} - 2u_2 - u_1$, and then add the vertex $A_{2,2} + 2u_2$ and edges between polygon vertices adjacent to it. A similar transformation can be applied if in figure 4.4(*a*) $A_{2,2}$ is joined by a path to $A_{2,3}$ within $v + R$ or if in figure 4.4(*b*) either $A_{2,1}$ is joined by a path to $A_{2,2}$ or $A_{1,2}$ is joined by a path to $A_{1,3}$ within $v + R$. Otherwise, one obtains the required polygon ω' from ω by deleting the three paths P_1, P_2 and P_3 from ω and adding new paths to create a new polygon. The former contact edge is used as an edge in one of the new paths and thus there is one less contact in the polygon. If the P_is are hooked up in ω as in figure 4.4(*a*), then the new path which uses the contact edge in $v + R$ is shown in figure 4.4(*c*). If the P_is are hooked up in ω as in figure 4.4(*b*), then the new path which uses the contact edge in $v + R$ is shown in figure 4.4(*d*). In either case, from a detailed case analysis[3] of all possible configurations of ω within $v + R$ it can be shown that figure 4.4(*c*) can be reconnected within $v + R$ to form a polygon ω' which has one less contact than ω and differs from ω only within $v + R$. □

Lemma 7. *Given $M_1 \geqslant 36$ and $M_2 \geqslant 5$ and given any tunnel-reduced polygon ω with n edges, $k \geqslant 1$ contacts, and with top contact vertex $v_t(\omega)$, one of the following two possibilities holds.*

(1) There is a tunnel-reduced polygon $\tilde{\omega}$ with $m \leqslant n$ edges, $k' < k$ contacts, and with its top contact vertex $v_t(\tilde{\omega}) < v_t(\omega)$, and such that $\tilde{\omega}$ equals ω everywhere outside the $2M_1 \times 2M_1$ box centred at $v_t(\omega)$ (that is, at least one contact can be removed from ω within a distance M_1 from v_t).

(2) There is a polygon $\tilde{\omega}$ with $m \leqslant n$ edges, $k' \leqslant k$ contacts such that $\tilde{\omega}$ equals ω everywhere outside the $2M_2 \times 2M_2$ box centred at $v_t(\omega)$ and $\tilde{\omega}$ contains exactly one r-tunnel, for some r such that $3 \leqslant r \leqslant 6$, within a distance M_2 of $v_t(\omega)$ and the lattice tree $\mathcal{T}$ associated with the r-tunnel is a lattice walk. Furthermore, let $T(\mathcal{T})$ be the tunnel polygon associated with $\mathcal{T}$. Then there is a unique m_1-edge, k_1-contact tunnel-reduced polygon ω_1 and a unique m_2-edge, k_2-contact tunnel-reduced polygon ω_2 both with their positions in Z^2 fixed and with $m_1 + m_2 + 2r = m$, $k_1 + k_2 + r \leqslant k'$, $v_t(\omega_2) < v_t(\omega_1) < v_t(\omega)$, and such that $\tilde{\omega} = [\omega_1 \cup \omega_2 \cup T(\mathcal{T})]'$, where the prime denotes that both edges of any double edges formed by the union of the edge sets of the graphs have been removed.

Proof. Given any tunnel-reduced polygon ω with n edges, $k \geqslant 1$ contacts, and with top contact vertex $v_t(\omega)$, the basic idea of the proof is to remove any contacts incident on $v_t(\omega)$ by either applying lemma 6 or by moving the contacts associated with $v_t(\omega)$ either to create an r-tunnel ($r \geqslant 3$) within a distance 5 of $v_t(\omega)$ or to isolate the contact(s) associated with $v_t(\omega)$ so that

[3] For the details, see http//math.usask.ca/∼soteros

lemma 6 can be applied to remove the contact(s). If an r-tunnel is created then two polygons, ω_1 and ω_2, can be obtained as in the tunnel reduction process described for lemma 4. The proof requires a detailed case analysis[4] dependent on the configuration of the polygon near $v_t(\omega)$. □

Lemma 8. *There exists an integer $\tilde{M} > 0$ such that given any tunnel-reduced polygon ω with n edges and k contacts, there exist non-negative integers $m > 0$, $b > 0$, j', $m_1 \geqslant 4, \ldots, m_b \geqslant 4$, $j_1, \ldots, j_b$, and $r_1 \leqslant j_1, r_2 < j_2, \ldots, r_b < j_b$ with $n - \tilde{M}^2 k \leqslant \sum_{i=1}^{b} m_i = m$, $2(b-1) \leqslant \sum_{i=1}^{b} j_i = j'$, $\sum_{i=1}^{b} r_i = b-1$, $m + 6(b-1) \leqslant n$, $j' + b - 1 \leqslant k$, and an algorithm for constructing from ω a b-tuple $((\tilde{\omega}_1, \mathcal{E}_1), \ldots, (\tilde{\omega}_b, \mathcal{E}_b))$ where $\tilde{\omega}_i$ is a polygon with m_i edges and 0 contacts; $\mathcal{E}_1$ is a j_1-tuple, $(\mathcal{E}_{1j}, j = 1, \ldots, j_1)$, of distinct vertices from the square lattice with $\mathcal{E}_{1j} > \mathcal{E}_{1j'}$ for any $j < j'$ and with r_1 of the vertices distinguished; $\mathcal{E}_i$ $(i > 1)$ is a j_i-tuple, $(\mathcal{E}_{ij}, j = 1, \ldots, j_i)$, of distinct vertices from the square lattice with one vertex designated as a root vertex, with $\mathcal{E}_{ij} > \mathcal{E}_{ij'}$ for any $j < j'$, and with r_i of the non-root vertices distinguished. Furthermore, the $(\tilde{\omega}_i, \mathcal{E}_i)$ satisfy the following.*

(1) Each vertex in $\mathcal{E}_i$ is either within a distance $\tilde{M}$ from another vertex which comes after it in $\mathcal{E}_i$ or within distance $\tilde{M}/2$ from a vertex of $\tilde{\omega}_i$.
(2) The last vertex in $\mathcal{E}_i$ is within a distance $\tilde{M}/2$ of a vertex of $\tilde{\omega}_i$.
(3) For $k \geqslant 1$, construct a graph Ω as follows. Translate $(\tilde{\omega}_1, \mathcal{E}_1)$ so that $\mathcal{E}_{11}$ coincides with the top vertex of the top contact of ω. Add the translated $\tilde{\omega}_1$ to Ω. For $i = 2, \ldots, r_1 + 1$, translate $(\tilde{\omega}_i, \mathcal{E}_i)$ so that the root vertex of $\mathcal{E}_i$ coincides with the $(i-1)$th distinguished vertex of the previously translated $\mathcal{E}_1$ and add the translated $\tilde{\omega}_i$ to Ω. Then for each $j = 2, \ldots, b$, and for $i = r_1 + \cdots + r_{j-1} + 2, \ldots, r_1 + \cdots + r_j + 1$, translate $(\tilde{\omega}_i, \mathcal{E}_i)$ so that the root vertex of $\mathcal{E}_i$ coincides with the $(i - 1 - \sum_{l=1}^{j-1} r_l)$th distinguished vertex of the previously translated $\mathcal{E}_{j-1}$ and add the translated $\tilde{\omega}_i$ to Ω. The resulting graph Ω differs from ω only within $j' - b + 1$ boxes of size $\tilde{M} \times \tilde{M}$ centred around the vertices specified by the translated $\mathcal{E}_i$s.

Proof. Consider a tunnel-reduced polygon ω with n edges and k contacts. For $k = 0$, set $b = 1$, $m = n$, $j' = j_1 = 0$, $\tilde{\omega}_1 = \omega$ and $\mathcal{E}_1 = \phi$. Otherwise, given a fixed $k \geqslant 1$, the goal is to remove all k contacts from this polygon and create the required b-tuple where the $\tilde{\omega}_i$s have no contacts.

The following is a description of the required algorithm for forming the b-tuple from ω. Initially, let the label set $L = \phi$. Starting at the top contact of ω we apply lemma 7 with $2M_1 = 2M_2 = \tilde{M} \equiv 72$. There are two possibilities, either (1) we obtain a tunnel-reduced polygon $\tilde{\omega}$ which has $k' \leqslant k-1$ contacts or (2) we obtain two tunnel-reduced polygons ω_1 and ω_2 with $v_t(\omega_2) < v_t(\omega_1) < v_t(\omega)$ and with k_1 and k_2 contacts, respectively, and m_1 and m_2 edges respectively such that $k_1 + k_2 \leqslant k - 3$ and $m_1 + m_2 \leqslant n - 6$. In the first case we let $v_t(\omega)$ be the first component of $\mathcal{E}_1$, add 1 to the label set L, and temporarily set $\tilde{\omega}_1 = \tilde{\omega}$. In the second case we let $v_t(\omega)$ be the first component of both $\mathcal{E}_1$ and $\mathcal{E}_2$, distinguish $v_t(\omega)$ in $\mathcal{E}_1$ and make it the root vertex in $\mathcal{E}_2$, add 1 and 2 to the label set L, and temporarily set $\tilde{\omega}_1 = \omega_1$ and $\tilde{\omega}_2 = \omega_2$. In this case, it is said that the distinguished vertex in $\mathcal{E}_1$ *leads to* the root vertex of $\tilde{\omega}_2$ or (equivalently) leads to $\tilde{\omega}_2$ and it is said that $(\tilde{\omega}_2, \mathcal{E}_2)$ is a *child* of $(\tilde{\omega}_1, \mathcal{E}_1)$. Note that in both cases, for each $i \in L$ the single component of $\mathcal{E}_i$ is within a distance $\tilde{M}/2$ of a vertex of $\tilde{\omega}_i$ so that properties (1) and (2) of the statement of this lemma are satisfied. Also $((\tilde{\omega}_i, \mathcal{E}_i), i \in L)$ satisfies property (3) of the statement of this lemma.

[4] The full details are provided at http//math.usask.ca/∼soteros

Assume an i'-tuple $((\tilde{\omega}_1, \mathcal{E}_1), \ldots, (\tilde{\omega}_{i'}, \mathcal{E}_{i'}))$ has been created with $\tilde{\omega}_i$ an m_i-edge, k_i-contact, tunnel-reduced polygon with: $\sum_{i=1}^{i'} k_i \leqslant k - 3(i'-1)$ and $n - \tilde{M}^2(k - \sum_{i=1}^{i'} k_i) \leqslant \sum_{i=1}^{i'} m_i \leqslant n - 6(i'-1)$; $\mathcal{E}_i$ a j_i-tuple of vertices of Z^2 with $2(i'-1) \leqslant \sum_{i=1}^{i'} j_i = j' \leqslant k-(i'-1)-\sum_{i=1}^{i'} k_i$ and for $i > 1$, one vertex designated as a root and for all i, r_i distinguished non-root vertices with $\sum_{i=1}^{i'} r_i = i' - 1$; and such that properties (1)–(3) of the statement of this lemma are satisfied. Let $L = \{1, 2, \ldots, i'\}$. Using the terminology introduced above, property (3) implies that for $j = 2, \ldots, i'$ and for $i = 2 + \sum_{l=1}^{j-1} r_l, \ldots, 1 + \sum_{l=1}^{j} r_l$, the $(i - 1 - \sum_{l=1}^{j-1} r_l)$th distinguished vertex of $\mathcal{E}_{j-1}$ leads to $\tilde{\omega}_i$ and that $(\tilde{\omega}_i, \mathcal{E}_i)$ is a child of $(\tilde{\omega}_{j-1}, \mathcal{E}_{j-1})$.

If for each $i \in L$, $\tilde{\omega}_i$ has 0 contacts then set $b = i'$ and stop because $((\tilde{\omega}_1, \mathcal{E}_1), \ldots, (\tilde{\omega}_{i'}, \mathcal{E}_{i'}))$ is the required b-tuple. Otherwise let i be the smallest number in L such that $\tilde{\omega}_i$ has at least one contact. Proceed to the top contact of $\tilde{\omega}_i$ and apply lemma 7. If case (1) of the lemma applies, then add $\tilde{v} \equiv v_t(\tilde{\omega}_i)$ to the end of $\mathcal{E}_i$ and redefine $\tilde{\omega}_i$ to be the polygon $\tilde{\omega}$ which results from the application of the lemma. If case (2) of the lemma applies, then consider the two polygons ω_1 and ω_2 which result from the application of the lemma. Each existing component of $\mathcal{E}_i$ is either within a distance $\tilde{M}$ from a later component of $\mathcal{E}_i$ or within a distance $\tilde{M}/2$ of a vertex of $\tilde{\omega}_i$. Thus each vertex $v_l^i = \mathcal{E}_{il}$ in $\mathcal{E}_i$ must be contained in a $2\tilde{M} \times 2\tilde{M}$ box centred at a vertex $v_{l'}^i = \mathcal{E}_{il'}, l' > l$ of $\mathcal{E}_i$ or contained in a $\tilde{M} \times \tilde{M}$ box centred at a vertex of $\tilde{\omega}_i$. Each $\mathcal{E}_i$ of this kind gives a unique set of planted plane trees, $t_1^i, \ldots, t_{s_i}^i$ ($s_i \leqslant j_i$), in the following way: if v_l^i is within a distance $\tilde{M}$ of some $v_{l'}^i$ ($l' > l$), then join v_l^i by an edge to $v_{l'}^i$ for the smallest such l'; otherwise (i.e. if there is no $l' > l$ such that v_l^i is within a distance $\tilde{M}$ of $v_{l'}^i$) join v_l^i by an edge to the closest vertex of $\tilde{\omega}_i$ (in case of ambiguity, choose the last vertex in a lexicographic ordering of the closest vertices). In the formation of this graph the vertices maintain their positions within the plane. (Note that if v_l^i is not within a distance $\tilde{M}$ of some $v_{l'}^i$ ($l' > l$) and if v_l^i is itself a vertex of $\tilde{\omega}_i$, then the vertex v_l^i is repeated in the graph but the duplicate vertex is placed in the plane in the location $v_l^i + (u_1 + u_2)/2$ and the two vertices are joined by an edge in the graph.) The resulting graph has no cycles (since all edges go from v_l^i to $v_{l'}^i$ for $l < l'$ or from v_l^i to a vertex of $\tilde{\omega}_i$) with up to j_i connected components all of which are plane trees. Each component ends at exactly one vertex of $\tilde{\omega}_i$ and each of these vertices has degree one (to see that this latter statement holds, suppose that a vertex v of $\tilde{\omega}_i$ has degree greater than one in the component t, then there are two vertices, v_l^i and $v_{l'}^i$ for $l < l'$, each within a distance $\tilde{M}/2$ of v, however, this means that v_l^i is within a distance $\tilde{M}$ of $v_{l'}^i$ and thus would have been joined by an edge to $v_{l'}^i$ and not to v in t). The vertices of $\tilde{\omega}_i$ associated with each component are distinct and are denoted $\rho_1^i > \cdots > \rho_{s_i}^i$; the component which contains ρ_l^i is planted at ρ_l^i and the resulting planted plane tree is called t_l^i. A vertex in $\mathcal{E}_i$ is said to be *associated* with the vertex ρ_l^i of $\tilde{\omega}_i$ if the vertex is on the planted plane tree t_l^i. If ρ_l^i is a vertex of ω_1 (ω_2) then all the vertices of $\mathcal{E}_i$ which are associated with ρ_l^i will also be considered to be associated with ω_1 (ω_2). If ρ_l^i is not a vertex of either ω_1 or ω_2, then it must be within a distance $\tilde{M}$ of $v_t(\tilde{\omega}_i)$ in which case it is said to be associated with the polygon ω_1. For $i > 1$ ($i = 1$), redefine $\tilde{\omega}_i$ to be the polygon ω_1 or ω_2 with which the root vertex of $\mathcal{E}_i$ (the first component of $\mathcal{E}_1$, $\mathcal{E}_{11}$) is associated and define $\tilde{\omega}_{i'+1}$ to be the other polygon. Define $\mathcal{E}_{i'+1}$ to be the subsequence of vertices of $\mathcal{E}_i$ associated with $\tilde{\omega}_{i'+1}$ and add $\tilde{v}$ to the end of $\mathcal{E}_{i'+1}$ as the root vertex of $\tilde{\omega}_{i'+1}$. Redefine $\mathcal{E}_i$ to be the subsequence of vertices of $\mathcal{E}_i$ associated with the new $\tilde{\omega}_i$ and add $\tilde{v}$ to the end of $\mathcal{E}_i$ as a distinguished vertex which leads to $\tilde{\omega}_{i'+1}$. Then $m_i, k_i, j_i, r_i, m_{i'+1}, k_{i'+1}, j_{i'+1}, r_{i'+1}$ are adjusted appropriately with now $n - \tilde{M}^2(k - \sum_{i=1}^{i'+1} k_i) \leqslant \sum_{i=1}^{i'+1} m_i = m \leqslant n - 6i'$, $\sum_{i=1}^{i'+1} k_i \leqslant k - i' - \sum_{i=1}^{i'+1} k_i$ and $2i' \leqslant \sum_{i=1}^{i'+1} j_i = j' \leqslant k - 2i'$. In order to ensure that property (3) holds, it is necessary next to relabel the 2-tuples $(\tilde{\omega}_l, \mathcal{E}_l)$ for $l = 1, \ldots, i' + 1$. This is done in a breadth-first fashion starting with the children of $(\tilde{\omega}_1, \mathcal{E}_1)$ and relabelling them with the numbers $2, \ldots, r_1 + 1$ in the order prescribed by the order of the distinguished vertices of $\mathcal{E}_1$ which lead to them. Then for each $j = 2, \ldots, i' + 1$, the children of the new $(\tilde{\omega}_j, \mathcal{E}_j)$ are relabelled with the numbers $r_1 + \cdots + r_{j-1} + 2, \ldots, r_1 + \cdots + r_j + 1$ in the order prescribed by the order of the distinguished vertices of $\mathcal{E}_j$ which lead to them. Add $i' + 1$ to L. If, for each $i \in L$, $\tilde{\omega}_i$ has 0 contacts then set $b = i' + 1$ and then $((\tilde{\omega}_1, \mathcal{E}_1), \ldots, (\tilde{\omega}_{i'+1}, \mathcal{E}_{i'+1}))$ is the required b-tuple; otherwise the process is repeated at most k times until the required b-tuple is obtained. □

Lemma 9. *For tunnel-reduced polygons in* Z^2*, for some constant* $C > 1$

$$\tilde{p}_n(k) \leqslant C^k \binom{2n}{k} p_n(0). \tag{2.49}$$

Proof. For $k \geqslant 1$, by the construction of lemma 8 each tunnel-reduced polygon with k contacts yields a b-tuple, for some $b > 0$, $((\tilde{\omega}_1, \mathcal{E}_1), \ldots, (\tilde{\omega}_b, \mathcal{E}_b))$ which depends on the index set of non-negative integers $S = \{m, j', b, m_1, \ldots, m_b, j_1, \ldots, j_b, r_1, \ldots, r_{b-1}\}$. To obtain an upper bound on $\tilde{p}_n(k)$ we note that

$$\tilde{p}_n(k) \leqslant \sum_{m=n-\tilde{M}^2 k}^{n} \sum_{j'=0}^{k} \sum_{b=1}^{b_{max}} \sum_{\{m_i\}} \sum_{\{j_i\}} \sum_{\{r_i\}} D_1(n, k, S) D_2(n, k, S) \tag{2.50}$$

where $D_1(n, k, S)$ is the maximum number of possible precursor n edge and k contact polygons of a b-tuple with index set S via the algorithm described in the proof of lemma 8; $D_2(n, k, S)$ is, for fixed n and k, the number of distinct b-tuples which result from the algorithm of lemma 8; and where $\sum_{\{m_i\}}$ denotes the sum over $\{m_i \geqslant 4, 1 \leqslant i \leqslant b | \sum_{i=1}^{b} m_i = m\}$, $\sum_{\{j_i\}}$ denotes the sum over $\{j_1 \geqslant 0, j_i > 0, 2 \leqslant i \leqslant b | \sum_{i=1}^{b} j_i = j'\}$, $\sum_{\{r_i\}}$ denotes the sum over $\{r_i \geqslant 0, 1 \leqslant i \leqslant b | \sum_{i=1}^{b} r_i = b - 1\}$, and $b_{max} = \min\{\frac{n-m}{6} + 1, k - j' + 1, \frac{j'}{2} + 1, \frac{m}{4}\}$. In fact, we calculate upper bounds $N_1(k) \geqslant D_1(n, k, S)$ and $N_2(n, k) \geqslant \sum_S D_2(n, k, S)$.

Since the vertices specified by the $\mathcal{E}_i$s determine the centres of $1 + \sum_{i=1}^{b}(j_i - 1) = j' - b + 1$ boxes in which changes to ω were made, an upper bound on the number of precursors to any b-tuple is thus given by $N_1(j' - b + 1) \equiv (2^{2\tilde{M}(\tilde{M}+1)})^{j'-b+1} \leqslant N_1(k)$, the number of ways to add or delete edges within each of the $j' - b + 1$ boxes.

Given $\tilde{\omega}_i$, then, as discussed in the proof of lemma 8, there is a one-to-one correspondence between $\mathcal{E}_i$ and a sequence of planted plane trees (with non-plant vertices in Z^2), $t_1^i, \ldots, t_{s_i}^i$ ($s_i \leqslant j_i$) such that each plant vertex is associated with a unique vertex of $\tilde{\omega}_i$ denoted, respectively, $\rho_1^i > \cdots > \rho_{s_i}^i$. Since the children of any non-plant vertex v of t_l^i (for some l) are vertices of $\mathcal{E}_i$ which are lexicographically larger than v and within a distance $\tilde{M}$ from v, thus the maximum number of children of a non-plant vertex of t_l^i is $V \equiv 2\tilde{M}(\tilde{M} + 1)$. The maximum number of choices for the child of the plant vertex is bounded above by $(\tilde{M}+1)^2 < V$. Thus, given $\tilde{\omega}_i$ and j_i, an upper bound on the number of ways to form $\mathcal{E}_i$ is given by the number of ways to do the following: (1) choose $s_i \leqslant j_i$ vertices of the polygon $\tilde{\omega}_i$ to be the plants for s_i planted plane trees, and then (2) choose a sequence of s_i abstract planted plane trees, $t_1^i, \ldots, t_{s_i}^i$, using a total of j_i non-plant vertices, and (3) starting with ρ_1^i and using the tree t_1^i, choose a vertex $u_{1,1}^i$ on the lattice within a distance $\tilde{M}/2$ of ρ_1^i to correspond to the child of the plant in t_1^i, choose vertices $u_{2,1}^i, \ldots, u_{2,c_1^i}^i$ on the lattice within a distance $\tilde{M}$ of $u_{1,1}^i$ to correspond to the c_1^i children of $u_{1,1}^i$ in t_1^i, ..., and similarly choose vertices on the lattice according to the remaining ρ_l^is and t_l^is, and (4) order the chosen vertices in decreasing lexicographic order (according to their coordinates). Let P_l be the number of abstract planted plane trees with l non-plant vertices, then (see, for example, [17])

$$P_{l_1} P_{l_2} \leqslant P_{l_1+l_2-1} \tag{2.51}$$

and for $l > 1$

$$P_l = \binom{2l-2}{l-1}\frac{1}{l} \tag{2.52}$$

and hence

$$P_l \leqslant 4^{l-1}. \tag{2.53}$$

Thus a bound on the number of ways to choose the vertices in $\mathcal{E}_i$ is

$$\begin{aligned}
\binom{V}{1}^{j_i} \sum_{s_i=1}^{j_i} \binom{m_i}{s_i} {\sum}' P_{e_1}\cdots P_{e_{s_i}} &\leqslant (V)^{j_i} P_{j_i} \sum_{s_i=1}^{j_i} \binom{m_i}{s_i}\binom{j_i-1}{s_i-1} \\
&= (V)^{j_i} P_{j_i} \sum_{s_i=1}^{j_i} \binom{m_i}{s_i}\binom{j_i-1}{j_i-s_i} \\
&= (V)^{j_i} P_{j_i} \binom{m_i+j_i-1}{j_i} \\
&\leqslant (16\tilde{M}^2)^{j_i} \binom{m_i+j_i-1}{j_i}
\end{aligned} \tag{2.54}$$

where the primed sum is over $\{e_l \geqslant 1, 1 \leqslant l \leqslant s_i \mid \sum_l e_l = j_i\}$. The number of ways to choose $\tilde{\omega}_i$ is $p_{m_i}(0)$ so that

$$U_i(m_i, j_i) = (16\tilde{M}^2)^{j_i} p_{m_i}(0) \binom{m_i+j_i-1}{j_i} \tag{2.55}$$

is an upper bound on the number of possible pairs $(\tilde{\omega}_i, \mathcal{E}_i)$ with m_i and j_i fixed but no vertices of $\mathcal{E}_i$ have been designated as a root or distinguished vertex.

The above argument gives an upper bound on the number of ways to choose the coordinates of the vertices of $\mathcal{E}_i$ relative to the coordinates of $\tilde{\omega}_i$. Next, by obtaining an upper bound on the number of ways to choose the root and distinguished vertices of $\mathcal{E}_i$ for $i = 1, \ldots, b$, an upper bound on the number of ways to position the $\tilde{\omega}_i$s relative to $\tilde{\omega}_1$ and hence relative to each other is obtained. Given the $\mathcal{E}_i$s, note that the number of ways to choose the root and distinguished vertices of $\mathcal{E}_i$ is given by $\binom{j_i}{1}\binom{j_i-1}{r_i}$ for $i \geqslant 2$ and is given by $\binom{j_i}{r_i}$ for $i = 1$. Thus we obtain the following upper bound on the number of distinct b-tuples $((\tilde{\omega}_i, \mathcal{E}_i), i = 1, \ldots, b)$ with parameter set S which could result from the algorithm of lemma 8,

$$\begin{aligned}
D_2(n, k, S) &\leqslant \binom{j_1}{r_1} \prod_{i=1}^{b} U_i(m_i, j_i) \left[\prod_{i=2}^{b} \binom{j_i}{1}\binom{j_i-1}{r_i}\right] \\
&= \binom{j_1}{r_1} (16\tilde{M}^2)^{j'} \prod_{i=1}^{b} p_{m_i}(0) \prod_{i=1}^{b} \binom{m_i+j_i-1}{j_i} \prod_{i=2}^{b} \binom{j_i}{1}\binom{j_i-1}{r_i}
\end{aligned} \tag{2.56}$$

and thus

$$
\begin{aligned}
\sum_S D_2(n,k,S) &\leqslant \sum_S p_m(0)(16\tilde{M}^2)^{j'}\binom{j_1}{r_1}\prod_{i=1}^{b}\binom{m_i+j_i-1}{j_i}\prod_{i=2}^{b}\binom{j_i}{1}\binom{j_i-1}{r_i}\\
&\leqslant \sum_m p_m(0)\sum_{j'}(16\tilde{M}^2)^{j'}\sum_b\sum_{\{m_i\}}\sum_{\{j_i\}}\prod_{i=1}^{b}\binom{m_i+j_i-1}{j_i}\\
&\quad\times\sum_{\{r_i\}}\binom{j_1}{r_1}\prod_{i=2}^{b}\binom{j_i}{1}\binom{j_i-1}{r_i}\\
&\leqslant \sum_m p_m(0)\sum_{j'}(16\tilde{M}^2)^{j'}\sum_b\binom{j'-b+1}{b-1}\sum_{\{m_i\}}\sum_{\{j_i\}}\prod_{i=1}^{b}\binom{m_i+j_i-1}{j_i}\prod_{i=2}^{b}\binom{j_i}{1}\\
&\leqslant \sum_m p_m(0)\sum_{j'}(16\tilde{M}^2)^{j'}\sum_b\binom{j'-b+1}{b-1}\binom{j'}{b}\sum_{\{m_i\}}\sum_{\{j_i\}}\prod_{i=1}^{b}\binom{m_i+j_i-1}{j_i}\\
&\leqslant \sum_m p_m(0)\sum_{j'}(16\tilde{M}^2)^{j'}\sum_b\binom{j'-b+1}{b-1}\binom{j'}{b}\sum_{\{m_i\}}\binom{m+j'-b}{j'}\\
&\leqslant \sum_m p_m(0)\sum_{j'}(16\tilde{M}^2)^{j'}\sum_b\binom{j'-b+1}{b-1}\binom{j'}{b}\binom{m+j'-b}{j'}\binom{m-1}{b-1}\\
&\leqslant \sum_m p_m(0)\sum_{j'}(64\tilde{M}^2)^{j'}\sum_b\binom{m+j'-b}{j'}\binom{m-1}{b-1}\\
&\leqslant p_n(0)(64\tilde{M}^2)^k\sum_m\sum_{j'}\sum_b\binom{m+j'-b}{j'}\binom{m-1}{b-1}\\
&\leqslant p_n(0)(64\tilde{M}^2)^k\sum_m\sum_{j'}\sum_b\binom{n+k-1}{j'}\binom{n-1}{b-1}\\
&\leqslant p_n(0)(64\tilde{M}^2)^k\sum_m\sum_{j'}\sum_b\binom{n+k-1}{j'}\binom{n-1}{k-j'}\\
&\leqslant p_n(0)(64\tilde{M}^2)^k\sum_m\sum_b\binom{2n+k-2}{k}\\
&\leqslant p_n(0)(64\tilde{M}^2)^k(\tilde{M}^2k+1)(k+1)\binom{2n+k-2}{k}\\
&= p_n(0)(64\tilde{M}^2)^k(\tilde{M}^2k+1)(k+1)\sum_{s=0}^{k}\binom{2n-2}{s}\binom{k}{k-s}\\
&\leqslant p_n(0)(64\tilde{M}^2)^k(\tilde{M}^2k+1)(k+1)2^k\binom{2n-2}{k}\\
&\leqslant p_n(0)(512\tilde{M}^2)^k\binom{2n-2}{k}\tilde{M}^2 \leqslant p_n(0)(2^{11}\tilde{M}^4)^k\binom{2n}{k} \equiv N_2(n,k).
\end{aligned}
\tag{2.57}
$$

Putting all the bounds together gives

$$\tilde{p}_n(k) \leqslant N_1(k)N_2(n,k) = (2^{11+2\tilde{M}(\tilde{M}+1)}\tilde{M}^4)^k \binom{2n}{k} p_n(0). \tag{2.58}$$

Thus we have the required result provided $C \geqslant 2^{11+2\tilde{M}(\tilde{M}+1)}\tilde{M}^4$. □

Lemma 10. *For polygons in* Z^2*, for some constant* $C' > 1$

$$p_n(k) \leqslant (C')^k \binom{6n}{k} p_n(0). \tag{2.59}$$

Proof. Applying lemmas 3, 5 and 9 yields

$$\begin{aligned} p_n(k) &\leqslant (64\lambda)^k \sum_{k'=0}^{k} \binom{2n}{k-k'} \hat{p}_n(k') \\ &\leqslant (64\lambda)^k \sum_{k'=0}^{k} \binom{2n}{k-k'} (256)^{k'} \sum_{j'=0}^{k'} \binom{2n}{k'-j'} \tilde{p}_n(j') \\ &\leqslant (64\lambda)^k \sum_{k'=0}^{k} \binom{2n}{k-k'} (256)^{k'} \sum_{j'=0}^{k'} \binom{2n}{k'-j'} C^{j'} \binom{2n}{j'} p_n(0) \\ &\leqslant (2^{18}C\lambda)^k p_n(0) \sum_{k'=0}^{k} \binom{2n}{k-k'} \sum_{j'=0}^{k'} \binom{2n}{k'-j'} \binom{2n}{j'} \\ &= (2^{18}C\lambda)^k \binom{6n}{k} p_n(0) \end{aligned} \tag{2.60}$$

which gives the required result for $C' \geqslant 2^{29+2\tilde{M}(\tilde{M}+1)}\tilde{M}^4\lambda$. □

We next prove a slightly weakened version of (b) for polygons in Z^2.

Theorem 5. *For polygons in* Z^2*, for fixed* k *there are constants* $B_1, B_2 > 0$ *independent of* n *and a positive integer* N *such that for* $n > N$

$$B_1 n^k p_n(0) \leqslant p_n(k) \leqslant B_2 n^k p_n(0). \tag{2.61}$$

Proof. This follows immediately from corollary 1 and lemma 10. □

3. Properties of the free energy

Let $Z_n^0(\beta) = \sum_k p_n(k)\mathrm{e}^{\beta k}$. The limit in equation (1.3) has been proved to exist [2, 3]. We now prove a corollary on the behaviour of $\mathcal{F}_0(\beta)$ as $\beta \to -\infty$.

Corollary 3. *For polygons in* Z^2*, for some constants* $C > 0$ *and* $\epsilon > 0$

$$\kappa_0 + \epsilon \log(1 + \mathrm{e}^{\beta}) \leqslant \mathcal{F}_0(\beta) \leqslant \kappa_0 + 6\log(1 + C\mathrm{e}^{\beta}). \tag{3.1}$$

Hence $\mathcal{F}_0(\beta)$ *is strictly greater than but asymptotic to* κ_0 *as* $\beta \to -\infty$*.*

Proof. From corollary 1 and lemma 10 with $C = C'$ we have the inequalities

$$\sum_k \binom{\lfloor \epsilon n \rfloor}{k} p_n(0) \mathrm{e}^{\beta k} \leqslant Z_n^0(\beta) \leqslant \sum_k \binom{6n}{k} C^k p_n(0) \mathrm{e}^{\beta k}. \tag{3.2}$$

Hence

$$p_n(0)(1 + \mathrm{e}^{\beta})^{\lfloor \epsilon n \rfloor} \leqslant Z_n^0(\beta) \leqslant p_n(0)(1 + C\mathrm{e}^{\beta})^{6n} \tag{3.3}$$

and the result follows by taking logarithms, dividing by n, and letting $n \to \infty$. □

The next corollary proves the analogue of (c) for polygons in Z^2 with $0 < a < 1$. This corollary implies $0 < \lim_{n\to\infty} \langle k \rangle_n / n < 1$, provided the limit exists.

Corollary 4. *If the free energy $\mathcal{F}_0(\beta)$ is differentiable at $\beta = 0$ then*

$$0 < \lim_{n\to\infty} \langle k \rangle_n / n < 1. \tag{3.4}$$

Otherwise

$$0 < \lim_{\beta\to 0^-} \mathcal{F}_0'(\beta) \leqslant \liminf_{n\to\infty} \langle k \rangle_n / n < \limsup_{n\to\infty} \langle k \rangle_n / n \leqslant \lim_{\beta\to 0^+} \mathcal{F}_0'(\beta) < 1. \tag{3.5}$$

Proof. Note that

$$\lim_{n\to\infty} \langle k \rangle_n / n = \lim_{n\to\infty} n^{-1} \left. \frac{\partial \log Z_n^0(\beta)}{\partial \beta} \right|_{\beta=0}. \tag{3.6}$$

$\mathcal{F}_0(\beta)$ is a convex, monotonically increasing function of β asymptotic to and bounded below by a line with slope one as β goes to infinity [2, 3]. This together with corollary 3 shows that $\mathcal{F}_0(\beta)$ is strictly monotonically increasing so the derivative, if it exists, at $\beta = 0$ must be positive and less than one. Since $\mathcal{F}_0(\beta)$ is convex, if the derivative at $\beta = 0$ exists, the order of the limit and derivative can be reversed in equation (3.6), so that $\lim_{n\to\infty} \langle k \rangle / n = \mathcal{F}_0'(0)$. Suppose that $\mathcal{F}_0(\beta)$ is not differentiable at $\beta = 0$. Convexity implies that there exists an interval $(0, \alpha)$ such that $\mathcal{F}_0(\beta)$ is differentiable inside this interval. Define

$$f_n(\beta) = n^{-1} \log Z_n^0(\beta). \tag{3.7}$$

Let $\beta \in (0, \alpha)$. Convexity of $f_n(\beta)$ implies that

$$f_n'(0) \leqslant f_n'(\beta) \tag{3.8}$$

so that

$$\limsup_{n\to\infty} f_n'(0) \leqslant \lim_{n\to\infty} f_n'(\beta) = \mathcal{F}_0'(\beta) \tag{3.9}$$

and hence

$$\limsup_{n\to\infty} f_n'(0) \leqslant \lim_{\beta\to 0^+} \mathcal{F}_0'(\beta). \tag{3.10}$$

Similarly, there exists $\gamma > 0$ such that $\mathcal{F}_0(\beta)$ is differentiable for all $\beta \in (-\gamma, 0)$ so that

$$\lim_{\beta\to 0^-} \mathcal{F}_0'(\beta) \leqslant \liminf_{n\to\infty} f_n'(0). \tag{3.11}$$

This completes the proof. □

4. Polygons with a density of contacts

In this section we consider polygons with a fixed density of contacts. We show that the number of such polygons grows exponentially and investigate the dependence of the exponential growth rate on the density of contacts. We first note that all except exponentially few polygons have a positive density of contacts confirming the observation of Douglas and Ishinabe [5] and Douglas *et al* [6]. This follows immediately from the pattern theorem for self-avoiding polygons [18] by taking the K-pattern $W = u_1 u_2 \bar{u}_1$. Our general approach is similar to that used by Madras *et al* [19] in the study of lattice animals with fixed cyclomatic index.

Let $q_n(\alpha) = p_n(\lfloor \alpha n \rfloor)$.

Lemma 11. *The connective constant $\kappa(\alpha)$ defined by*

$$\lim_{n\to\infty} n^{-1} \log q_n(\alpha) \equiv \kappa(\alpha) \tag{4.1}$$

exists.

Proof. Any polygon with n_1 edges and k_1 contacts can be concatenated with any polygon with n_2 edges and k_2 contacts to create a polygon with $n_1 + n_2$ edges and $k_1 + k_2 + 2$ contacts. This implies the inequality

$$\frac{p_{n_1}(k_1) p_{n_2}(k_2)}{d-1} \leqslant p_{n_1+n_2}(k_1 + k_2 + 2) \tag{4.2}$$

where the factor of $d - 1$ accounts for rotations [7]. Setting $k_1 = \lfloor \alpha n_1 \rfloor$ and $k_2 = \lfloor \alpha n_2 \rfloor$, we obtain the generalized supermultiplicative inequality

$$\frac{q_{n_1}(\alpha) q_{n_2}(\alpha)}{d-1} \leqslant q_{n_1+n_2}(\alpha + f(\alpha, n_1, n_2)) \tag{4.3}$$

where $0 \leqslant f(\alpha, n_1, n_2) \leqslant \frac{3}{n_1+n_2}$ so that $\lim_{n_1+n_2\to\infty} f(\alpha, n_1, n_2) = 0$.

Since $q_n(\alpha) \leqslant p_n$ it is exponentially bounded and the existence of the limit then follows from standard subadditivity arguments [8–10]. □

Lemma 12. *$\kappa(\alpha)$ is a concave function of α.*

Proof. Setting $k_1 = \lfloor \alpha_1 n \rfloor$ and $k_2 = \lfloor \alpha_2 n \rfloor$ in equation (4.2), we obtain

$$\frac{q_n(\alpha_1) q_n(\alpha_2)}{d-1} \leqslant q_{2n}\left(\frac{\alpha_1 + \alpha_2}{2} + f\left(\frac{\alpha_1 + \alpha_2}{2}, n, n\right)\right) \tag{4.4}$$

where the function f is as in lemma 11. Taking logarithms, dividing by $2n$, and letting n go to infinity gives

$$\frac{\kappa(\alpha_1) + \kappa(\alpha_2)}{2} \leqslant \kappa\left(\frac{\alpha_1 + \alpha_2}{2}\right). \tag{4.5}$$

□

Lemma 13. *For $d = 2$,*

$$\lim_{\alpha\to 0^+} \kappa(\alpha) = \kappa_0. \tag{4.6}$$

For $d \geqslant 3$

$$\lim_{\alpha\to 0^+} \kappa(\alpha) \geqslant \kappa_0. \tag{4.7}$$

Proof. For $d = 2$, from lemma 10 and lemma 2.4 of Madras *et al* [19]

$$\lim_{n\to\infty} n^{-1} \log q_n(\alpha) \leqslant \alpha \log C' + 6 \log 6 - \alpha \log \alpha - (6-\alpha)\log(6-\alpha) + \kappa_0. \tag{4.8}$$

For all d, from corollary 1 for any $\alpha < \epsilon$

$$\lim_{n\to\infty} n^{-1} \log q_n(\alpha) \geqslant \epsilon \log \epsilon - \alpha \log \alpha - (\epsilon - \alpha)\log(\epsilon - \alpha) + \kappa_0. \tag{4.9}$$

Hence, letting $\alpha \to 0^+$ in equations (4.8) and (4.9), for $d = 2$ we obtain continuity at $\alpha = 0$ (i.e. equation (4.6)). Letting $\alpha \to 0^+$ in equation (4.9), we obtain equation (4.7). □

Theorem 6. *For $d = 2$,*

(a)
$$\lim_{\alpha\to 0^+} \frac{\mathrm{d}\kappa(\alpha)}{\mathrm{d}\alpha} = \infty. \tag{4.10}$$

For all d

(b)
$$\max_{\alpha} \kappa(\alpha) = \kappa. \tag{4.11}$$

Proof.

(a) The right derivative of $\kappa(\alpha)$ exists by concavity. Differentiating equation (4.9) then shows that the right derivative must be infinite.
(b) Define $\alpha_n^* = \min\{\alpha | q_n(\alpha) \geqslant q_n(\beta), \forall \beta\}$. Then

$$q_n(\alpha_n^*) \leqslant p_n = \int_0^{d-1} q_n(\alpha)\,\mathrm{d}\alpha \leqslant (d-1) q_n(\alpha_n^*) \tag{4.12}$$

so that

$$\kappa = \lim_{n\to\infty} n^{-1} \log q_n(\alpha_n^*) \tag{4.13}$$

and since

$$\max_{\alpha} \kappa(\alpha) = \lim_{n\to\infty} n^{-1} \log q_n(\alpha_n^*) \tag{4.14}$$

(b) follows.

□

Corollary 5. *For $d = 2$,*

$$\lim_{n\to\infty; k=o(n)} n^{-1} \log p_n(k) = \kappa_0. \tag{4.15}$$

5. Conclusions

With regard to the conjectures for self-avoiding walks with a fixed number of contacts, made by Douglas *et al* [5, 6], we have proved (a) for self-avoiding walks and polygons in Z^d and somewhat weakened versions of (b) and (c) for polygons in Z^2. We also investigated the form of the connective constant, $\kappa(\alpha)$, for polygons with a density, α, of contacts. We showed that the connective constant exists, is a concave function of α, and is equal to the connective constant of self-avoiding walks for some value of α. For $d = 2$, we showed that $\lim_{\alpha\to 0^+} \kappa(\alpha) = \kappa_0$ and that $\kappa(\alpha)$ has infinite derivative at $\alpha = 0$.

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