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J. Phys. A: Math. Theor. 40 (2007) 8621-8634

doi:10.1088/1751-8113/40/30/002

New pattern theorems for square lattice self-avoiding walks and self-avoiding polygons

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Received 12 March 2007, in final form 11 June 2007 Published 12 July 2007 Online at stacks.iop.org/JPhysA/40/8621

Abstract

A general pattern theorem for weighted self-avoiding polygons (SAPs) and selfavoiding walks (SAWs) in \mathbb{Z}^2 is obtained. The pattern theorem for SAPs fits into the general framework of the pattern theorem for lattice clusters introduced by Madras (1999 *Ann. Comb.* **3** 357–84). Note that, unlike other pattern theorems proved for SAPs, this pattern theorem does not rely on first establishing a relationship between SAPs and SAWs. These results are applied to obtain pattern theorems for self-interacting SAPs and self-interacting SAWs.

PACS numbers: 05.50.+q, 05.70.Fh, 61.25.Hq

1. Introduction

Self-avoiding walk (SAW) and self-avoiding polygon (SAP) lattice models are known to be useful statistical mechanics models for studying the phase behaviour and asymptotic (as polymer size grows) configurational properties of linear and ring polymers in solution respectively [1–3]. One advantage of these models is that it has been possible to prove rigorous results about partition functions, especially in the large polymer limit. In this regard, one of the most powerful mathematical tools is a 'pattern theorem'. One such theorem, due to Kesten [4], is for self-avoiding walks in \mathbb{Z}^d , $d \ge 2$, and states: for an appropriately defined pattern *P*, there exists an $\epsilon > 0$ such that all but exponentially few sufficiently long *n*-step self-avoiding walks contain the pattern *P* at least ϵn times. Kesten's pattern theorem has been used, for example, to establish results about knotting probabilities for self-avoiding polygons in \mathbb{Z}^3 [5] and to help establish relationships between entropic critical exponents for various lattice models [6].

More recently, Madras [7] has developed a general pattern theorem that holds for sets of lattice clusters (finite subgraphs of a lattice) that satisfy a set of axioms. For a suitable

1751-8113/07/308621+14\$30.00 © 2007 IOP Publishing Ltd Printed in the UK

set of clusters and pattern *P* it states that: there exists an $\epsilon > 0$ such that the limiting (as $n \to \infty$) free energy per monomer for size *n* clusters which contain less than ϵn translates of *P* is strictly less than that for the full set of size *n* clusters. This theorem [7, theorem 2.1], referred to herein as the *Madras pattern theorem*, was shown in [7] to be applicable for several sets of 'interacting' (or weighted) clusters on a variety of lattices (including \mathbb{Z}^d , $d \ge 2$). For example for $d \ge 2$, the full set of axioms is shown to hold for the set of self-interacting bond animals in the hypercubic lattice \mathbb{Z}^d , in which the interaction energy is proportional to the number of nearest-neighbour contacts (see [7, proposition 3.1]); hence the Madras pattern theorem follows for this set of weighted clusters. The arguments presented in [7] do not, however, establish that the full set of axioms holds for SAWs or SAPs. In fact, one of the axioms (namely (CA4)) used in [7, theorem 2.1] cannot be satisfied for self-avoiding walks [7] in \mathbb{Z}^d , $d \ge 2$. Note, however, that the full set of axioms has recently been proved to hold for SAPs in pseudo-one-dimensional sublattices of \mathbb{Z}^3 known as tubes or prisms [9].

In this paper, we establish a general pattern theorem for weighted self-avoiding polygons in the square lattice, \mathbb{Z}^2 , by showing that the axioms defined in [7] hold for this set of clusters. In addition, we relax one of the axioms and note that a modified general pattern theorem still holds; this allows us to establish a general pattern theorem for weighted square lattice selfavoiding walks. The new pattern theorem for SAPs has the advantage that its proof does not rely on establishing any relationships between weighted SAPs and weighted SAWs, in contrast to previous approaches for establishing pattern theorem to SAPs [1, 3]. For example, the previously cited applications of Kesten's pattern theorem to self-avoiding polygons [5, 6] each rely on the fact that the limiting entropy per site for self-avoiding polygons (or exponential growth rate of the number of self-avoiding polygons) is equal to that for self-avoiding walks. Hence the pattern theorem for SAPs established herein can be applied to cases for which it is not known whether the limiting free energies for SAWs and SAPs are equal, as is the case for example, when the interaction energy is proportional to the number of nearest-neighbour contacts [3, 8], i.e. for self-interacting SAPs. The SAP results can also be extended to obtain a pattern theorem for self-avoid.

The first goal of this paper is to establish cluster axiom 4 (CA4) of [7] for square lattice SAPs. That is, roughly speaking, we show that, given an appropriately defined (i.e. proper) SAP pattern *P* and an arbitrary vertex *y* in an arbitrary polygon ω , one can insert *P* into ω at a location near *y*. For appropriate choices of weights (i.e. those satisfying cluster axiom 2 (CA2) of [7]), this will then imply the Madras pattern theorem [7, theorem 2.1].

Establishing (CA4) for square lattice SAPs requires a constructive argument. In order to virtually eliminate the detailed case analysis which might otherwise be required, we take advantage of the detailed case analysis on the square lattice that was employed in a recent paper [6]. In [6], combinatorial bounds were derived which related the number of open or closed *n*-step trails with a fixed number of vertices of degree 4 to the number of *n*-step self-avoiding walks (*n*-SAWs) or *n*-edge self-avoiding polygons (*n*-SAPs), respectively. In order to accomplish this, it was first established, via a detailed case analysis, that it was possible to remove vertices of degree 4 'locally' from a trail (or rather its underlying graph) to ultimately obtain either a SAP or a SAW in \mathbb{Z}^2 . In this paper, the closed trail results [6, lemma 7] are used to establish (CA4) for self-avoiding polygons in \mathbb{Z}^2 .

Our second goal will be to establish a modified version of (CA4) for SAWs in \mathbb{Z}^2 . Based on [6, lemma 8] and the arguments used to establish that (CA4) holds for SAPs, a modified version of (CA4) is shown to hold for USAWs (undirected SAWs); the modification needed is that the set of all proper patterns is replaced by the set of proper SAP patterns. Then, the proof of the Madras pattern theorem in [7] implies that its consequences will also hold for USAWs, provided the patterns are restricted to the proper SAP patterns. From this, the fact that each USAW corresponds to two distinct SAWs allows the pattern theorem for USAWs to be extended immediately to a pattern theorem for SAWs.

These results then give, for example, pattern theorems for interacting SAPs and SAWs with interaction energy proportional to the number of nearest-neighbour contacts. Applications of these results to the study of open and closed trails with a fixed number of vertices of degree 4 will be presented in a subsequent paper.

The paper is structured as follows. In the next section, the notation, cluster axioms and the Madras pattern theorem from [7] are briefly reviewed. In section 3, the necessary definitions for our main results are introduced and the lemmas needed to establish the new pattern theorems of this paper are stated and proved. Finally, in section 4 some applications to interacting SAPs (ISAPs) and SAWs (ISAWs), with interaction energy proportional to the number of nearest-neighbour contacts, are explored.

2. Brief overview of the Madras general pattern theorem

Unless stated otherwise, the terminology and notation follow that given in [6] and [7] with dimension d = 2. In particular for G a subgraph of \mathbb{Z}^2 , V(G) (or V_G) and $\mathcal{E}(G)$ (or \mathcal{E}_G) are used to denote the vertex set and edge set of G, respectively. For convenience, we give a brief review of Madras' notation and general pattern theorem results and refer the reader to [7] for the complete details.

Let C_n denote a set of size *n* clusters (finite subgraphs) of a lattice *L*. For example, clusters may be SAPs with their size measured by the number of edges in the SAP.

A set of clusters, C_n , which is invariant under translations on L is said to satisfy the *first* cluster axiom (CA1).

Let C_n^* denote a subset of C_n that contains exactly one translate of each cluster in C_n .

Let *wt* be a weight function, $wt : C_{<\infty} \to (0, \infty)$, that assigns a positive weight to each cluster in $C_{<\infty} = \bigcup_{n=1}^{\infty} C_n$ and that is invariant under translation. The *second cluster axiom* (*CA2*) is satisfied if for each $m \ge 0$ there is a finite positive constant γ_m with the property that

$$\frac{1}{\gamma_m}wt(G) \leqslant wt(G') \leqslant \gamma_m wt(G), \tag{2.1}$$

whenever G and G' differ by at most m vertices and edges.

Let G_n denote the weighted sum of all clusters of size *n* (up to translation),

$$\mathcal{G}_n = \sum_{G \in C^*} wt(G), \tag{2.2}$$

and define

$$\lambda = \limsup_{n \to \infty} (\mathcal{G}_n)^{\frac{1}{n}}.$$
(2.3)

The *third cluster axiom* (*CA3*) is that $\lim_{n\to\infty} (\mathcal{G}_n)^{\frac{1}{n}}$ exists and is finite (and equals λ).

We consider very general patterns as defined in [7] so that a pattern can exclude some lattice edges and vertices as well as include others. Specifically, given the lattice L, an ordered pair $P = (P_1, P_2)$ is a *pattern* for any pair of finite disjoint subsets, P_1 and P_2 , of $V(L) \cup \mathcal{E}(L)$ (the union of the vertex set and edge set of the lattice L), with P_1 nonempty. Note that $P_i(i = 1, 2)$ need not be a subgraph of L since knowing that the edge $\{v, w\} \in P_i$ does not necessarily imply that the vertices v and w are in P_i . A cluster in C_n is said to *contain* a pattern P if it contains all the vertices and edges in P_1 and none of the vertices and edges in P_2 . If one is only interested in patterns consisting of vertices and edges that actually occur in



Figure 1. Two examples of proper SAP patterns: (*a*) pattern $U = (U_1, U_2)$ where U_1 consists of the solid edges and circles and U_2 consists of the open circles, and (*b*) pattern $V = (V_1, V_2)$ where V_1 is the solid edges and circles and V_2 is the open circles.

a cluster, then one can set $P_2 = \emptyset$. See figures 1(*a*) and (*b*) for two examples of patterns with respect to the set of SAPs in $L = \mathbb{Z}^2$.

Given a set of clusters $C_{<\infty}$, $P = (P_1, P_2)$ is called a *proper pattern* with respect to $C_{<\infty}$ if there are infinitely many values of *n* such that *P* is contained in some size *n* cluster. For $L = \mathbb{Z}^2$ and C_n equal to the set of square lattice *n*-edge SAPs, the proper patterns with respect to $C_{<\infty}$ are referred to as *proper SAP patterns*. (The patterns given in figures 1(*a*) and (*b*) are each examples of proper SAP patterns.) Note that any subgraph \tilde{P} obtained from a *Kesten pattern* by ignoring the orientation of its edges (see, for example, section 3 of [6]) can be represented by the proper pattern $P = (V_{\tilde{P}} \cup \mathcal{E}_{\tilde{P}}, \emptyset)$, where \emptyset is the empty set.

Let \mathcal{P} be the set of proper patterns associated with $C_{<\infty}$. We further define a pattern $P \in \mathcal{P}$ to be a *Madras pattern* with respect to $C_{<\infty}$ if the following is true. There exists a finite set D of vertices and edges of L which contains P and has the following property: for every cluster $G \in C_{<\infty}$ and every vertex y in G, there is another cluster G' and a translation vector t (dependent on y) such that $y \in D+t$, G' contains P+t, and $G' \setminus (D+t) = G \setminus (D+t)$. That is, one can obtain from G a new cluster G' which contains a translate of P within a fixed distance from y such that G' differs from G only within D + t.

Given a set of clusters $C_{<\infty}$, the *fourth cluster axiom* (CA4) can now be simply stated as follows: every proper pattern P is a Madras pattern with respect to $C_{<\infty}$.

Theorem 1 (Madras [7]). Assume that cluster axioms (CA1), (CA2) and (CA4) hold for a set of clusters $C_{<\infty}$. Let P be a proper pattern. Let $\mathcal{G}_n[\leqslant m, P]$ be the weighted sum of the set of clusters in C_n^* which contain at most m translates of P. Then there exists an $\epsilon > 0$ such that

$$\limsup_{n \to \infty} (\mathcal{G}_n[\leqslant \epsilon n, P])^{\frac{1}{n}} < \lambda.$$
(2.4)

We will need to relax the assumption of (CA4), i.e. that every proper pattern must be a Madras pattern. This is possible as a direct consequence of the results presented in [7]. Namely, the proof of theorem 1 in [7, theorem 2.1] implies the following corollary.

Corollary 1. Assume that cluster axioms (CA1) and (CA2) hold for a set of clusters $C_{<\infty}$. Let *P* be a Madras pattern. Let $\mathcal{G}_n[\leqslant m, P]$ be the weighted sum of the set of clusters in C_n^* which contain at most *m* translates of *P*. Then there exists an $\epsilon > 0$ such that

$$\limsup_{n \to \infty} (\mathcal{G}_n[\leqslant \epsilon n, P])^{\frac{1}{n}} < \lambda.$$
(2.5)

3. New pattern theorems for SAPs and SAWs

An *n*-step self-avoiding walk, ω , in the square lattice \mathbb{Z}^2 is a sequence of *n* distinct edges $\alpha_1, \alpha_2, \ldots, \alpha_n$ in $\mathcal{E}(\mathbb{Z}^2)$ such that $\alpha_i = \{s_{i-1}, s_i\}$ for $i = 1, \ldots, n$ and s_0, s_1, \ldots, s_n are distinct vertices in $V(\mathbb{Z}^2)$. The *n*-SAW ω is said to start at s_0 and end at s_n and, for $i = 1, \ldots, n$, the edge from s_{i-1} to s_i is called the *i*th step of the walk. The number of *n*-SAWs in \mathbb{Z}^2 starting at the origin is denoted by c_n . For a given *n*-SAW σ , there is a corresponding reverse SAW rev(σ) $\equiv (\alpha_n, \alpha_{n-1}, \ldots, \alpha_1)$ and $\{\sigma, rev(\sigma)\}$ forms a set of 2 distinct *n*-SAWs originating from σ . This set of *n*-SAWs can be regarded as a single geometrical entity, which is called an *n*-edge undirected self-avoiding walk (*n*-USAW). Equivalently an *n*-USAW is a connected *n*-edge, (n + 1)-vertex subgraph of \mathbb{Z}^2 in which all vertices have degree at most two. Two *n*-USAWs in \mathbb{Z}^2 is denoted by u_n . Note that $c_n = 2u_n$.

For any positive even integer *n*, an *n*-step *self-avoiding circuit* (*n*-SAC) σ is a sequence of *n* distinct edges $\alpha_1, \alpha_2, \ldots, \alpha_n$ in $\mathcal{E}(\mathbb{Z}^2)$ such that $\alpha_i = \{s_{i-1}, s_i\}$ for $i = 1, \ldots, n, s_n = s_0$ and $s_0, s_1, \ldots, s_{n-1}$ are distinct vertices in $V(\mathbb{Z}^2)$. The number of *n*-SACs in \mathbb{Z}^2 starting at the origin is denoted by q_n . The *n*-SAC 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 SAC* of σ . For any $i = 1, \ldots, n$, the *n*-SAC cyc_{*s*_{*i*-1}(σ) $\equiv (\alpha_i, \alpha_{i+1}, \ldots, \alpha_n, \alpha_1, \alpha_2, \ldots, \alpha_{i-1})$, obtained from an *n*-SAC σ by a cyclic permutation of its edges, is referred to as the *cyclic permutation of* σ starting at s_{i-1} . For a given *n*-SAC σ , {cyc_{*s*_{*i*-1}(σ), cyc_{*s*_{*i*-1}(rev (σ)), $i = 1, \ldots, n$ } forms a set of 2*n* distinct *n*-SACs originating from σ . 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 two. 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 . Note that $q_n = 2np_n$.}}}

We also refer to any finite connected subgraph of \mathbb{Z}^2 with no (exactly two) odd degree vertices as a *closed (open) eulerian embedding*.

With regard to a general pattern theorem, the main clusters of interest here are SAPs and hence we let C_n denote the set of square lattice SAPs with *n* edges, and C_n^* be the set of all elements of C_n whose lexicographically smallest vertex is the origin. Thus the number of square lattice *n*-edge SAPs (up to translation) is given by $p_n = |C_n^*|$, with *n* even. Since the square lattice is invariant under all translations in \mathbb{Z}^2 then cluster axiom 1 (CA1) of [7] is satisfied. As discussed in [7], cluster axiom 2 (CA2) holds for a wide class of weight functions. Thus we are interested in establishing cluster axiom 4 (CA4) of [7] for SAPs. For this, we show next that it is possible to insert any properly defined SAP pattern at (roughly) an arbitrary location in an arbitrary square lattice SAP.

First define the *square* R(a, b, M) to be the subgraph of \mathbb{Z}^2 induced by the vertex set $\{v = (v_1, v_2) \in V(\mathbb{Z}^2) | a \leq v_1 \leq a + M, b \leq v_2 \leq b + M\}$ for $a, b \in \mathbb{Z}$ and non-negative integer M; M is referred to as the *side-length* of the square. The *boundary* of the square R(a, b, M) is denoted by $\partial R(a, b, M)$ and defined to be the subgraph of \mathbb{Z}^2 induced by the vertex set $\{v = (v_1, v_2) \in V(R(a, b, M)) | v_1 \in \{a, a + M\}$ or $v_2 \in \{b, b + M\}$.

The next lemma establishes (CA4) for SAPs.

Lemma 1. Every proper SAP pattern $P = (P_1, P_2)$ is a Madras pattern with respect to the set of all finite size self-avoiding polygons in \mathbb{Z}^2 . That is, given any SAP G and vertex y in G, it is possible to insert a translate of the pattern P into G at a position which is 'near' the vertex y.

The details of the proof are given after the proof of lemma 3. However, an outline of the proof is as follows: delete all edges and vertices of *G* lying inside a prespecified square centred at vertex *y*; reconnect the resulting subgraph by making changes near the boundary of the square to produce a new connected subgraph, \tilde{G} , having only even degree vertices (vertices of degree 4 are allowed); next, in order to insert the pattern *P* into the embedding, translate (using translation vector *t*) a polygon containing *P* into the square and then concatenate it to \tilde{G} ; finally, create a SAP *G'* by removing any vertices of degree 4 (by applying [6, lemma 7]) without affecting the pattern. The set *D* required for *P* to be a Madras pattern is then defined so that D + t is the subgraph of the lattice where changes were made to *G*.

As pointed out in [7], lemma 1 does not hold for SAWs or USAWs. This is due to the fact that *end patterns* (patterns which can only appear either at the start or end of a walk) would fall into the class of proper patterns for USAWs. However, it is clearly not possible to insert an end pattern at an arbitrary location in a USAW. Instead, we prove a modified version of lemma 1, namely that it is possible to insert any proper SAP pattern at an arbitrary location in a USAW. With this, corollary 1 then establishes that a pattern theorem (i.e. equation (2.4)) holds for USAWs with the applicable pattern set restricted to the set of proper SAP patterns. The modified version of lemma 1 is as follows.

Lemma 2. Every proper SAP pattern $P = (P_1, P_2)$ is a Madras pattern with respect to the set of all finite size undirected self-avoiding walks (USAWs) in \mathbb{Z}^2 . That is, given any USAW *G* and vertex *y* in *G*, it is possible to insert a translate of the pattern *P* into *G* at a position which is 'near' the vertex *y*.

The method of proof for both lemmas 1 and 2 is essentially the same with some minor modifications needed for the USAW case. Hence, we prove both these lemmas at the same time with the required USAW case modifications set off in square brackets. The proof in either case requires that the following lemma be established first. Essentially this lemma allows for the erasure of a region containing y in order to make room for inserting the pattern P.

Lemma 3. Given any SAP [USAW] G in \mathbb{Z}^2 and any vertex $y = (y_1, y_2)$ in V_G , let $D_N \equiv R(y_1 - N/2, y_2 - N/2, N)$ (a square centred at y with even sidelength N) for any N > 0. Then for every even $N \ge 6$ such that $V_{\partial D_N} \cap V_G \ne \emptyset$ [and V_{D_N} does not contain any degree one vertices of the USAW], there is a closed [open] Eulerian embedding \tilde{G} in \mathbb{Z}^2 such that $G \setminus D_N = \tilde{G} \setminus D_N$ and $V_{\tilde{G}} \cap V_{D_{N-6}} = \emptyset$. Also, any vertices of degree greater than 2 in \tilde{G} are either in ∂D_N or ∂D_{N-2} or or ∂D_{N-4} .

Proof. Let G, y, N and D_N be as in the statement of the lemma (see, for example, figure 2(*a*)). Since $y \in V_G$ and $V_{\partial D_N} \cap V_G \neq \emptyset$, it follows that $V_{\partial D_K} \cap V_G \neq \emptyset$ for all $K \leq N$.

Denote the four corners of ∂D_N by $\Lambda_N \equiv \{(y_1 - N/2, y_2 - N/2), (y_1 - N/2, y_2 + N/2), (y_1 + N/2, y_2 - N/2), (y_1 + N/2, y_2 + N/2)\}.$

Now, we define the procedure for constructing \tilde{G} . First, remove all the edges of G in D_N except for those incident on the four corner vertices in Λ_N . Then remove any resulting isolated vertices to create a subgraph G_1 of G (see, for example, figure 2(*b*)). Note that G_1 may be empty, however, this does not change our construction of \tilde{G} .

 G_1 may now have vertices of odd degree [beyond the two outside D_N] and it is not necessarily connected. The ultimate goal is to create a connected graph \tilde{G} having no odd degree vertices [beyond the two outside D_N] and which is the same as G_1 outside D_N . To do this, we need to examine the connectedness of G_1 and some properties of its odd degree vertices.



Figure 2. Example construction for the proof of lemma 3: begin with (*a*) SAP *G* and, in the following order, transform to (*b*) G_1 , (*c*) G_2 , (*d*) G_3 , (*e*) G_4 and then (*f*) eulerian embedding \tilde{G} . In (*c*), $v_1 \in \Lambda_{N-2}$ is corner vertex *X* as in figure 3(*a*) and v_2 is *X* in figure 3(*b*).

By the definition of G_1 , we can say the following about the degree of any vertex $v \in V_{G_1}$. If $v \notin V_{\partial D_N} \setminus \Lambda_N$, then $\deg_{G_1}(v) = \deg_G(v)$. In particular, for $v \in V_{G_1} \cap \Lambda_N$, $\deg_{G_1}(v) = \deg_G(v) = 2$. If $v \in V_{\partial D_N} \setminus \Lambda_N$ then either v is a neighbour to a corner in Λ_N and $\deg_{G_1}(v) \in \{1, 2\}$ or else v is not a neighbour to a corner and $\deg_{G_1}(v)$ must be one. If $\deg_{G_1}(v) = 2$ then clearly $\deg_{G_1}(v) = \deg_G(v)$ (since G is a SAP [USAW]).

Note that for any graph the number of odd degree vertices is even. Furthermore, since $V_{\partial D_{N-2}} \cap V_G \neq \emptyset$, if $V_{G_1} \neq \emptyset$ then there must be at least one odd degree vertex, w_0 say, in $V_{G_1} \cap (V_{\partial D_N} \setminus \Lambda_N)$. Finally, for each vertex $v \in V_{G_1}$ there is a path in G_1 from v to an odd degree vertex in $V_{\partial D_N} \setminus \Lambda_N$. To see why this last claim is true, suppose $v \in V_{G_1}$ is not itself an odd degree vertex in $V_{\partial D_N} \setminus \Lambda_N$. Consider a path in G from v to w_0 , denoted by the sequence of vertices $(v, w_j, \ldots, w_1, w_0)$ with $j \ge 0$; such a path exists because G is connected and, by the choice of v, it must have length at least one. Consider the smallest value of l such that the path (v, w_j, \ldots, w_l) is in G_1 . Note that the edge $\{w_{l+1}, w_l\} \in \mathcal{E}_{G_1}$ while $\{w_l, w_{l-1}\} \notin \mathcal{E}_{G_1}$.



Figure 3. The corner transformations needed to create G_3 from G_2 in the proof of lemma 3. The vertex marked (×) is an odd degree vertex X in $\Lambda_{N-2} \cap V_{G_2}$. Solid edges and vertices in the configurations shown on the left are edges and vertices in G_2 ; hash marks and open circles indicate, respectively, edges and vertices which are not unoccupied. The configurations on the right are the transformations needed for constructing G_3 from G_2 in the two cases (*a*) $Y' \in V(G_2)$ and (*b*) $Y' \notin V(G_2)$.

Therefore, deg_{*G*₁}(w_l) = 1, and hence there is a path in *G*₁ from v to an odd degree vertex in $V_{\partial D_N} \setminus \Lambda_N$.

Next, create a new subgraph G_2 of \mathbb{Z}^2 by adding an edge from each odd degree vertex in $V_{G_1} \cap \partial D_N$ to its square lattice neighbour in ∂D_{N-2} (this is possible because the corners of ∂D_N have the same degree in G_1 as in G and hence necessarily have even degree). (See an example of G_2 in figure 2(c).)

Thus all vertices in G_2 have degree one or two, its odd degree vertices [beyond the two outside D_N] are in ∂D_{N-2} , and there are no edges of G_2 in ∂D_{N-2} . Furthermore all the vertices of G_2 in ∂D_{N-2} have degree one except possibly the corner vertices Λ_{N-2} . For example, the corner vertex $(y_1 - (N-2)/2, y_2 - (N-2)/2)$ would have degree two if the neighbours of $(y_1 - N/2, y_2 - N/2)$ in ∂D_N both had degree one in G_1 . (For example in figure 2(*c*), see the vertex in the bottom left corner of ∂D_{N-2} .)

For the next step of the construction of \tilde{G} , we need to create a graph G_3 from G_2 having no edges in ∂D_{N-2} and only even degree corner vertices Λ_{N-2} . Suppose that there is a corner vertex X in $\Lambda_{N-2} \cap G_2$ with odd degree (ie degree one) in G_2 . Then X is joined by an edge in G_2 to exactly one vertex, say Y, and it is in ∂D_N . This is illustrated (modulo lattice symmetries) in figure 3, where X is marked by a cross (×). For the construction of G_3 , we only need to consider whether the vertex $Y' = X + (X - Y) \in \mathbb{Z}^2$ is occupied in G_2 or not. These two cases lead respectively to the configurations shown on the left in figures 3(a) and (b). The transformations indicated on the right of these figures can then be performed so that the corner vertex X now has even degree (degree two). This results in a new subgraph, G_3 , in which every vertex in G_3 is joined by a path in G_3 to a vertex in ∂D_{N-2} and there are no edges of the graph in ∂D_{N-2} , as desired. By this construction, neighbours of the corners Λ_N



Figure 4. An example of ω_P associated with pattern $P = (P_1, P_2)$. P_1 is the bold U-shaped USAW, P_2 consists of the open circles, and the bold edge at the bottom left is the required edge in $\partial R(a_P, b_P, M_P)$ (as in the definition of ω_P).

in ∂D_N may have degree 4 in G_3 . (For an example of this construction see figures 2(c) and (d) where the vertex v_1 is in the configuration of figure 3(a) and vertex v_2 is in the configuration of figure 3(b).)

Next add in every edge of ∂D_{N-2} to create a connected subgraph G_4 . Note that it is possible that a vertex of degree 4 will be created at a corner of ∂D_{N-2} . Then, to create G_5 , add an edge from ∂D_{N-2} to ∂D_{N-4} for each vertex of $V_{G_4} \cap \partial D_{N-2}$ of odd degree (recall that the corner vertices of $\Lambda_{N-2} \cap V_{G_4}$ have even degree). Since there must be an even number of odd degree vertices, we can now connect them up in pairs, by proceeding clockwise around ∂D_{N-4} starting at the top-most left-most odd degree vertex. Each time an odd degree vertex is encountered it is connected to the next odd degree vertex using a path in ∂D_{N-4} . Call the resulting embedding \tilde{G} . Clearly \tilde{G} has all [except for the two end vertices of the USAW which were untouched] even degree vertices and is connected and thus it is a closed [open] eulerian embedding in \mathbb{Z}^2 . Finally, the construction also guarantees that $G \setminus D_N = \tilde{G} \setminus D_N$ and $V_{\tilde{G}} \cap V_{D_{N-6}} = \emptyset$, and the only vertices of degree 4 introduced are in $\partial D_N \cup \partial D_{N-2} \cup \partial D_{N-4}$.

In order to prove lemmas 1 and 2, we need some additional notation. Let $P = (P_1, P_2)$ be a proper SAP pattern. Since P is proper, there must exist at least one choice of $a \in \mathbb{Z}$, $b \in \mathbb{Z}$, integer $m \ge 1$, and an associated SAP, ω , such that the following conditions hold: (1) ω contains P and is a subgraph of the square R(a, b, 2m); (2) P_2 is composed of vertices and edges of R(a, b, 2m) and no edges or vertices of either P_1 or P_2 are contained in $\partial R(a, b, 2m)$; and (3) the edge from the vertex (a, b) to the vertex (a, b + 1) is in ω . Fix any (but preferably one in which m is as small as possible) a, b, m, and ω satisfying these conditions and set $a_P = a, b_P = b, M_P = 2m$, and $\omega_P = \omega$. (See for example figure 4 with P_1 being the thick walk and P_2 the two empty sites surrounded by P_1 .) We need also one more lemma that follows immediately from the proofs in [6, lemma 7, lemma 8]. This will be stated for closed Eulerian embeddings with the required open Eulerian embedding modifications set off in square brackets.

Lemma 4 (James and Soteros [6]). Let M = 10 [M = 12] and let σ be any closed [open] Eulerian embedding in \mathbb{Z}^2 with l vertices of degree 4. Let $\xi_i \in \mathbb{Z}^2, i = 1, ..., l$ denote the locations of the l vertices of degree 4. Then there exists a SAP [USAW] $\tilde{\omega}$ such that $\tilde{\omega} = \sigma$ everywhere outside a set of squares of sidelength M centred at the vertices of degree 4, ie $\tilde{\omega} = \sigma$ in $\mathbb{Z}^2 \setminus \bigcup_{i=1}^{l} (\xi_i + R(-M/2, -M/2, M)).$

Now we are ready to prove lemmas 1 and 2. These will both be proved simultaneously below, with (once again) the required USAW modifications set off in square brackets.

Lemma 1 [lemma 2]

Proof. Let M = 10 [M = 12]. Consider any proper SAP pattern $P = (P_1, P_2)$ and a corresponding choice of a_P, b_P, M_P and ω_P , as defined above. Since M_P is even, $R(a_P, b_P, M_P)$ is centred at the vertex $r = (r_1, r_2) \equiv (a_P + M_P/2, b_P + M_P/2)$.

Let *G* be any SAP [USAW] and $y = (y_1, y_2)$ any vertex in V_G . Define t = t(y) to be the translation vector in \mathbb{Z}^2 such that y = r + t, i.e. $t = (y_1 - a_P - M_P/2, y_2 - b_P - M_P/2)$. The *D* that we require is such that $D + t = D_{N'} = R(y_1 - N'/2, y_2 - N'/2, N')$ with $N' = M_P + 2M + 4 [N' = M_P + 2M + 6]$. Thus $D = R(r_1 - N'/2, r_2 - N'/2, N')$, that is the square of side length N' centred at the vertex *r*. Note that $y \in D + t$ and that $\omega_P + t$ is a SAP contained within $D_{M_P} \subset D + t = D_{N'}$ which contains the pattern P + t and has at least one edge in ∂D_{M_P} .

Since $y \in D + t = D_{N'}$, if $V_{\partial D_{N'}} \cap V_G = \emptyset$, then G must be a subgraph of D + t so that $G \setminus (D + t) = \emptyset$. In this case, define G' to be $\omega_P + t$ [with one of its edges in ∂D_{M_P} removed to create a USAW] and the lemma is proved. Otherwise, $V_{\partial D_K} \cap V_G \neq \emptyset$ for all $K \leq N'$.

[Next, for the case of *G* a USAW, if one or both of the degree one vertices of the USAW are in $V_{D_{N'-2}}$, create a new USAW *G*^{*}, which is the same as *G* outside $D_{N'}$, by deleting any path in $D_{N'} \cap G$ that goes from a degree one vertex inside $D_{N'-2}$ to a vertex in $\partial D_{N'}$.]

Consider $N = M_P + M + 4$. Then we have $M_P < N < N'$ and N > 6. Therefore, lemma 3 can be applied using G [or G^* , if appropriate], y, and D_N . Consider \tilde{G} obtained according to the proof of lemma 3. \tilde{G} is a connected closed [open] Eulerian embedding such that any vertex of degree 4 of \tilde{G} is contained in $\partial D_N \cup \partial D_{N-2} \cup \partial D_{N-4}$ and $\tilde{G} \cap D_{N-6} = \emptyset$.

Next consider the SAP $\omega_P + t$. (See for example figure 5(*a*).) By its definition, it is contained in D_{M_P} and it contains the edge from $v \equiv y - (M_P/2, M_P/2)$ to v + (0, 1). Create a new SAP, ω' , from $\omega_P + t$ by first deleting the edge from v to v + (0, 1) and then adding the following sequences of edges: (a) the edge from v - (k - 1, 0) to v - (k, 0), for each $k = 1, \ldots, M/2$; (b) the edge from v - (k - 1, -1) to v - (k, -1), for each $k = 1, \ldots, M/2$; and (c) the edge, *e*, from $u \equiv y - ((N - 4)/2, M_P/2)$ to u + (0, 1). (See figure 5(*b*).) Clearly ω' contains P + t, is contained in D_{N-4} , and has only the edge *e* contained in ∂D_{N-4} . Thus \tilde{G} can intersect ω' at the edge *e* or one or more of its end points but nowhere else.

The goal now is to concatenate \tilde{G} and ω' to create a new connected embedding, G'', with all [except the two endpoints of the USAW] of its vertices even degree. Thus there are three cases: (1) e is in the edge set of \tilde{G} , namely $e \in \mathcal{E}_{\tilde{G}}$; (2) $e \notin \mathcal{E}_{\tilde{G}}$, however, at least one vertex in $V_{\tilde{G}}$ is incident on e; or (3) \tilde{G} and ω' are disjoint graphs. In case (1), to construct G'' take the union of the respective vertex and edge sets of \tilde{G} and ω' but then delete the edge e. In case (2), take the union of the vertex and edge sets of both graphs to create G''. In this case, at least one and at most six vertices of degree 4 exist in $V_{G''} \cap V_{\partial D_{N-4}}$. In case (3), since $e \notin \mathcal{E}_{\tilde{G}}$ and



Figure 5. (*a*) Boundaries of the squares used in the proof of lemmas 1 and 2 are shown. Thin solid edges represent the boundaries ∂D_{M_P} , ∂D_N and $\partial D_{N'}$, while thin dashed edges represent the boundaries ∂D_{N-2} and ∂D_{N-4} , as indicated in the diagram. The SAP, $\omega_P + t$, lies within D_{M_P} ; an example is indicated using thick solid edges. The thick dotted edges are the ones which are added to connect $\omega_P + t$ to the graph \tilde{G} as indicated in the proof of lemmas 1 and 2. (*b*) The lower left-hand portion of the corridor given by $\partial D_N \setminus \partial D_{M_P}$ is magnified to show the details of the construction outlined in the proof of lemmas 1 and 2. The double hash mark indicates the edge has been removed between vertices v and v + (0, 1). Also indicated in the diagram are the edge e from u to u + (0, 1) and the edge f from w to w + (0, 1).

since the edge, f, from $w \equiv u - (1, 0)$ to w + (0, 1) is in $\mathcal{E}_{\tilde{G}}$, G'' can be created by uniting the edge and vertex sets of the two graphs, deleting the edges e and f, and adding the edge from u to w and the edge from u + (0, 1) to w + (0, 1) (see figure 5(b)). In all cases, G'' is a connected embedding, with only [except for the two endpoints of the USAW] even degree vertices, which contains P + t within D_{M_P} , and is such that all (except the two endpoints of the USAW) its vertices outside $\partial D_N \cup \partial D_{N-2} \cup \partial D_{N-4}$ have degree two. Furthermore, $G'' \setminus D_N = \tilde{G} \setminus D_N = G \setminus D_N$ [or $G^* \setminus D_N$, if appropriate].

Finally, lemma 4 can be applied to obtain a SAP [USAW], G', which is the same as G'' everywhere except possibly in $\bigcup_{v=(v_1,v_2)\in V(\partial D_N\cup\partial D_{N-2}\cup\partial D_{N-4})} R(v_1 - M/2, v_2 - M/2, M) = D_{N+M} \setminus D_{N-4-M}$. Note that N + M = N' [N + M = N' - 2] and $N - 4 - M = M_P$. [Therefore the degree one vertices of the USAW outside $D_{N'-2}$ remained untouched.] Thus $G' \setminus D_{N'} = G' \setminus D_{N'} = G \setminus D_{N'}$ and G' contains P + t.

Lemma 1 establishes cluster axiom 4 for square lattice SAPs and hence the Madras pattern theorem (theorem 1) will hold for any weight function that satisfies cluster axiom 2 (CA2). More specifically this proves the following pattern theorem for square lattice SAPs.

Theorem 2. Let wt be any weight function satisfying (CA2) for SAPs and let P be a proper SAP pattern. Let \mathcal{G}_n be the weighted sum over all the square lattice n-SAPs in C_n^* and let $\mathcal{G}_n[\leq m, P]$ be the weighted sum over the n-SAPs in C_n^* which contain at most m translates of P. Then there exists an $\epsilon > 0$ such that

$$\limsup_{n \to \infty} (\mathcal{G}_{2n}[\leqslant \epsilon n, P])^{\frac{1}{2n}} < \lambda_p \equiv \limsup_{n \to \infty} (\mathcal{G}_{2n})^{\frac{1}{2n}}.$$
(3.6)

Lemma 2 establishes that each proper SAP pattern is also a Madras pattern with respect to the set of all USAWs. Thus corollary 1 yields a corresponding pattern theorem for USAWs.

Let U_n^* denote the set of all *n*-edge USAWs whose lexicographically smallest vertex is at the origin.

Theorem 3. Let wt be any weight function satisfying (CA2) for USAWs and let P be a proper SAP pattern. Let \mathcal{G}_n be the weighted sum over all the square lattice n-USAWs in U_n^* and let $\mathcal{G}_n[\leq m, P]$ be the weighted sum over all n-USAWs in U_n^* which contain at most m translates of P. Then there exists an $\epsilon > 0$ such that

$$\limsup_{n \to \infty} (\mathcal{G}_n[\leqslant \epsilon n, P])^{\frac{1}{n}} < \lambda_u \equiv \limsup_{n \to \infty} (\mathcal{G}_n)^{\frac{1}{n}}.$$
(3.7)

4. Applications to ISAPs and ISAWs

To illustrate the usefulness of theorems 2 and 3, the specific choice of weights corresponding to self-interacting SAPs with a nearest-neighbour contact interaction is discussed next.

Given a SAP π in the square lattice, any edge in \mathbb{Z}^2 which is not in π but which is incident on two vertices of π is called a *contact* edge of π . The number of *n*-SAPs in C_n^* containing *k* contact edges is denoted by $p_n(k)$ (note that this is non-zero only for *n* even). Then the partition function for self-interacting *n*-SAPs is given by

$$\mathcal{G}_n^o(\beta) = \sum_k p_n(k) \,\mathrm{e}^{\beta k}.\tag{4.8}$$

For this model, it has been proved [8] that the limit

$$\lambda^{o}(\beta) \equiv \lim_{n \to \infty} \left[\mathcal{G}_{2n}^{o}(\beta) \right]^{\frac{1}{2n}} \tag{4.9}$$

exists and is finite for all finite β . Thus cluster axiom 3 holds. (Note that the proofs in [8] are for \mathbb{Z}^3 but they extend *mutatis mutandis* to \mathbb{Z}^d , $d \ge 2$.)

The corresponding model for self-interacting *n*-SAWs has the partition function

$$\mathcal{G}_n(\beta) = \sum_k c_n(k) \,\mathrm{e}^{\beta k},\tag{4.10}$$

where $c_n(k)$ is the number of *n*-step SAWs, starting at the origin, with *k* contact edges. For this model, it has been proved [8] for $\beta \leq 0$ that the limit

$$\lambda(\beta) \equiv \lim_{n \to \infty} [\mathcal{G}_n(\beta)]^{\frac{1}{n}} \tag{4.11}$$

exists and is finite and is equal to $\lambda^{o}(\beta)$. Thus (CA3) holds for $\beta \leq 0$. However, for $\beta > 0$ the standard subadditivity argument used to establish the existence of the limit when $\beta \leq 0$ now fails. Thus the proof of (CA3) in this case ($\beta > 0$) remains an open problem.

Note that for both cases, the partition function is a weighted sum over a specific set of clusters with the weight function being given by $wt(G) = e^{\beta k}$, where k is the number of contacts in the cluster G. This choice of weights has the form shown in [7, equation (1.4)] with $z_s = 1$ and $z_m = e^{\beta} \in (0, \infty)$, and as indicated in [7], for any finite β , such a weight function satisfies (CA2). In fact, for $wt(G) = e^{\beta k}$ the choice of $\gamma_m = e^{\max\{-4m\beta, 4m\beta\}}$ in equation (2.1) works. To see this, let m be any positive integer. Let G and G' be two SAPs (or SAWs) which differ in size by at most m vertices and edges, i.e. $|V(G)\setminus V(G')| + |V(G')\setminus V(G)| + |\mathcal{E}(G)\setminus \mathcal{E}(G')| + |\mathcal{E}(G')\setminus \mathcal{E}(G)| \leq m$. Then to convert G' to G one removes the edges in $\mathcal{E}(G')\setminus \mathcal{E}(G)$ and the vertices in $V(G)\setminus V(G')$ and the edges in $\mathcal{E}(G)\setminus \mathcal{E}(G')$. In so doing, at most 4 contacts are introduced for each vertex added and at most 1 contact for each edge removed; thus at most 4m contacts are introduced. Similarly, at most 4 contacts are deleted for each vertex removed and at most 1 contact for each edge added; thus at most 4m contacts are deleted. Hence

 $wt(G') \leq e^{\max\{-4m\beta, 4m\beta\}}wt(G)$ and by symmetry $wt(G) \leq e^{\max\{-4m\beta, 4m\beta\}}wt(G')$. Thus for fixed β equation (2.1) is satisfied with $\gamma_m = e^{\max\{-4m\beta, 4m\beta\}}$.

Previous approaches (see [1, section 7.2] and [3, section 5.2]) for obtaining pattern theorems for interacting SAWs have relied on the subadditivity properties of the logarithm of the model's partition function and/or the fact that the limiting free energy is the same for SAWs and unfolded SAWs. These approaches can be used to establish a pattern theorem for the model of self-interacting SAWs given above in the case that $\beta \leq 0$ but have not been successful for $\beta > 0$. The previous approaches for obtaining pattern theorems for interacting SAPs have relied on either relating the limiting free energy for SAPs to that of SAWs or to that of unfolded SAWs. These approaches have not worked for the self-interacting SAP model above, in the case $\beta > 0$.

In contrast, establishing (CA4) for SAPs in \mathbb{Z}^2 did not rely on establishing any relationship between SAPs and SAWs. Furthermore, since (CA2) holds for $wt(G) = e^{\beta k}$ for any finite β , then theorem 2 holds. In particular, given a proper pattern $P = (P_1, P_2)$, let $p_n (\leq m, P, k)$ be the number of square lattice *n*-SAPs in C_n^* with exactly *k* contact edges and that contain at most *m* translates of *P*. Define

$$\mathcal{G}_n^o(\leqslant m, P, \beta) = \sum_k p_n(\leqslant m, P, k) \,\mathrm{e}^{\beta k}. \tag{4.12}$$

Theorem 2 implies the following.

Theorem 4. Given a proper SAP pattern $P = (P_1, P_2)$ in \mathbb{Z}^2 and any finite β , there exists an $\epsilon > 0$ such that

$$\limsup_{n \to \infty} \left(\mathcal{G}_{2n}^{o} (\leqslant \epsilon n, P, \beta) \right)^{\frac{1}{2n}} < \lambda^{o}(\beta).$$
(4.13)

Since the limit in equation (4.9) exists for all finite β , (CA3) is satisfied. Also, by [7, proposition 3.5], given any fixed finite β , there exists a constant A such that $\mathcal{G}_{2n+2}^{o}(\beta) \ge A\mathcal{G}_{2n}^{o}(\beta)$ for all sufficiently large *n*. Then, using the proper SAP patterns U and V as defined in figure 1 (see also [1, figure 7.4]) along with [7, theorem 2.2], the following ratio limit theorem is one direct consequence of theorem 4 (for $\beta \leq 0$ this result was also given in [7, corollary 3.6]):

Corollary 2. For all finite
$$\beta$$
,

$$\lim_{n \to \infty} \frac{\mathcal{G}_{2n+2}^{o}(\beta)}{\mathcal{G}_{2n}^{o}(\beta)} = [\lambda^{o}(\beta)]^{2}.$$
(4.14)

Now, given a proper SAP pattern $P = (P_1, P_2)$, let $c_n (\leq m, P, k)$ be the number of *n*-SAWs, starting at the origin, with *k* contact edges and whose underlying graph (ie associated USAW) contains at most *m* translates of *P*. Define

$$\mathcal{G}_n(\leqslant m, P, \beta) = \sum_k c_n(\leqslant m, P, k) e^{\beta k}.$$
(4.15)

Then, using the fact that there are precisely 2 distinct *n*-SAWs for each *n* edge USAW, theorem 3 leads to the following pattern theorem for self-interacting SAWs.

Theorem 5. Given a proper SAP pattern $P = (P_1, P_2)$ in \mathbb{Z}^2 and any finite β , there exists an $\epsilon > 0$ such that

$$\limsup_{n \to \infty} (\mathcal{G}_n(\leqslant \epsilon n, P, \beta))^{\frac{1}{n}} < \limsup_{n \to \infty} (\mathcal{G}_n(\beta))^{\frac{1}{n}} \equiv \lambda(\beta).$$
(4.16)

In the case that $\beta \leq 0$, the right-hand side of equation (4.16) is equal to $\lambda^{o}(\beta)$.

For $\beta \leq 0$, a ratio limit theorem for SAWs analogous to corollary 2 was given in [7, corollary 3.6]; however, (CA3) has yet to be proved for $\beta > 0$ and thus the corresponding ratio limit theorem remains unproved for this case.

In summary, although theorems 4 and 5 can be proved by alternate methods for $\beta \leq 0$, the results above for $\beta > 0$ are new. The method of proof used for lemmas 1 and 2 is so far only applicable to the square lattice since lemma 4 has only been proved for \mathbb{Z}^2 . It is expected that a detailed case analysis would lead to similar conclusions for \mathbb{Z}^3 , however, this has not been proved. Further consequences of these results will be explored in a subsequent paper.

Acknowledgments

The authors wish to acknowledge helpful discussions with Stu Whittington and Neal Madras. CES would like to thank the Chemical Physics Theory Group, Department of Chemistry, University of Toronto, for their hospitality during two sabbatical visits when this work was carried out. EWJ acknowledges financial support from the Fields Institute for her participation in 'Lattices and Trajectories: A Symposium of Mathematical Chemistry in honour of Ray Kapral and Stu Whittington' after which work on this paper was completed. This research was supported by a grant from NSERC of Canada.

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