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The statistics of collapsing square lattice trails with a fixed number of vertices of degree 4

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Abstract

A trail on the square lattice with a fixed number, k, of vertices of degree 4 is called a k-trail. We model polymer collapse using k-trails by incorporating an interaction energy which is proportional to the number of nearest-neighbour contact edges of the trail. It is known that the number of square lattice n-edge closed (open) k-trails can be bounded above and below (to $O(n^k)$) by the number of n-step self-avoiding circuits (walks). This along with pattern theorems for self-interacting self-avoiding circuits and walks are used herein to establish upper and lower bounds (to $O(n^k)$) for the collapsing free energy of k-trails in terms of self-avoiding circuits or walks, as appropriate. We also use pattern theorems to obtain bounds on the limiting nearest-neighbour contact density for collapsing k-trails. Finally, we investigate k-trails with a fixed density of nearest-neighbour contacts and show that their limiting entropy per monomer is independent of k.

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1. Introduction

High molecular weight polymers in dilute solution have been observed to undergo a *collapse transition* as the solvent quality is reduced [1–3]. In these experiments, a linear polymer is typically in an expanded coil state under good solvent conditions but *collapses* into a globular state (minimizing monomer–solvent interactions) under poor solvent conditions. Lattice models of polymers have been used to model and understand this transition (see [4] and references therein). One question of interest has been determining how the collapsing free energy and ultimately the transition temperature depend on the polymer structure [5, 6], i.e. such as whether the polymer is linear, branched or a ring polymer. In this paper, we focus on how the collapsing free energy depends on polymer structure in the case that the structure is determined by a set of planar Eulerian graphs, i.e. trails. As in the standard model for interacting self-avoiding walks (ISAWs) [5], the models for collapse studied here incorporate an interaction energy which is proportional to the number of nearest-neighbour contact edges (lattice edges which are incident on two vertices of the trail but which are not edges of the trail).

Recently [7], we focused on the number of n-step trails with a fixed number, k, of vertices of degree 4 (k-trails) and derived combinatorial bounds relating the number of such trails to the number of n-step self-avoiding walks or circuits. In particular, we established that the number of square lattice n-edge closed (open) k-trails can be bounded above and below (to $O(n^k)$) by the number of n-step self-avoiding circuits (walks). This work extended and improved the arguments first given by Zhao and Lookman [8] on a similar question. Zhao and Lookman [8] also studied the collapsing free energy of closed (open) k-trails and found bounds for the free energy in terms of that for self-avoiding circuits (walks). In this paper, we use the arguments in [7] and the pattern theorems in [9] to establish tighter bounds (to $O(n^k)$) between the collapsing free energy of closed (open) k-trails and that of self-avoiding circuits (walks). These results indicate that for trails, the limiting collapsing free energy and the collapse transition temperature, if they exist, are independent of the fixed number of vertices of degree 4 while the collapsing free energy critical exponent, if it exists, is increased by 1 for each vertex of degree 4.

Soteros and Whittington [10] obtained bounds on the limiting density of contacts for the collapsing free energy of self-avoiding polygons (SAPs). We extend their arguments to k-trails and using the pattern theorem for collapsing SAPs [9], establish new bounds on the contact density for k-trails.

In addition, we investigate k-trails with a fixed density of contacts and show that their limiting entropy per monomer is independent of k.

Since a trail is a walk with no repeated edges, trails can be viewed as an intermediate model between random walks (edges and vertices can be traversed more than once) and self-avoiding walks (no repeated vertices or edges) for incorporating the excluded volume property into a polymer model. Based on this, another approach for investigating the collapse of trails is one which incorporates an interaction energy which is proportional to the number of repeated vertices (or intersections) in the trail [11–13] instead of the number of contact edges. For closed k-trails on the square lattice, the number of repeated vertices is k while for open k-trails it is the number of degree 3 vertices plus k (which is at most $k+2$). Recent numerical evidence [14, 15] reinforces earlier arguments [11–13] that this model of collapsing trails is in a different universality class from ISAWs. While our model of collapsing trails cannot be used to address this universality class issue, our results are a first step towards analysing a two-variable model which can be used for this purpose. Such a two-variable model would incorporate an interaction energy proportional to the number of nearest-neighbour contact edges and an interaction energy proportional to the number of degree 4 vertices; this is similar to a two-variable model that has been used to study lattice animal models of branched polymer collapse [16]. However, since the two-variable model is not investigated directly in this work, we do not discuss it further here.

In order to introduce our results more precisely, some terminology and definitions are required first. These and a more detailed description of our results are presented next.

1.1. Terminology and statement of results

The notation used is similar to that in [7] with a focus on $\mathbb{Z}^2$. For $v = (v_1, v_2), w = (w_1, w_2) \in \mathbb{R}^2$, define $\|v - w\| = |v_1 - w_1| + |v_2 - w_2|$. The square lattice $\mathbb{Z}^2$ will be viewed as the infinite graph with a vertex set $V(\mathbb{Z}^2) = \{(x_1, x_2)|x_i \in \mathbb{Z}, i = 1, 2\}$ and an edge set $\mathbb{E}(\mathbb{Z}^2) = \{\{v, w\}|v, w \in V(\mathbb{Z}^2), \|v - w\| = 1\}$.

An n-step *self-avoiding walk* (n-SAW), ω, in the square lattice is a sequence of distinct vertices $r_0, r_1, \ldots, r_n$ in $V(\mathbb{Z}^2)$ such that r_{i-1} and r_i are joined by an edge in $\mathbb{E}(\mathbb{Z}^2)$ for $i = 1, \ldots, n$. The n-SAW ω is said to start at r_0 and end at r_n and, for $i = 1, \ldots, n$, the edge from r_{i-1} to r_i is called the ith step of the walk. The number of n-SAWs in $\mathbb{Z}^2$ starting at the origin is denoted by c_n. Given a SAW ω, an edge in $\mathbb{Z}^2$ which is incident on two vertices of ω but is not a step of ω is called a *contact* edge of ω. The number of n-SAWs in $\mathbb{Z}^2$ starting at the origin and containing l contact edges is denoted by $c_n(l)$.

Given any n-SAW, ω, one may ignore the direction on its edges in order to obtain $\tilde{\omega}$, the n-step *undirected self-avoiding walk* (n-USAW), which is the underlying graph of ω. Two n-USAWs are considered equivalent if one is a translate of the other. The number of distinct n-USAWs in $\mathbb{Z}^2$ is denoted by u_n and the number of these containing l contacts is denoted by $u_n(l)$. Note that there are exactly two possible orientations which could be chosen for $\tilde{\omega}$ in order to create two distinct n-SAWs. Therefore, $c_n = 2u_n$ and $c_n(l) = 2u_n(l)$.

An n-step *trail*, σ, in $\mathbb{Z}^2$ starting at s_0 is a sequence of n distinct edges $\alpha_1, \alpha_2, \ldots, \alpha_n$ in $\mathrm{E}(\mathbb{Z}^2)$ such that $\alpha_i = \{s_{i-1}, s_i\}$ for $i = 1, ..., n$. The n-step trail $\mathrm{rev}(\sigma) \equiv (\alpha_n, \alpha_{n-1}, \ldots, \alpha_1)$, obtained by reversing the order of σ's edges, is referred to as the *reverse trail* of σ. Note that if $s_0, s_1, \ldots, s_n$ are distinct vertices in $V(\mathbb{Z}^2)$, then σ is an n-SAW. The number of n-step trails in $\mathbb{Z}^2$ starting at the origin is denoted by t_n and the number of n-step k-trails (trails containing k vertices of degree 4) with l contact edges is denoted $t_n(k, l)$. An n-step closed trail or *trailgon* is a trail such that $s_0 = s_n$. The number of n-step trailgons in $\mathbb{Z}^2$ starting at the origin is denoted t_n° and the number of such trailgons containing k vertices of degree 4 (k-trailgons or closed k-trails, for short) and l contact edges is denoted $t_n^\circ(k, l)$. For any $i = 1, \ldots, n$, the n-step trailgon $\mathrm{cyc}_{s_{i-1}}(\sigma) \equiv (\alpha_i, \alpha_{i+1}, \ldots, \alpha_n, \alpha_1, \alpha_2, \ldots, \alpha_{i-1})$, obtained from an n-step trailgon σ by a cyclic permutation of its edges, is referred to as the *cyclic permutation of* σ starting at s_{i-1}. A trail which is not closed is called an *open trail*. The number of n-step open trails in $\mathbb{Z}^2$ starting at the origin is denoted by $\check{t}_n$ and the number of n-step open k-trails with l contact edges is denoted $\check{t}_n(k, l)$.

An n-step *self-avoiding circuit* (n-SAC) is a trailgon such that the vertices $s_0, \ldots, s_{n-1}$ are all distinct. The number of n-SACs in $\mathbb{Z}^2$ starting at the origin is denoted by q_n and $q_n(l)$ denotes the number of these containing l contact edges. For a given n-SAC σ, $\{\mathrm{cyc}_{s_{i-1}}(\sigma), \mathrm{cyc}_{s_{i-1}}(\mathrm{rev}(\sigma)), i = 1, \ldots, n\}$ forms a set of $2n$ distinct n-SACs. This set of n-SACs can be regarded as a single geometrical entity, which is called an n-edge *self-avoiding polygon* (n-SAP). Equivalently an n-SAP is a connected n-edge, n-vertex subgraph of $\mathbb{Z}^2$ in which each vertex has degree 2. Two n-SAPs are considered equivalent if one is a translate of the other. The number of distinct n-SAPs in $\mathbb{Z}^2$ is denoted by p_n and the number of these containing l contact edges is denoted by $p_n(l)$. Note that $q_n = 2np_n$ and $q_n(l) = 2np_n(l)$.

An abstract-connected graph τ is said to be *homeomorphically irreducible* if it has no vertices of degree 2, or if it has exactly one vertex, and this vertex has degree 2 (i.e. a *loop graph*). Let $\mathcal{G}$ be the set of all homeomorphically irreducible abstract-connected planar graphs having at least one edge and with maximum vertex degree less than or equal to 4. Given a graph $\tau \in \mathcal{G}$, an n-tau in $\mathbb{Z}^2$ is defined to be an n-edge subgraph of $\mathbb{Z}^2$ which is *homeomorphic* to τ (i.e., isomorphic to τ when vertices of degree 2 are suppressed). An n-SAP is considered an embedding of the loop graph. The number of distinct (up to translation) n-taus in $\mathbb{Z}^2$ is denoted by $g_n(\tau)$ and the number of these containing l contact edges is denoted $g_n(\tau, l)$.

Let $\mathcal{G}_i(k)$ be the subset of $\mathcal{G}$ consisting of graphs with i vertices of odd degree and exactly k vertices of degree 4. For any $\tau \in \mathcal{G}_2(k)$ ($\mathcal{G}_0(k)$), Euler's theorem [18] implies that τ contains an open (closed) *Euler trail* which uses every edge of the graph exactly once and hence each

n-tau may be converted to an open (closed) n-step trail, by finding an Euler trail of the n-tau. We thus refer to $\tau \in \mathcal{G}_2(k)$ ($\mathcal{G}_0(k)$) as an *open (closed) Eulerian graph with k vertices of degree 4*, or an *open (closed) k-graph*, for short. The number (up to translation) of n-edge embeddings in $\mathbb{Z}^2$ of all open k-graphs is defined by

$$\check{E}_n(k) \equiv \sum_{\tau \in \mathcal{G}_2(k)} g_n(\tau), \tag{1.1}$$

while the number (up to translation) of n-edge embeddings in $\mathbb{Z}^2$ of all closed k-graphs is defined by

$$\mathring{E}_n(k) \equiv \sum_{\tau \in \mathcal{G}_0(k)} g_n(\tau). \tag{1.2}$$

Similarly, the number (up to translation) of n-edge embeddings in $\mathbb{Z}^2$ of all open k-graphs with l contacts is defined by

$$\check{E}_n(k, l) \equiv \sum_{\tau \in \mathcal{G}_2(k)} g_n(\tau, l), \tag{1.3}$$

and the number (up to translation) of n-edge embeddings in $\mathbb{Z}^2$ of all closed k-graphs with l contacts is defined by

$$\mathring{E}_n(k, l) \equiv \sum_{\tau \in \mathcal{G}_0(k)} g_n(\tau, l). \tag{1.4}$$

Bounds relating k-trails and k-graphs were established in [7, equation (1.18)] and those arguments lead *mutatis mutandis* to

$$2\check{E}_n(k, l) \leqslant \check{t}_n(k, l) \leqslant 4(3)^{k+1}\check{E}_n(k, l) \tag{1.5}$$

and

$$2n\mathring{E}_n(k, l) \leqslant \mathring{t}_n(k, l) \leqslant 2(3)^k n\mathring{E}_n(k, l). \tag{1.6}$$

Hammersley [19, 20] proved (see also [21]) that

$$0 < \lim_{n\to\infty} n^{-1} \log c_n = \lim_{n\to\infty} n^{-1} \log p_n \equiv \log \mu < \log 3, \tag{1.7}$$

where the second limit is taken through even values of n. Given any $\tau \in \mathcal{G}$, there exists $n > 0$ such that $g_n(\tau) > 0$ [17, section 4). Hence the arguments given in the proof of [22, theorem 4.2] can be applied to establish that for any $\tau \in \mathcal{G}$,

$$0 < \lim_{n\to\infty} n^{-1} \log g_n(\tau) = \log \mu, \tag{1.8}$$

where the limit is taken through all values of n for which $g_n(\tau) > 0$. Hence the number of n-taus increases exponentially with n, at a rate which is independent of τ, and at the same rate as that for n-SAWs. Guttmann [23] proved the existence of the following limit for lattice trails and Zhao and Lookman [8] proved the second inequality in

$$0 < \log \mu < \lim_{n\to\infty} n^{-1} \log t_n \equiv \log \mu_T. \tag{1.9}$$

For each of these models, we define a collapsing free energy by introducing an interaction energy which is proportional to the number of contact edges. In particular, we define the following partition functions:

$$P_n(\beta) = \sum_{l=0}^{n} p_n(l)\, \mathrm{e}^{\beta l}; \qquad U_n(\beta) = \sum_{l=0}^{n+2} u_n(l)\, \mathrm{e}^{\beta l}; \tag{1.10}$$

$$Q_n(\beta) = \sum_{l=0}^{n} q_n(l)\,\mathrm{e}^{\beta l}; \qquad C_n(\beta) = \sum_{l=0}^{n+2} c_n(l)\,\mathrm{e}^{\beta l}; \tag{1.11}$$

$$T_n^o(k,\beta) = \sum_{l=0}^{n-2k} t_n^o(k,l)\,\mathrm{e}^{\beta l}; \qquad \check{T}_n(k,\beta) = \sum_{l=0}^{n-2k+2} \check{t}_n(k,l)\,\mathrm{e}^{\beta l}; \tag{1.12}$$

$$T_n^o(\beta) = \sum_{k} T_n^o(k,\beta); \qquad \check{T}_n(\beta) = \sum_{k} \check{T}_n(k,\beta); \tag{1.13}$$

$$\mathring{\mathcal{E}}_n(k,\beta) = \sum_{l=0}^{n-2k} \mathring{E}_n(k,l)\,\mathrm{e}^{\beta l}; \qquad \check{\mathcal{E}}_n(k,\beta) = \sum_{l=0}^{n-2k+2} \check{E}_n(k,l)\,\mathrm{e}^{\beta l}; \tag{1.14}$$

$$T_n(\beta) = \sum_{l=0}^{n+2} t_n(l)\,\mathrm{e}^{\beta l}; \qquad G_n(\tau,\beta) = \sum_{l=0}^{n-2k+i-j} g_n(\tau,l)\,\mathrm{e}^{\beta l}, \tag{1.15}$$

where $\tau \in \mathcal{G}$ and i, j, k denote, respectively, the number of degree 1, 3, 4 vertices in τ. To get the upper bounds for l in the above summations, note first that any n-tau of $\mathbb{Z}^2$ has $n - 2k - \frac{3j+i}{2}$ degree 2 vertices (by the handshaking lemma, see, for example, [18]). Then each vertex of degree $m \in \{1, 2, 3\}$ is an end point of at most $4 - m$ contacts so that the number of contact edge end points in a given n-tau is at most $2n - 4k + 2i - 2j$ and the number of contact edges is at most $n - 2k + i - j$ (since each contact edge has two end points). For closed k-graphs and trailgons, $i = j = 0$ while for open k-graphs and trails, $i - j \in \{-2, 0, 2\}$ so that $i - j \leqslant 2$.

Taking the logarithm and then dividing by n for any one of the partition functions above yields the reduced *collapsing free energy* per monomer for the corresponding model. It is known that [5, 24]

$$\lim_{n\to\infty} n^{-1} \log P_n(\beta) \equiv \mathcal{P}(\beta) \tag{1.16}$$

exists and is finite for all finite β. It has also been proved that

$$\lim_{n\to\infty} n^{-1} \log C_n(\beta) = \mathcal{P}(\beta) \tag{1.17}$$

for all $\beta \leqslant 0$ [5, 24, 25]; however, the existence of the limit on the left-hand side has yet to be proved to exist for $\beta > 0$. Arguments given in Zhao and Lookman [8] lead to

$$\lim_{n\to\infty} n^{-1} \log g_n\big(\tau_k^0,\beta\big) = \lim_{n\to\infty} n^{-1} \log T_n^o(k,\beta) = \mathcal{P}(\beta) \tag{1.18}$$

for all β, and to

$$\lim_{n\to\infty} n^{-1} \log g_n\big(\tau_k^2,\beta\big) = \lim_{n\to\infty} n^{-1} \log \check{T}_n(k,\beta) = \mathcal{P}(\beta) \tag{1.19}$$

for $\beta \leqslant 0$, where (as in [7]) $\tau_k^i \in \mathcal{G}_i(k)$ is a k-loop daisy graph (see figure 1(b)) when $i = 0$ and a k-loop twin-tailed tadpole graph (see figure 1(a)) when $i = 2$, with i referring to the number of odd degree vertices in the graph.

In [7] it was established that there exist positive constants $\epsilon, \tilde{C}, \tilde{D}, C, D_0, D, N_\epsilon$ such that for all $n \geqslant N_\epsilon$ and for any $k \geqslant 0$,

$$\tilde{C}\binom{\lfloor \epsilon n \rfloor}{k} p_n \leqslant g_n\big(\tau_k^0\big) \leqslant \mathring{E}_n(k) \leqslant C^k \binom{2n}{k} p_n, \tag{1.20}$$

and

$$\tilde{D}\binom{\lfloor \epsilon n \rfloor}{k} c_n \leqslant g_n\big(\tau_k^2\big) \leqslant \check{E}_n(k) \leqslant D_0 (D)^k \binom{2n}{k} c_n, \tag{1.21}$$

where the lower bounds hold for all $\mathbb{Z}^d$ with $d \geqslant 2$ and the upper bounds hold for $d = 2$.

(a) (b)

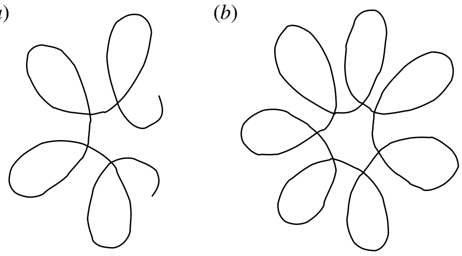


Figure 1. (a) An example of a k-loop twin-tailed tadpole (τ_k^2), with $k = 4$. (b) An example of a k-loop daisy (τ_k^0), with $k = 7$.

In this paper, we use the arguments that lead to the above result along with the new pattern theorems for SAWs and SAPs in $\mathbb{Z}^2$ [9] to establish bounds to $O(n^k)$ for $\mathring{\mathcal{E}}_n(k, \beta)$ and $\breve{\mathcal{E}}_n(k, \beta)$ in terms of $P_n(\beta)$ and $C_n(\beta)$, respectively. In particular, we establish the following results.

Given any fixed $\beta \in \mathbb{R}$, there exist positive constants $\epsilon > 0$, $N > 0$, $D_0(\beta) > 0$, $D(\beta) > 0$ and $D'(\beta) > 0$ such that for any integers $k \geqslant 0$ and $n \geqslant N$,

$$\frac{1}{2}\binom{\lfloor \epsilon n \rfloor}{k} P_n(\beta) \leqslant G_n\left(\tau_k^0, \beta\right) \leqslant \mathring{\mathcal{E}}_n(k, \beta) \leqslant (D(\beta))^k \binom{2n}{k} P_n(\beta) \tag{1.22}$$

and, for $\beta \leqslant 0$,

$$\frac{1}{4}\binom{\lfloor \epsilon n \rfloor}{k} C_n(\beta) \leqslant G_n\left(\tau_k^2, \beta\right) \leqslant \breve{\mathcal{E}}_n(k, \beta) \leqslant D_0(\beta)(D'(\beta))^k \binom{2n}{k} C_n(\beta). \tag{1.23}$$

Now applying equations (1.5) and (1.6) leads to the following results for closed and open k-trails:

$$\frac{1}{2}\binom{\lfloor \epsilon n \rfloor}{k} Q_n(\beta) \leqslant 2nG_n\left(\tau_k^0, \beta\right) \leqslant \mathring{T}_n(k, \beta) \leqslant (3D(\beta))^k \binom{2n}{k} Q_n(\beta) \tag{1.24}$$

and, for $\beta \leqslant 0$,

$$\frac{1}{2}\binom{\lfloor \epsilon n \rfloor}{k} C_n(\beta) \leqslant 2G_n\left(\tau_k^2, \beta\right) \leqslant \breve{T}_n(k, \beta) \leqslant 12D_0(\beta)(3D'(\beta))^k \binom{2n}{k} C_n(\beta), \tag{1.25}$$

where the constants are as defined in equations (1.22) and (1.23).

Hence, given any $\beta \in \mathbb{R}$, we have that

$$\mathring{T}_n(k, \beta) = \Theta(n^k Q_n(\beta)) = \Theta(n\mathring{\mathcal{E}}_n(k, \beta)) = \Theta(n^{k+1} P_n(\beta)) \tag{1.26}$$

and, for $\beta \leqslant 0$,

$$\breve{T}_n(k, \beta) = \Theta(n^k C_n(\beta)) = \Theta(\breve{\mathcal{E}}_n(k, \beta)) = \Theta(n^k U_n(\beta)), \tag{1.27}$$

where we define the notation $f_n = \Theta(g_n)$ to mean that there exist constants (independent of n) $A, B, N \geqslant 0$ such that $Ag_n \leqslant f_n \leqslant Bg_n$ for all $n \geqslant N$. It is generally believed, for example, that $P_n(\beta) = \Theta(n^{\theta(\beta)} e^{\mathcal{P}(\beta)n})$, with *collapsing free energy critical exponent* $\theta(\beta)$. Hence our results indicate that this critical exponent, if it exists, goes up by 1 for each vertex of degree 4 in the k-trail or k-graph.

We also use the pattern theorem for collapsing n-SAPs [9] to obtain bounds on the average n-SAP contact density, $\langle l \rangle_\beta / n$. For example, we show that there exist $1 > \epsilon_1 > 0$ and $1 > \epsilon_2 > 0$ such that if $\mathcal{P}(\beta)$ is differentiable at $\beta \in \mathbb{R}$ then

$$\epsilon_1 \leqslant \mathcal{P}'(\beta) = \lim_{n \to \infty} \frac{\langle l \rangle_\beta}{n} \leqslant 1 - \epsilon_2. \tag{1.28}$$

Then, using equations (1.18) and (1.19) this can be extended to yield the same conclusion regarding the average contact density for collapsing k-graphs and k-trails.

Finally, we investigate k-graphs with a fixed density of contacts. Here we show that the limiting entropy per monomer is independent of k.

The remainder of the paper is organized as follows. The upper and lower bounds of equations (1.22) and (1.23) on the collapsing free energies of k-graphs are derived in the following section. In the third section the results concerning the density of contacts are presented. In the last section, the properties of k-graphs with a fixed density of contacts are explored.

2. Main results on the collapsing free energy of *k*-graphs

2.1. Upper bounds

James and Soteros [7, lemma 7] proved that, there exists $M > 0$ such that given any $n > 0, k \geqslant 0, \tau \in \mathcal{G}_0(k)$ and any n-tau, σ, with l contacts, there is a map Φ which takes σ to a triple $(\tilde{\omega}, \Xi, \mathcal{T})$ where $\tilde{\omega}$ is a polygon which only differs from σ in up to k square boxes of side length M. Hence $\tilde{\omega}$ has l' contacts for some l' such that $l - kA \leqslant l' \leqslant l + kA$, where $A = 2(M+1)(M+2)$ is the number of edges contained inside or touching the boundary of a square box of side length M. Using this and following the proof of [7, lemma 10], one obtains the upper bound for $\overset{\circ}{E}_n(k,l)$ stated below in equation (2.1). From this one can obtain an upper bound for $\overset{\circ}{\mathcal{E}}_n(k,\beta)$, the partition function for n-edge closed k-graphs, as defined in equation (1.14).

Lemma 1. *There exists a constant $C > 1$, such that for all $k \geqslant 0, n \geqslant 1$ and $l \geqslant 0$*

$$\overset{\circ}{E}_n(k,l) \leqslant C^k \binom{2n}{k} \sum_{m=n-4k}^{n} \sum_{l'=l-kA}^{l+kA} p_m(l'), \tag{2.1}$$

and hence, given any fixed $\beta \in \mathbb{R}$, there exists a constant $D(\beta) > 0$ such that for all $k \geqslant 0$ and $n \geqslant 1$,

$$\overset{\circ}{\mathcal{E}}_n(k,\beta) = \sum_{l=0}^{n-2k} \overset{\circ}{E}_n(k,l) e^{\beta l} \leqslant (D(\beta))^k \binom{2n}{k} P_n(\beta). \tag{2.2}$$

Proof. As discussed above, equation (2.1) follows directly from [7, lemma 7] and the proof of [7, lemma 10]. Summing over l on both sides of equation (2.1) gives the following results:

$$\begin{aligned}
\overset{\circ}{\mathcal{E}}_n(k,\beta) = \sum_{l=0}^{n-2k} \overset{\circ}{E}_n(k,l)\, \mathrm{e}^{\beta l} &\leqslant C^k \binom{2n}{k} \sum_{l=0}^{n-2k} \sum_{m=n-4k}^{n} \sum_{l'=l-kA}^{l+kA} p_m(l')\, \mathrm{e}^{\beta l} \\
&= C^k \binom{2n}{k} \sum_{l=0}^{n-2k} \sum_{m=n-4k}^{n} \sum_{j=0}^{2kA} p_m(j+l-kA)\, \mathrm{e}^{\beta l} \\
&= C^k \binom{2n}{k} \sum_{m=n-4k}^{n} \sum_{j=0}^{2kA} \mathrm{e}^{\beta(kA-j)} \sum_{l=0}^{n-2k} p_m(j+l-kA)\, \mathrm{e}^{\beta(j+l-kA)} \\
&\leqslant C^k \binom{2n}{k} \sum_{m=n-4k}^{n} \sum_{j=0}^{2kA} \mathrm{e}^{\beta(kA-j)} P_m(\beta) \\
&= C^k \binom{2n}{k} \left(\sum_{m=n-4k}^{n} P_m(\beta) \right) \sum_{j=0}^{2kA} \mathrm{e}^{\beta(kA-j)}.
\end{aligned} \tag{2.3}$$

A standard concatenation of a unit square onto the bottom most of the left-most edges of a polygon leads to

$$p_{N-2}(l) \leqslant p_N(l+1) \tag{2.4}$$

for any even integer $N \geqslant 6$. This, in turn, implies that $P_{N-2s}(\beta) \leqslant \mathrm{e}^{-s\beta} P_N(\beta)$, for any choice of integers s and N (N even) such that $N - 2s \geqslant 4$ and $s \geqslant 0$. Therefore, equation (2.3) is bounded as follows:

$$\begin{aligned}\mathring{\mathcal{E}}_n(k,\beta) &\leqslant C^k \binom{2n}{k} \left(P_n(\beta) \sum_{s=0}^{2k} \mathrm{e}^{-s\beta} \right) \sum_{j=0}^{2kA} \mathrm{e}^{\beta(kA-j)} \\ &= C^k \binom{2n}{k} P_n(\beta) \sum_{s=0}^{2k} \sum_{j=0}^{2kA} \mathrm{e}^{-\beta(s+j-kA)}. \end{aligned} \tag{2.5}$$

Next, because the quantity $s + j$ is not larger in magnitude than $2k + 2kA$, we have that $|s + j - kA| \leqslant k(A + 2)$, and hence $|\beta(s + j - kA)| \leqslant |\beta|k(A + 2)$. Therefore, $\mathrm{e}^{-\beta(s+j-kA)} \leqslant \mathrm{e}^{|\beta(s+j-kA)|} \leqslant \mathrm{e}^{|\beta|k(A+2)}$, which allows the last term of the inequality in (2.5) to be bounded as follows:

$$\begin{aligned}\mathring{\mathcal{E}}_n(k,\beta) &\leqslant C^k \binom{2n}{k} P_n(\beta) \sum_{s=0}^{2k} \sum_{j=0}^{2kA} \mathrm{e}^{|\beta|k(A+2)} \\ &= C^k \binom{2n}{k} P_n(\beta)(2k+1)(2kA+1)\, \mathrm{e}^{|\beta|k(A+2)} \\ &\leqslant C^k \binom{2n}{k} P_n(\beta)(12)^k(2A+1)^k\, \mathrm{e}^{|\beta|k(A+2)} \\ &\leqslant (D(\beta))^k \binom{2n}{k} P_n(\beta), \end{aligned} \tag{2.6}$$

where $D(\beta) \geqslant 12C\, \mathrm{e}^{|\beta|(A+2)}(2A+1)$. The second-to-last inequality in equation (2.6) is found as follows. First, observe that the function $y = \frac{\log(x)}{x}$ is bounded above by its maximum value of $1/e$ (obtained at $x = e$). Therefore,

$$\log(a+1) + \log(k) \leqslant k(\log(a+1) + 1/e), \qquad \text{for any } a > 0, k \geqslant 1. \tag{2.7}$$

By exponentiating both sides of equation (2.7) and using $\mathrm{e}^{1/e} \leqslant 2$, it follows that:

$$ak + 1 \leqslant (a+1)k \leqslant (2(a+1))^k, \qquad \text{for any } a > 0, k \geqslant 1. \tag{2.8}$$

In fact, note that the inequality involving the left-most and right-most ends of equation (2.8) holds true for $k = 0$, as well. In other words,

$$ak + 1 \leqslant (2(a+1))^k, \qquad \text{for any } a > 0 \quad \text{and for any integer } k \geqslant 0. \tag{2.9}$$

In particular, we conclude from equation (2.9) that $2k+1$ is bounded above by 6^k and $2kA+1$ is bounded above by $(2(2A+1))^k$, for all integers $k \geqslant 0$, as desired. □

In exactly the same way as described for lemma 1, we may obtain the following upper bound for $\check{\mathcal{E}}_n(k,\beta)$, the partition function for n-edge open k-graphs, as defined in equation (1.14).

Lemma 2. *There exist constants $D_0 > 0$ and $D > 1$, such that for all $k \geqslant 0$, $n \geqslant 1$ and $l \geqslant 0$*

$$\check{E}_n(k,l) \leqslant D_0(D)^k \binom{2n}{k} \sum_{m=n-220k-2}^{n} \sum_{l'=l-kA}^{l+kA} c_m(l'), \tag{2.10}$$

and hence, given any fixed $\beta \in \mathbb{R}$, there exist constants $D_0(\beta) > 0$ and $D(\beta) > 0$ such that for all $k \geqslant 0$ and $n \geqslant 1$,

$$\breve{\mathcal{E}}_n(k,\beta) = \sum_{l=0}^{n-2k+2} \breve{E}_n(k,l)\,\mathrm{e}^{\beta l} \leqslant D_0(\beta)(D'(\beta))^k \binom{2n}{k} C_n(\beta). \tag{2.11}$$

Proof. For this case, equation (2.10) follows directly from [7, lemma 8] and the proof of [7, lemma 11]. Next, the steps given in equation (2.3) work the same way for SAWs as for SAPs. Thus, we have the following inequality, which corresponds to the last line in equation (2.3):

$$\breve{\mathcal{E}}_n(k,\beta) = \sum_{l=0}^{n-2k+2} \breve{E}_n(k,l)\,\mathrm{e}^{\beta l} \leqslant D_0 D^k \binom{2n}{k} \left(\sum_{m=n-220k-2}^{n} C_m(\beta) \right) \sum_{j=0}^{2kA} \mathrm{e}^{\beta(kA-j)}. \tag{2.12}$$

Now, given any $(N-2)$-SAW with l contacts, let e denote the bottom most of its left-most edges. If e is horizontal (vertical), then a concatenation of a horizontal 2-SAW (a unit square) onto the $(N-2)$-SAW at e can be used to obtain a unique N-SAW with l $(l+1)$ contacts. Thus, we have

$$c_{N-2}(l) \leqslant c_N(l+1) + c_N(l). \tag{2.13}$$

In turn, this gives

$$C_{N-2}(\beta) \leqslant (1+\mathrm{e}^{-\beta}) C_N(\beta). \tag{2.14}$$

Repeated applications of equation (2.14) gives, for any nonnegative integer, $t \geqslant 0$:

$$C_{N-2t}(\beta) \leqslant (1+\mathrm{e}^{-\beta})^t C_N(\beta). \tag{2.15}$$

Thus, equation (2.15) can be used to bound equation (2.12) as follows:

$$\begin{aligned}
\breve{\mathcal{E}}_n(k,\beta) &\leqslant D_0 D^k \binom{2n}{k} \left(\sum_{m=n-220k-2}^{n} C_m(\beta) \right) \sum_{j=0}^{2kA} \mathrm{e}^{\beta(kA-j)} \\
&= D_0 D^k \binom{2n}{k} \left(\sum_{s=0}^{2(110k+1)} C_{n-s}(\beta) \right) \sum_{j=0}^{2kA} \mathrm{e}^{\beta(kA-j)} \\
&\leqslant D_0 D^k \binom{2n}{k} \left(\sum_{t=0}^{110k+1} (C_{n+1-2t}(\beta) + C_{n-2t}(\beta)) \right) \sum_{j=0}^{2kA} \mathrm{e}^{\beta(kA-j)} \\
&\leqslant D_0 D^k \binom{2n}{k} [C_{n+1}(\beta) + C_n(\beta)] \sum_{t=0}^{110k+1} (1+\mathrm{e}^{-\beta})^t \sum_{j=0}^{2kA} \mathrm{e}^{\beta(kA-j)}.
\end{aligned} \tag{2.16}$$

Note next that removing the last edge of an $(n+1)$-SAW with l contacts yields an n-SAW with $l-i$ contacts for some $i \in \{0,1,2,3\}$. Since at most three distinct $(n+1)$-SAWs will result in the same n-SAW, this argument leads to

$$c_{n+1}(l) \leqslant 3[c_n(l) + c_n(l-1) + c_n(l-2) + c_n(l-3)]. \tag{2.17}$$

Therefore, we have the following bound:

$$C_{n+1}(\beta) \leqslant 3C_n(\beta)(1+\mathrm{e}^{\beta}+\mathrm{e}^{2\beta}+\mathrm{e}^{3\beta}). \tag{2.18}$$

We can use equation (2.18) to bound equation (2.16) as follows:

$$\begin{aligned}
\breve{\mathcal{E}}_n(k,\beta) &\leqslant D_0 D^k \binom{2n}{k} C_n(\beta) \left[1 + 3\sum_{s=0}^{3} \mathrm{e}^{s\beta} \right] \sum_{t=0}^{110k+1} (1+\mathrm{e}^{-\beta})^t \sum_{j=0}^{2kA} \mathrm{e}^{\beta(kA-j)} \\
&\leqslant D_0 D^k \binom{2n}{k} C_n(\beta) [13\,\mathrm{e}^{3|\beta|}](110k+2)(2\,\mathrm{e}^{|\beta|})^{110k+1} \sum_{j=0}^{2kA} \mathrm{e}^{\beta(kA-j)},
\end{aligned} \tag{2.19}$$

where the final bound in equation (2.19) is found by noting that $1 + 3\sum_{s=0}^{3} \mathrm{e}^{s\beta} \leqslant 1 + 3\sum_{s=0}^{3} \mathrm{e}^{3|\beta|} \leqslant 1 + 12\,\mathrm{e}^{3|\beta|} \leqslant 13\,\mathrm{e}^{3|\beta|}$ and that $(1+\mathrm{e}^{-\beta})^t \leqslant (1+\mathrm{e}^{|\beta|})^{110k+1} \leqslant (2\,\mathrm{e}^{|\beta|})^{110k+1}$.

Next, by equation (2.9), $110k + 2 \leqslant 1 + (222)^k \leqslant 2(222)^k$. Therefore, we may bound equation (2.19) as follows:

$$\breve{\mathcal{E}}_n(k,\beta) \leqslant D_0 D^k \binom{2n}{k} C_n(\beta) 52\,\mathrm{e}^{4|\beta|}[222(2^{110})\,\mathrm{e}^{110|\beta|}]^k \sum_{j=0}^{2kA} \mathrm{e}^{\beta(kA-j)}. \tag{2.20}$$

Finally, we may bound equation (2.20) by first observing that, because $0 \leqslant j \leqslant 2kA$, we have $\mathrm{e}^{\beta(kA-j)} \leqslant \mathrm{e}^{|\beta|kA}$, and then applying equation (2.9) yields

$$\begin{aligned}\breve{\mathcal{E}}_n(k,\beta) &\leqslant D_0 D^k \binom{2n}{k} C_n(\beta) 52\,\mathrm{e}^{4|\beta|}(222(2^{110})\,\mathrm{e}^{110|\beta|})^k (2kA+1)\,\mathrm{e}^{|\beta|kA} \\ &\leqslant D_0 D^k \binom{2n}{k} C_n(\beta) 52\,\mathrm{e}^{4|\beta|}(444(2^{110})\,\mathrm{e}^{110|\beta|})^k (2A+1)^k\,\mathrm{e}^{|\beta|kA} \\ &\leqslant D_0(\beta)(D'(\beta))^k \binom{2n}{k} C_n(\beta),\end{aligned} \tag{2.21}$$

where $D_0(\beta) \geqslant D_0 52\,\mathrm{e}^{4|\beta|}$ and $D'(\beta) \geqslant 444 D 2^{110}\,\mathrm{e}^{(110+A)|\beta|}(2A+1)$. This yields the desired bound. □

2.2. Lower bounds

We next wish to obtain appropriate lower bounds for $\mathring{\mathcal{E}}_n(k,\beta)$ and for $\breve{\mathcal{E}}_n(k,\beta)$. We will rely on the new pattern theorems for SAPs and SAWs derived recently in [9] and refer the reader to this reference for a definition of the term *pattern* for SAPs or SAWs (but for examples of proper SAP patterns see figure 2). It is also necessary to introduce some new notation here. First, let P denote a fixed pattern that can occur in a SAP. Given P, let $p_n(\leqslant m, P, l)$ denote the number of n-edge SAPs having l contacts and containing at most m translates of the pattern P. Also, let $p_n(>m, P, l)$ denote the number of n-edge SAPs having l contacts and containing more than m translates of the pattern P. The notation $c_n(\leqslant m, P, l)$ and $c_n(>m, P, l)$ is used *mutatis mutandis* for SAWs. Also, for any $\epsilon > 0$, define $C_n(\beta,\epsilon,P) \equiv \sum_l c_n(>\lfloor \epsilon n\rfloor, P, l)\,\mathrm{e}^{\beta l}$ to be the partition function for self-interacting n-SAWs with more than $\lfloor \epsilon n\rfloor$ copies of the pattern, P.

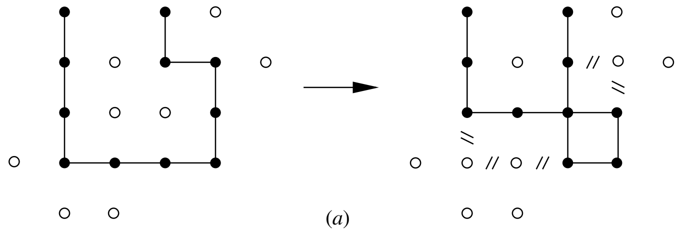
Using the pattern theorems of [9] combined with arguments similar to those described in [7, section 3] and a judicious choice of pattern $P = (P_1, P_2)$ (see figure 2(*a*)), we obtain the following lemmas for SAPs and SAWs. (Note that P is chosen so that both the number of edges and the number of contacts remain unchanged during the L-to-loop transformation depicted in figure 2(*a*).)

Lemma 3. *Given any fixed $\beta \in \mathbb{R}$ there exists an $\epsilon > 0$ and an $N > 0$ such that for any integer $k \geqslant 0$ and any integer $n \geqslant N$, the following inequality holds:*

$$\frac{1}{2}\binom{\lfloor \epsilon n\rfloor}{k} P_n(\beta) \leqslant \mathring{\mathcal{E}}_n(k,\beta). \tag{2.22}$$

Lemma 4. *Let P be the pattern as defined in figure 2(a). Given any fixed $\beta \in \mathbb{R}$, any $\epsilon > 0$ and any $n > 0$, the following inequality holds:*

$$\frac{1}{2}\binom{\lfloor \epsilon n\rfloor}{k} C_n(\beta,\epsilon,P) \leqslant \breve{\mathcal{E}}_n(k,\beta). \tag{2.23}$$



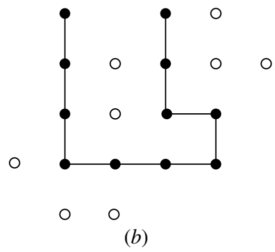


Figure 2. (*a*) Pattern P is defined on the left. The result of the 'L-to-loop transformation' (needed for the proofs of lemmas 3 and 4) is shown on the right. $P = (P_1, P_2)$, where P_1 is the L-shaped set of solid vertices and edges and P_2 is given by the empty circles surrounding the L-shape. P_2 has been chosen so that no contacts are created or destroyed during the transformation. Solid lines represent edges which are occupied. Solid (empty) circles represent vertices which are occupied (unoccupied). Double hash-marks represent edges which have been removed during the transformation. (*b*) Pattern $\hat{P}$ used in section 3 is shown here.

Furthermore, for any finite nonpositive $\beta \leqslant 0$ there exists an $\epsilon_P > 0$ and an $N_P > 0$ such that for any integer $k \geqslant 0$ and any integer $n \geqslant N_P$, the following inequality holds:

$$\frac{1}{4}\binom{\lfloor \epsilon_P n \rfloor}{k} C_n(\beta) \leqslant \breve{\mathcal{E}}_n(k, \beta). \tag{2.24}$$

In order to prove lemmas 3 and 4, the following two theorems from [9] and their corresponding corollaries are needed.

Theorem 1 (James and Soteros [9])**.** *Given any proper SAP pattern $P = (P_1, P_2)$ in $\mathbb{Z}^2$ and any finite β, there exists an $\epsilon_P > 0$ such that*

$$\limsup_{n\to\infty} \frac{1}{n} \log \sum_l p_n(\leqslant \lfloor \epsilon_P n \rfloor, P, l)\, \mathrm{e}^{\beta l} < \mathcal{P}(\beta). \tag{2.25}$$

As a consequence of this and equation (1.16), the arguments given by Sumners and Whittington [26], equations (3.8) and (3.9) lead to the following corollaries.

Corollary 1. *Given any proper SAP pattern $P = (P_1, P_2)$ in $\mathbb{Z}^2$ and any finite β, there exists an $\epsilon_P > 0$ such that*

$$\lim_{n\to\infty} \frac{\sum_l p_n(> \lfloor \epsilon_P n \rfloor, P, l)\, \mathrm{e}^{\beta l}}{P_n(\beta)} = 1. \tag{2.26}$$

Corollary 2. *Given any proper SAP pattern $P = (P_1, P_2)$ in $\mathbb{Z}^2$ and any finite β, there exists an $\epsilon_P > 0$ and $M_P > 0$ such that for all $n \geqslant M_P$,*

$$\frac{1}{2} P_n(\beta) \leqslant \sum_l p_n(> \lfloor \epsilon_P n \rfloor, P, l)\, \mathrm{e}^{\beta l}. \tag{2.27}$$

As mentioned above, the proof for corollary 1 is the same as that given in [26, equations (3.8) and (3.9)]. The crux of this proof, however, occurs in the bound given in [26, equation (3.8)] and depends on the known asymptotic behaviour of the denominator term in equation (2.26). In other words, the proof works because we know that $\lim_{n\to\infty} n^{-1}\log P_n(\beta)$ exists and is equal to the finite value, $\mathcal{P}(\beta)$, for any finite β (see equation (1.16)).

So far, the corresponding corollaries for SAWs, stated next, are only proved for nonpositive β. This is because the asymptotic behaviour for the denominator, in the SAW case, is not known for positive β. In other words, it has only been proved for $\beta \leqslant 0$ that $\lim_{n\to\infty} n^{-1}\log C_n(\beta)$ exists and is equal to the finite value, $\mathcal{P}(\beta)$ (see equation (1.17)).

Theorem 2 (James and Soteros [9])**.** *Given any proper SAP pattern $P = (P_1, P_2)$ in $\mathbb{Z}^2$ and any finite β, there exists an $\epsilon_P > 0$ such that*

$$\limsup_{n\to\infty}\frac{1}{n}\log\sum_l c_n(\leqslant\lfloor\epsilon_P n\rfloor, P, l)\,\mathrm{e}^{\beta l} < \limsup_{n\to\infty}\frac{1}{n}\log C_n(\beta). \tag{2.28}$$

Corollary 3. *Given any proper SAP pattern $P = (P_1, P_2)$ in $\mathbb{Z}^2$ and any finite nonpositive $\beta \leqslant 0$, there exists an $\epsilon_P > 0$ such that*

$$\lim_{n\to\infty}\frac{\sum_l c_n(>\lfloor\epsilon_P n\rfloor, P, l)\,\mathrm{e}^{\beta l}}{C_n(\beta)} = 1. \tag{2.29}$$

Corollary 4. *Given any proper SAP pattern $P = (P_1, P_2)$ in $\mathbb{Z}^2$ and any finite nonpositive $\beta \leqslant 0$, there exists an $\epsilon_P > 0$ and $N_P > 0$ such that for all $n \geqslant N_P$,*

$$\frac{1}{2}C_n(\beta) \leqslant \sum_l c_n(>\lfloor\epsilon_P n\rfloor, P, l)\,\mathrm{e}^{\beta l} = C_n(\beta, \epsilon_P, P). \tag{2.30}$$

We now prove lemma 3 and then lemma 4.

Lemma 3

Proof. Fix any $\beta \in \mathbb{R}$ and let $P = (P_1, P_2)$ be the proper pattern shown on the left side of figure 2(*a*). Let $M_P > 0$ and $\epsilon_P > 0$ be as required for the result of corollary 2. Using the L-to-loop transformation shown in figure 2(*a*) and the arguments given in [7, section 3], given any $n \geqslant M_P$ and $m > \lfloor\epsilon_P n\rfloor$, we convert any n-SAP containing m translates of P into an n-edge k-daisy graph in $\binom{m}{k} > \binom{\lfloor\epsilon_P n\rfloor}{k}$ possible ways, without changing the number of edges or the number of contacts in the graph. We thus obtain the following lower bound for $\mathring{E}_n(k, l)$, the number of n-edge closed k-graphs with l contacts. For any $k \geqslant 0$ and $n \geqslant M_P$,

$$\begin{aligned}\binom{\lfloor\epsilon_P n\rfloor}{k} p_n(>\lfloor\epsilon_P n\rfloor, P, l) &\leqslant g_n\big(\tau_k^0, l\big)\\ &\leqslant \sum_{\tau\in\mathcal{G}_0(k)} g_n(\tau, l)\\ &= \mathring{E}_n(k, l).\end{aligned} \tag{2.31}$$

Next, multiply equation (2.31) by $\mathrm{e}^{\beta l}$, sum over all the choices for l, and apply corollary 2 to make the following lower bound estimate. For any $k \geqslant 0$ and $n \geqslant M_P$,

$$\begin{aligned}\frac{1}{2}\binom{\lfloor\epsilon_P n\rfloor}{k}\sum_l p_n(l)\,\mathrm{e}^{\beta l} &\leqslant \binom{\lfloor\epsilon_P n\rfloor}{k}\sum_l p_n(>\lfloor\epsilon_P n\rfloor, P, l)\,\mathrm{e}^{\beta l}\\ &\leqslant \sum_l g_n\big(\tau_k^0, l\big)\,\mathrm{e}^{\beta l}\end{aligned}$$

$$\leqslant \sum_{l} \sum_{\tau \in \mathcal{G}_0(k)} g_n(\tau, l)\, \mathrm{e}^{\beta l}$$
$$= \sum_{l} \mathring{E}_n(k, l)\, \mathrm{e}^{\beta l}. \tag{2.32}$$

This is the lower bound inequality, as promised in lemma 3. □

Lemma 4

Proof. Fix any $\beta \in \mathbb{R}$ and any $\epsilon > 0$ and let $P = (P_1, P_2)$ be the proper pattern shown on the left side of figure 2(*a*). Using the *L*-to-loop transformation shown in figure 2(*a*) and the arguments given in [7, section 3], given any $n \geqslant 0$ and $m > \lfloor \epsilon n \rfloor$, we convert any n-USAW containing m translates of P into an n-edge k-loop twin-tailed tadpole graph in $\binom{m}{k} > \binom{\lfloor \epsilon n \rfloor}{k}$ possible ways, without changing the number of edges or the number of contacts in the graph. We thus obtain the following lower bound for $\breve{E}_n(k, l)$, the number of n-edge open k-graphs with l contacts. For any n and $k \geqslant 0$,

$$\begin{aligned}\binom{\lfloor \epsilon n \rfloor}{k} \left(\frac{1}{2}\right) c_n(>\lfloor \epsilon n \rfloor, P, l) &\leqslant g_n\left(\tau_k^2, l\right) \\ &\leqslant \sum_{\tau \in \mathcal{G}_2(k)} g_n(\tau, l) \\ &= \breve{E}_n(k, l).\end{aligned} \tag{2.33}$$

Note that the number of n-USAWs is equal to half the number of n-SAWs, hence the factor of $1/2$ given in the inequality in (2.33). Next, multiply equation (2.33) by $\mathrm{e}^{\beta l}$ and sum over all the choices for l, to obtain the following lower bound estimate. For any n and $k \geqslant 0$,

$$\begin{aligned}\binom{\lfloor \epsilon n \rfloor}{k} \left(\frac{1}{2}\right) \sum_{l} c_n(>\lfloor \epsilon n \rfloor, P, l)\, \mathrm{e}^{\beta l} &\leqslant \sum_{l} g_n\left(\tau_k^2, l\right) \mathrm{e}^{\beta l} \\ &\leqslant \sum_{l} \sum_{\tau \in \mathcal{G}_2(k)} g_n(\tau, l)\, \mathrm{e}^{\beta l} \\ &= \sum_{l} \breve{E}_n(k, l)\, \mathrm{e}^{\beta l}.\end{aligned} \tag{2.34}$$

Therefore, for any n and $k \geqslant 0$,

$$\frac{1}{2}\binom{\lfloor \epsilon n \rfloor}{k} C_n(\beta, \epsilon, P) \leqslant \breve{\mathcal{E}}_n(k, \beta), \tag{2.35}$$

which guarantees the first lower bound promised in lemma 4. In particular, for $\beta \leqslant 0$, let $\epsilon_P > 0$ and $N_P > 0$ be as required for the result of corollary 4. Then we have for $k \geqslant 0$ and all $n \geqslant N_P$,

$$\frac{1}{4}\binom{\lfloor \epsilon_P n \rfloor}{k} C_n(\beta) \leqslant \frac{1}{2}\binom{\lfloor \epsilon_P n \rfloor}{k} C_n(\beta, \epsilon_P, P) \leqslant \breve{\mathcal{E}}_n(k, \beta). \tag{2.36}$$

This is the second lower bound inequality, as promised in lemma 4. □

2.3. Combining the upper and lower bounds

Thus for fixed β and k, lemmas 1 and 3 and the asymptotic properties of $\binom{\alpha n}{k}$ (see, for example, [27, equation (2.16)]), imply that

$$\mathring{\mathcal{E}}_n(k, \beta) = \Theta(n^k P_n(\beta)), \tag{2.37}$$

i.e. there exists constants (independent of n) A, B, N such that for all $n \geqslant N$, $An^k P_n(\beta) \leqslant \overset{\circ}{\mathcal{E}}_n(k,\beta) \leqslant Bn^k P_n(\beta)$.

Furthermore, given a fixed β such that the limiting free energy of walks exists, and a fixed k we also have by lemmas 2 and 4 that

$$\breve{\mathcal{E}}_n(k,\beta) = \Theta(n^k C_n(\beta)), \tag{2.38}$$

i.e. there exists constants A', B', N' such that for all $n \geqslant N'$, $A'n^k C_n(\beta) \leqslant \breve{\mathcal{E}}_n(k,\beta) \leqslant B'n^k C_n(\beta)$.

3. The density of contacts in collapsing *k*-graphs

Given any $\beta \in \mathbb{R}$ and integers $n, k \geqslant 0$, we investigate next the asymptotic properties of the average number of contacts per vertex, *the contact density*, for closed and open k-graphs, respectively:

$$\frac{\langle l \rangle_{n,k,0,\beta}}{n} = \frac{1}{n} \frac{\sum_l l \overset{\circ}{E}_n(k,l)\,\mathrm{e}^{\beta l}}{\overset{\circ}{\mathcal{E}}_n(k,\beta)} \tag{3.1}$$

$$\frac{\langle l \rangle_{n,k,2,\beta}}{n} = \frac{1}{n} \frac{\sum_l l \breve{E}_n(k,l)\,\mathrm{e}^{\beta l}}{\breve{\mathcal{E}}_n(k,\beta)}. \tag{3.2}$$

The proof of [10, corollary 4] combined with equations (1.18) and (1.19) lead immediately to the following result.

Corollary 5. *Consider any finite β^* and any integer $k \geqslant 0$. If $\beta^* > 0$, consider $i = 0$ and otherwise consider any $i \in \{0, 2\}$.*

If $\mathcal{P}(\beta)$ is differentiable at $\beta = \beta^*$, then

$$0 < \lim_{n\to\infty} \frac{\langle l \rangle_{n,k,i,\beta^*}}{n} = \mathcal{P}'(\beta^*) < 1, \tag{3.3}$$

i.e. the limiting density exists, is strictly positive and less than 1, and is independent of i and k. Otherwise, the left and right derivatives exist at $\beta = \beta^*$ and

$$0 < \lim_{\beta\to(\beta^*)^-} \mathcal{P}'(\beta) \leqslant \liminf_{n\to\infty} \frac{\langle l \rangle_{n,k,i,\beta^*}}{n} < \limsup_{n\to\infty} \frac{\langle l \rangle_{n,k,i,\beta^*}}{n} \leqslant \lim_{\beta\to(\beta^*)^+} \mathcal{P}'(\beta) < 1. \tag{3.4}$$

In this section we use the pattern theorem, theorem 1, to derive this result by an alternate approach, and we obtain further bounds on $\frac{\langle l \rangle_{n,0,0,\beta}}{n}$.

Consider patterns P and $\hat{P}$ as in figures 2(a) and (b), respectively. We focus on the case $i = 0$ and $k = 0$. Given any fixed $\beta^* \in \mathbb{R}$, let ϵ_P and $\epsilon_{\hat{P}}$ be as required for the results of theorem 1.

Note that an n-SAP containing more than $\lfloor \epsilon_{\hat{P}} n \rfloor$ translates of $\hat{P}$ must contain at least $\lfloor \epsilon_{\hat{P}} n \rfloor$ contacts (one for each translate). Hence, for $\beta = \beta^*$ and $n \geqslant M_{\hat{P}}$ (as needed for corollary 2),

$$\sum_l l p_n(l)\,\mathrm{e}^{\beta l} \tag{3.5}$$

$$= \sum_{l \leqslant \lfloor \epsilon_{\hat{P}} n \rfloor} l p_n(l)\,\mathrm{e}^{\beta l} + \sum_{l > \lfloor \epsilon_{\hat{P}} n \rfloor} l p_n(l)\,\mathrm{e}^{\beta l} \tag{3.6}$$

$$\geqslant \lfloor \epsilon_{\hat{P}} n \rfloor \sum_{l > \lfloor \epsilon_{\hat{P}} n \rfloor} p_n(l)\, \mathrm{e}^{\beta l} \tag{3.7}$$

$$\geqslant \lfloor \epsilon_{\hat{P}} n \rfloor \sum_{l} p_n(>\lfloor \epsilon_{\hat{P}} n \rfloor, \hat{P}, l)\, \mathrm{e}^{\beta l} \geqslant \frac{\lfloor \epsilon_{\hat{P}} n \rfloor}{2} P_n(\beta), \tag{3.8}$$

where the last inequality follows from corollary 2. Thus for $\beta = \beta^*$ and any $n \geqslant M_{\hat{P}}$

$$\frac{\langle l \rangle_{n,0,0,\beta^*}}{n} \geqslant \frac{\lfloor \epsilon_{\hat{P}} n \rfloor}{2n}. \tag{3.9}$$

For an upper bound, note first that for any square lattice n-SAP with s solvent-contact edges (edges from a polygon vertex to a vertex not part of the polygon) and l contact edges we have (see, for example, [28])

$$s + 2l = 2n. \tag{3.10}$$

Each occurrence of P contributes at least 12 distinct solvent-contact edges, hence an n-SAP containing more than $\lfloor \epsilon_P n \rfloor$ translates of P contains at most $(n - 6\lfloor \epsilon_P n \rfloor)$ contact edges. Define $\epsilon_2 = \min\{\epsilon_P, 1/6\} < 1$, and hence $p_n(l) \geqslant p_n(>\lfloor \epsilon_2 n \rfloor, P, l) \geqslant p_n(>\lfloor \epsilon_P n \rfloor, P, l)$ so that corollaries 1 and 2 hold for $\sum_l p_n(>\lfloor \epsilon_2 n \rfloor, P, l)\, \mathrm{e}^{\beta^* l}$. Thus, for $\beta = \beta^*$,

$$\sum_l l p_n(>\lfloor \epsilon_2 n \rfloor, P, l)\, \mathrm{e}^{\beta l} = \sum_{l=0}^{n-6\lfloor \epsilon_2 n \rfloor} l p_n(>\lfloor \epsilon_2 n \rfloor, P, l)\, \mathrm{e}^{\beta l} \tag{3.11}$$

$$\leqslant (n - 6\lfloor \epsilon_2 n \rfloor) \sum_l p_n(>\lfloor \epsilon_2 n \rfloor, P, l)\, \mathrm{e}^{\beta l}, \tag{3.12}$$

and thus

$$\frac{\sum_l l p_n(>\lfloor \epsilon_2 n \rfloor, P, l)\, \mathrm{e}^{\beta^* l}}{\sum_l p_n(>\lfloor \epsilon_2 n \rfloor, P, l)\, \mathrm{e}^{\beta^* l}} \leqslant (n - 6\lfloor \epsilon_2 n \rfloor). \tag{3.13}$$

As discussed in the proof of [10, corollary 4], if $\mathcal{P}(\beta)$ is differentiable at $\beta = \beta^*$ then the order of the differentiation and the limit as n goes to infinity can be interchanged. Thus

$$\mathcal{P}'(\beta^*) = \frac{\mathrm{d}}{\mathrm{d}\beta} \lim_{n\to\infty} n^{-1} \log P_n(\beta) \bigg|_{\beta=\beta^*} \tag{3.14}$$

$$= \frac{\mathrm{d}}{\mathrm{d}\beta} \lim_{n\to\infty} n^{-1} \log \sum_l p_n(>\lfloor \epsilon_2 n \rfloor, P, l)\, \mathrm{e}^{\beta l} \bigg|_{\beta=\beta^*} \tag{3.15}$$

$$= \lim_{n\to\infty} n^{-1} \frac{\mathrm{d}}{\mathrm{d}\beta} \log \sum_l p_n(>\lfloor \epsilon_2 n \rfloor, P, l)\, \mathrm{e}^{\beta l} \bigg|_{\beta=\beta^*} \tag{3.16}$$

$$= \lim_{n\to\infty} n^{-1} \frac{\sum_l l p_n(>\lfloor \epsilon_2 n \rfloor, P, l)\, \mathrm{e}^{\beta^* l}}{\sum_l p_n(>\lfloor \epsilon_2 n \rfloor, P, l)\, \mathrm{e}^{\beta^* l}} \tag{3.17}$$

$$\leqslant \lim_{n\to\infty} n^{-1}(n - 6\lfloor \epsilon_2 n \rfloor) = 1 - 6\epsilon_2, \tag{3.18}$$

where for equation (3.15) we have used corollary 1. Combining this upper bound with equation (3.9) yields

$$\epsilon_1 \leqslant \lim_{n\to\infty} \frac{\langle l \rangle_{n,0,0,\beta^*}}{n} = \mathcal{P}'(\beta^*) \leqslant 1 - 6\epsilon_2, \tag{3.19}$$

where $\epsilon_1 = \epsilon_{\hat{P}}/2$.

Using equations (1.18) and (1.19), the conclusions from equation (3.19) are now essentially the same as the conclusions of corollary 5, however, the arguments above provide an alternate approach for determining the bounds and, at least in the case of equation (3.9), also give bounds on the density of contacts at finite n for SAPs.

4. Closed k-graphs with a fixed density of contacts

Given k and $0 \leqslant \alpha \leqslant 1$ fixed, we define a new function

$$\phi_n(k,\alpha) = \overset{\circ}{E}_n(k, \lfloor \alpha n \rfloor). \tag{4.1}$$

$\phi_n(k,\alpha)$ is thus the number (up to translation) of n-edge closed k-graphs with a fixed limiting (as $n \to \infty$) contact density α. We are interested in the existence and other properties of the *limiting entropy per monomer at fixed density* α given by

$$\kappa(k,\alpha) \equiv \lim_{n\to\infty} \frac{1}{n} \log \phi_n(k,\alpha). \tag{4.2}$$

For $k = 0$ (SAPs), Soteros and Whittington [10, section 4] established that the following limit exists and is a concave function of α,

$$\kappa(0,\alpha) \equiv \lim_{n\to\infty} \frac{1}{n} \log \phi_n(0,\alpha) = \lim_{n\to\infty} \frac{1}{n} \log p_n(\lfloor \alpha n \rfloor). \tag{4.3}$$

In many cases [4, 27], the limiting collapsing free energy can be connected to the limiting entropy per monomer at a fixed density through the Legendre transform. Since the limiting collapsing free energy is independent of k, we thus expect that the limiting entropy per monomer at a fixed density will also be independent of k. We show next that this is in fact the case.

For an appropriate upper bound we note that, by combining equations (2.1) and (2.4), there exist constants $A > 0$ and $C > 0$ such that for all $k \geqslant 0$, $l \geqslant 0$ and $n \geqslant 0$

$$\overset{\circ}{E}_n(k,l) \leqslant C^k \binom{2n}{k} \sum_{m=n-4k}^{n} \sum_{l'=l-kA}^{l+kA} p_m(l') = C^k \binom{2n}{k} \sum_{s=0}^{2k} \sum_{l'=l-kA}^{l+kA} p_{n-2s}(l') \tag{4.4}$$

$$\leqslant C^k \binom{2n}{k} \sum_{s=0}^{2k} \sum_{l'=l-kA}^{l+kA} p_n(l'+s). \tag{4.5}$$

For a lower bound, consider any fixed 0-contact embedding, σ, of a k-loop daisy and let m be the number of edges in σ. Now consider any $(l-2)$-contact $(n-m)$-edge polygon ω. Let e_1 be the top most of the right-most edges of σ and e_2 be the bottom most of the left-most edges of ω. Translate ω so that e_2 is exactly one lattice unit to the right of e_1. Now *concatenate* σ and ω, by deleting e_1 and e_2 and adding in two new horizontal edges, to create an l-contact n-edge k-graph. Since ω is arbitrary and the result of the transformation is unique, this gives the bound

$$p_{n-m}(l-2) \leqslant \overset{\circ}{E}_n(k,l), \tag{4.6}$$

where m is fixed and $n \geqslant m > 0$, $l \geqslant 2$.

Thus there exist constants $m > 0$, $A > 0$ and $C > 0$, such that for all $k \geqslant 0$, $l \geqslant 2$ and $n \geqslant m$

$$p_{n-m}(l-2) \leqslant \overset{\circ}{E}_n(k,l) \leqslant C^k \binom{2n}{k} (2k+1)(2kA+1) \max_{l-kA \leqslant l' \leqslant l+k(A+2)} p_n(l'). \tag{4.7}$$

Setting $l = \lfloor \alpha n \rfloor$ in equation (4.7), taking logarithms, dividing by n and then taking the limit as $n \to \infty$, yields

$$\kappa(k, \alpha) = \lim_{n\to\infty} n^{-1} \log \overset{\circ}{E}_n(k, \lfloor \alpha n \rfloor) = \lim_{n\to\infty} n^{-1} \log \phi_n(k, \alpha) = \kappa(0, \alpha), \tag{4.8}$$

where we have used the following lemma.

Lemma 5. *Let* $l_n \in [0, n]$ *be a sequence of integers such that* $lim_{n\to\infty} l_n/n = \alpha$ *with* $\alpha \in (0, 1)$. *Then*

$$\lim_{n\to\infty} n^{-1} \log p_n(l_n) = \kappa(0, \alpha). \tag{4.9}$$

Proof. This follows from [4, theorem 3.6] and the fact that $r_n(l) \equiv [1 + p_n(l - 2)]/5$, for $2 \leqslant l \leqslant n$, satisfies [4, assumptions 3.1] (see also [10, 27]). □

Equation (4.4) gives an appropriate upper bound for establishing that $\phi_n(k, \alpha) = O(n^k \phi_n(0, \alpha))$. We expect that an appropriate lower bound can be established to yield $\phi_n(k, \alpha) = \Theta(n^k \phi_n(0, \alpha))$, but this is left for future work.

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