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Composite models of polygons

E J Janse van Rensburg
Mathematics and Statistics, York University, Toronto, ON, Canada M3J 1P3

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Abstract. A composite polygon is composed of a lattice polygon in the square lattice, which contains in its interior an internal structure, which may also be a lattice polygon, or a lattice tree or a lattice animal, or a lattice disc (or a collection of these). The properties of composite polygons are considered in this manuscript. In particular, I shall consider the growth constants and generating functions of these models, as well as the statistical mechanics of interacting models of composite polygons. It is shown that there is an adsorption transition of the internal structure on the containing polygon, and a transition which corresponds to the inflation of the containing polygon (by the internal structure).

1. Introduction

Models of lattice polygons continue to attract much attention in the mathematical and physical literature. They have served as models of ring polymers in a good solvent and have been investigated for a variety of different reasons, see for example Sumners and Whittington (1988), Guttmann (1989), Orlandini *et al* (1998). Interacting polygons also received attention. Recent work includes the use of a lattice polygon as a model of two-dimensional vesicles (Fisher *et al* 1991), models of three-dimensional vesicles were studied in Leibler (1987), Orlandini and Tesi (1992), Stella *et al* (1992) Orlandini *et al* (1993), Whittington (1993), Orlandini *et al* (1996) and Janse van Rensburg (1997, 1998b). Models of interacting polygons, similar to models of walks with a nearest neighbour interaction between vertices (originally introduced by Mazur and McCrackin (1968), see also Tesi *et al* (1996)), and models of adsorbing walks (Hammersley *et al* 1982, Vrbová and Whittington 1996, 1998a, b, Janse van Rensburg 1998a), have also been considered.

In this paper I consider a variant of two-dimensional polygons (or vesicles). One such possible variant is illustrated in figure 1; it is a composite of a lattice polygon and a lattice tree, which is contained in its interior. Other variants are obtained by replacing the tree with a polygon, or an animal, or a disc, or a collection of these. Such objects will be called *composite polygons*. Models of composite polygons will also be closely related to models of dense walks, polygons, trees or animals in a confined area, such as a square or rectangle. These models were introduced by Welsh (1985), and studied by Whittington and Guttmann (1990) and Madras (1995). Related studies on dense walks were carried out by Duplantier and Saleur (1987), Burkhardt and Guim (1991), Prentis (1991), Batchelor (1994) and Batchelor and Yung (1994). A composite polygon may also be viewed as a model of a polymer or a branched polymer in a random geometry (of the containing polygon). In this context, an interaction between the internal structure and the containing polygon is a model of a polymer or branched polymer interacting with a substrate of random (fractal) geometry, see for example Nakanishi and Moon (1992).

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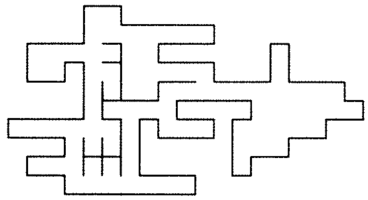

Figure 1. A composite two-dimensional polygon.

The composite polygon consists of two parts; the first is a *containing polygon*, and it encloses an *internal structure* in its interior (in figure 1 this is a tree). If the internal structure is a connected object, then the composite polygon will be called a *simple composite model*; if it need not be connected, then a *complex composite model* is considered†.

The first questions about composite polygons concern the existence of growth constants. In particular, if there are $p_n(m)$ composite polygons‡ consisting of a polygon of length n containing an internal structure of size m, does the limit

$$\lim_{n\to\infty} \frac{1}{n} \log p_n(\lfloor \epsilon n \rfloor) = \log \mathcal{P}(\epsilon) \tag{1.1}$$

exist? The number $\epsilon > 0$ is fixed and real, and $\lfloor q \rfloor$ is the larger integer smaller than or equal to q. Are there related limits to the one presented above? The existence of the growth constant of lattice walks and polygons are closely related to these questions (Hammersley 1960, 1961, Hammersley and Welsh 1962), as are the existence of growth constants of other embedded graphs such as θ-graphs, tadpoles and so on (Soteros 1993, 1998). Limits of this type were also considered by Madras (1995) for walks that cross (and are confined) to a square.

An interacting model of composite polygons can be obtained by the introduction of an activity z conjugate to the size of the internal structure: the partition function in such a model is defined by

$$p_n(z) = \sum_{m\geqslant 0} p_n(m) z^m. \tag{1.2}$$

In this model the existence of a limiting free energy is also an important question, and I shall show that the limit

$$\mathcal{F}(z) = \lim_{n\to\infty} \frac{1}{n} \log p_n(z) \tag{1.3}$$

exists if $z < z_c$ in simple composite models, where $z_c \geqslant 0$ is a critical value of the activity. A more interesting case is found if there is an interaction between the internal structure and the polygon; this interaction could be defined by introducing an activity y conjugate to the number of nearest neighbour contacts between vertices in the internal structure and the polygon. The partition function in such a model is

$$p_n(y, z) = \sum_{k,m} p_n(k, m) y^k z^m \tag{1.4}$$

† Notice that the internal structure is confined to the interior of the polygon, and is disjoint with the polygon. In this paper the internal structure will be imagined to be a polygon, tree or animal. In complex composite polygons a self-avoiding walk can also be used, but the arguments in this paper will not apply for a simple composite polygon with an internal structure which is a walk. That model would not submit to the methods in this paper, and a different approach may be necessary. A hint about this can also be found in the study of walks that cross a square (Madras 1995).

‡ The number of simple composite polygons will be denoted by $p_n^s(m)$, and the number of complex composite polygons by $p_n^c(m)$; if the superscript is left away, then a generic model, which may be either simple or complex, is obtained.

where $p_n(k, m)$ is the number of composite polygons containing a structure of size m and with k nearest neighbour contacts between the internal structure and the containing polygon. The existence of a free energy in these models is a particularly interesting question, and I shall show that it exists for a certain range of the activities in simple composite models. In addition, I shall show that there are critical lines in the phase diagram of this model. If z is increased, then a line of transitions to a phase of inflated simple composite polygons is encountered; if y is increased (with $z < z_c$) there is also an adsorption transition of the internal structure on the polygon.

The existence of growth constants and free energies rely on a generalized super-multiplicative inequality involving $p_n(k, m)$. It is a challenge to show that such a relation exists in simple composite models, and section 2 is devoted to an *unfolding* of a polygon which will be the key to a proof that there is a super-multiplicative relation in these models. In particular, I shall show that a polygon can be *unfolded* through its convex hull, and if it is augmented by adding a small number of edges, then two unfoldings will produce a polygon which contains the original convex hull in its interior, and is otherwise disjoint with it. The most important fact about the unfolding is that it can be done in $o(n)$ operations, a fact which is proven using the result in appendix A. In section 3 the existence of growth constants and limits such as the limit in equation (1.1) are considered. A model of simple composite polygons with an interaction between the containing polygon and the internal structure is considered in section 4. The phase diagram of this model is found to contain at least two critical lines; one a line of transitions to an inflated phase, and the second a line of transitions to a deflated and adsorbed phase (where the internal structure adsorbs on the containing polygon). The line of adsorption transitions meet the line of transitions to an inflated phase at a critical endpoint.

2. Unfolding polygons

Let A be a polygon and let $C(A)$ be its convex hull (see figure 2). The *interior* of $C(A)$ will be denoted by $\tilde{C}(A)$, and the closure of $\tilde{C}(A)$ is $\bar{C}(A) = C(A) \cup \tilde{C}(A)$. The unfolding of the polygon A will be a sequence of steps which will change A into a polygon A^{uu} such that the closure of the convex hull of A is contained entirely in the interior of the convex hull of A^{uu}: $\bar{C}(A) \subset \tilde{C}(A^{uu})$. The basic construction is the reflection of parts of A through the convex hull, but there are many technical details which must be considered in this process. For example, if A is a square, then it is equal to its convex hull, and it cannot be changed into a different

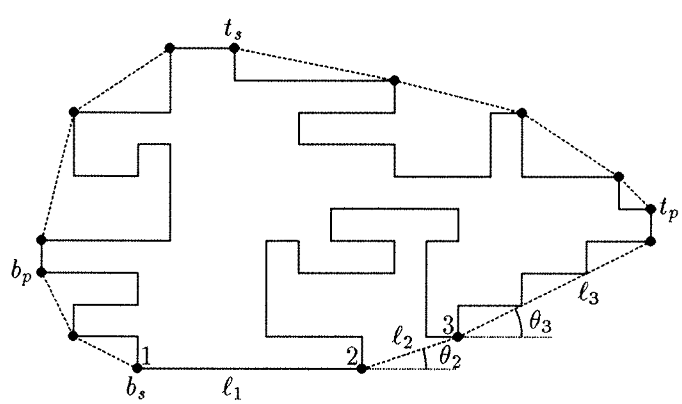

Figure 2. The convex hull of a polygon. Pivot points are indicated by ●.

polygon using reflections through its convex hull.

The construction will be presented in several stages. I first discuss the convex hull of a lattice polygon, before the basic constructions are presented. The unfolding will not make ‘too many’ changes to a polygon, and this will be useful in the study of composite models in section 3.

2.1. The convex hull of a polygon

The convex hull of a lattice polygon A is the minimum length (off-lattice) polygon which contains A. $C(A)$ consists of straight line segments joined into a convex plane polygon (as opposed to a lattice polygon); the first and last vertices of each line segment are vertices in the polygon A, and they are called *pivot points*. Note that exactly two line segments in the convex hull are horizontal (parallel to the X-axis), and two are vertical (parallel to the Y-axis).

A lexicographic ordering of the vertices in A, first with respect to the X-direction, and then with respect to the Y-direction, will define a unique ‘lexicographic most’ vertex, which is called the *primary top vertex* t_p of A, and a unique ‘lexicographic least’ vertex, which is called the *primary bottom vertex* b_p of A. Similarly, a *secondary top vertex* t_s and a *secondary bottom vertex* b_s can be defined by doing the lexicograhic ordering first in the Y-direction, and then in the X-direction. These vertices are indicated in figure 2. It is possible that the top vertices t_p and t_s are coincident, and that the bottom vertices b_p and b_s are coincident. These top and bottom vertices divide the polygon into four sections, of which two may be empty.

Lemma 2.1. *Let A be a polygon of length n and with convex hull $C(A)$. Then there is a constant $K_0 > 0$ such that $C(A)$ is the union of at most $K_0\lfloor n^{2/3}\rfloor$ line segments. Thus, there are at most $K_0\lfloor n^{2/3}\rfloor$ pivot points in the convex hull.*

Proof. Let the primary and secondary top and bottom vertices of A be defined as above. In addition, consider the subwalk of the polygon between b_s and t_p. Label the pivot points in this subwalk by $1, 2, \ldots,$ starting at b_s (see figure 2). The pivot points are lattice points in the square lattice (with integer coordinates), and they are the endpoints of the line segments whose union is the segment of $C(A)$ between the vertices b_s and t_p. Let ℓ_i be the line segment between pivot points i and $i+1$. Let θ_i be the angle between ℓ_i and the positive X-direction; then $\tan\theta_i$ is a rational number. Define

$$\tan\theta_i = \frac{q_i}{p_i}$$

with (p_i, q_i) relative primes, and suppose that there are M such line segments and angles with $\tan\theta_i \leqslant 1$. By definition, $\tan\theta_1 = 0$, in this case define $q_1 = 0$ and $p_1 = 1$. Since $C(A)$ is convex,

$$0 = \tan\theta_1 < \tan\theta_2 < \cdots < \tan\theta_M \leqslant 1$$

or in other words

$$0 = \frac{q_1}{p_1} < \frac{q_1}{p_2} < \cdots < \frac{q_M}{p_M} \leqslant 1. \qquad (\dagger)$$

The number of edges in the part of the polygon ω which joins the endpoints of ℓ_i is at least $p_i + q_i$, so that

$$\sum_{i=1}^{M}(p_i + q_i) \leqslant n. \qquad (\ddagger)$$

Thus, the M distinct points (p_i, q_i) with $q_i \leqslant p_i$ satisfy the constraints in equations (†) and (‡). The largest number of distinct points satisfying these constraints is bounded from above

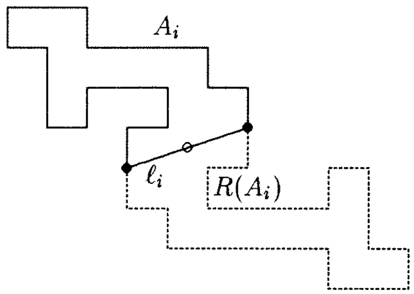

Figure 3. The reflected image of a subwalk.

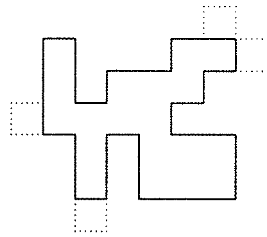

Figure 4. The augmentation of a polygon.

by $C_0\lfloor n^{2/3}\rfloor$; a fact which is proven in appendix A. Thus $M \leqslant C_0\lfloor n^{2/3}\rfloor$. By reflecting or rotating the polygon, the number of line segments in the subwalk of the polygon between b_s and t_p which makes angles greater than $\pi/4$ with the positive X-direction can be bounded by $C_0\lfloor n^{2/3}\rfloor$. Thus there are at most $2C_0\lfloor n^{2/3}\rfloor$ such line segments in the section of the convex hull between b_s and t_p. Therefore, the total number of line segments in the convex hull is at most $8C_0\lfloor n^{2/3}\rfloor$. □

Lemma 2.1 states that if a lattice polygon A has length n, and convex hull $C(A)$, then $C(A)$ is an M-gon, where $M \leqslant K_0\lfloor n^{2/3}\rfloor$, for some fixed number K_0 independent of A and n. The next step is the unfolding of subwalks of A through the sides of $C(A)$; since there are at most $K_0\lfloor n^{2/3}\rfloor$ such sides, this will limit the number of unfolding of subwalks.

2.2. *The unfolding of a polygon*

Let the convex hull of a polygon A of length n be $C(A)$, and suppose that $C(A)$ is an M-gon composed of line segments $\{\ell_i\}_{i=1}^{M}$, where $M \leqslant K_0\lfloor n^{2/3}\rfloor$. The endpoints of a line segment ℓ_i are pivot points, and they are vertices in A; they are also the endpoints of a subwalk A_i of A which is entirely in the closure $\bar{C}(A)$. The basic operation in an unfolding of a polygon is a reflection of A_i through the midpoint of the line segment ℓ_i as illustrated in figure 3. The reflected image of A_i, denoted by $R(A_i)$, is disjoint with $\tilde{C}(A_i)$.

There are potential problems with the operation in figure 3 only if the line ℓ_i is parallel to a lattice axis; in that case the entire subwalk A_i might be contained in ℓ_i (that is, $A_i = \ell_i$), and so $R(A_i) = A_i$). For every other ℓ_i in the convex hull, every edge (except for possibly one of its endpoints) in A_i is in $\tilde{C}(A)$, and so every edge is moved outside $\tilde{C}(A)$ in the reflection. Only vertices in $R(A_i)$ may still be in $C(A)$. To avoid the problems above when ℓ_i is parallel to a lattice axis, I shall slightly change A by adding eight new edges to it.

In the previous section the primary and secondary top and bottom vertices of A were defined. The *primary top and bottom edges* of A are similarly defined: they are the lexicographic most and least edges with respect to an ordering of their midpoints; first in the X-direction, and then in the Y-direction. Similarly, the *secondary top and bottom edges* of A are the lexicographic most and least edges with respect to an ordering of the midpoints of the edges; first in the Y-direction, and then in the X-direction. A polygon A is *augmented* when two edges are added at each of the primary and secondary top and bottom edges as illustrated in figure 4. This increases the length of the polygon by eight edges, and the augmented polygon derived from A will be denoted by A^a. An augmented polygon has the important property that *only* its primary and secondary top and bottom edges are contained in its convex hull. Every other edge in A^a is either disjoint with the convex hull, or has at most one endpoint in the convex hull. The unfolding of a polygon A always proceeds by operating on the augmented polygon A^a derived from A. The following lemma states the basic construction in an unfolding.

Lemma 2.2. *Let A be an arbitrary polygon, and let $C(A)$ be its convex hull. Then any edge in A^a can be reflected through the convex hull $C(A^a)$ to an image which is disjoint with the interior $\tilde{C}(A)$ of the convex hull of A, and which has at most one endpoint in the closure $\bar{C}(A)$ of the convex hull of A.*

Proof. Suppose that $C(A) = \cup_{i=1}^{M} \ell_i$ is the union of straight line segments ℓ_i joined at pivot points in A, and let the pivot points cut A into subwalks A_i, where the first and last vertices of A_i are the endpoints of ℓ_i (see figure 3). Augment A to A^a, and similarly let $C(A^a) = \cup_{i=1}^{M_a} \ell_i^a$ be its convex hull, consisting of $M_a \leqslant M$ line segments ℓ_i^a, with pivots points which cut A^a into subwalks A_i^a. Let e be an arbitrary edge in A^a. There are two possibilities: in the first case, e may be a top or a bottom edge (primary or secondary), or be adjacent to a top or a bottom edge of A^a. By the construction of the augmented polygon, e is then disjoint with $\tilde{C}(A)$, and there is nothing to prove. In the second case, e is contained in some subwalk A_i of A. But A_i is a subwalk of some A_i^a in the augmented polygon, and so e has at most one endpoint in $C(A^a)$. Reflecting A_i^a through the midpoint of ℓ_i^a to $R(A_i^a)$ gives $R(e)$ disjoint with $\tilde{C}(A^a)$. But since $\tilde{C}(A) \subset \tilde{C}(A^a)$, $R(e) \cap \tilde{C}(A) = \emptyset$. If one endpoint of e is in $\bar{C}(A^a)$, then one endpoint of $R(e)$ will also be in $\bar{C}(A^a)$. □

Lemma 2.2 suggests that by reflecting subwalks in an augmented polygon through the convex hull, the polygon can be mapped to an image which is disjoint with the interior of the convex hull of the initial polygon. The result will be a polygon which is *unfolded* with respect to the initial polygon.

Theorem 2.3. *Let A be an arbitrary polygon, and let it be augmented to A^a. Suppose that A has length n. Then there exists a constant K_0 such that at most $K_0\lfloor (n+8)^{2/3}\rfloor$ reflections of subwalks in A^a is necessary to produce a polygon A^u of length $n+8$, with the properties that $A^u \cap \tilde{C}(A) = \emptyset$, and $\tilde{C}(A^u) \supset A$. Moreover, no edge in A^u are contained in $\bar{C}(A)$ (but some vertices in A^u may be contained in $\bar{C}(A)$).*

Proof. Let $C(A^a) = \cup_{i=1}^{M} \ell_i^a$ where the ℓ_i^a are straight line segments. Then $M \leqslant K_0\lfloor (n+8)^{2/3}\rfloor$ by lemma 2.1, since A has length n. Order the ℓ_i^a lexicographically with respect to their midpoints, and label the least by 1, the next least by 2 and so on, until the most gets label M. Since A^a is an augmented polygon, exactly four of the ℓ_i^a are parallel to a lattice axis, and they are all of length one. Let A_i^a be that subwalk of A^a with endpoints the endpoints of ℓ_i^a. By the definition of A^a, ℓ_1^a is a vertical line segment of length one, and it consists of the primary bottom edge of A^a. This is illustrated in figure 5. Since this edge, and its endpoints, are already disjoint with $\bar{C}(A)$, nothing needs to be done here. Reflect A_2^a through the midpoint of ℓ_2^a to $R(A_2^a)$, and let $A^{(2)} = (A^a \setminus A_2^a) \cup R(A_2^a)$ be the new polygon. By lemma 2.2, all the edges in $R(A_2^a)$ are disjoint with $\tilde{C}(A^a)$, and at best has one endpoint in $\bar{C}(A^a)$. Continue this process: at the ith step proceed as follows. Let the convex hull of $A^{(i-1)}$ be composed of line segments $\ell_j^{(i-1)}$: $C(A^{(i-1)}) = \cup_j \ell_j^{(i-1)}$. Let $A_j^{(i-1)}$ be that subwalk of $A^{(i-1)}$ which has the same endpoints as $\ell_j^{(i-1)}$; and let $A_i^{(i-1)}$ be that subwalk of $A^{(i-1)}$ such that $\ell_i^{(i-1)}$ is that line segment in $C(A^{(i-1)})$ with the lexicographic least midpoint and where $A_i^{(i-1)}$ has edges in $\tilde{C}(A)$. Now form the polygon $A^{(i)} = (A^{(i-1)} \setminus A_i^{(i-1)}) \cup R(A_i^{(i-1)})$. This is illustrated in figure 5. Finally, one finds the polygon $A^{(M')} = (A^{(M'-1)} \setminus A_{M'}^{(M'-1)}) \cup R(A_{M'}^{(M'-1)})$, for some M'. The number of these reflections will not exceed the number of sides in the convex hull of

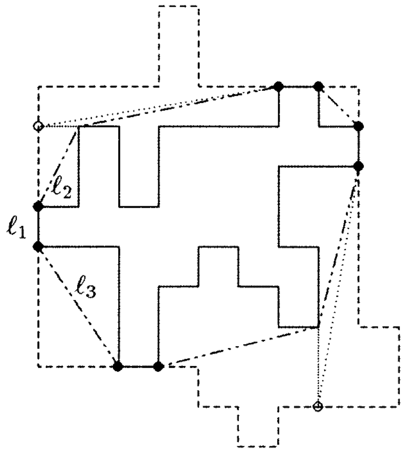

Figure 5. Unfolding a polygon. The dashed lines are images of subwalks in the polygon reflected through the convex hull, which is indicated by the dash-dotted lines. The reflections of subwalks takes place in increasing lexicographic order of the midpoints of the line segments which makes up the convex hull. Closely dotted lines are images of subwalks which were later reflected again, while the two wider spaced dotted lines are parts of the convex hull of a partly unfolded polygon encountered midway through the construction.

A^a, since each subwalk A_i^a will be mapped outside of the convex hull in a single reflection of a subwalk $A_j^{(i-1)}$. Thus $M' \leqslant M \leqslant K_0\lfloor(n+8)^{2/3}\rfloor$. Since each $R(A_i^{(i-1)})$ is disjoint with $\tilde{C}(A)$, and since each edge in $R(A_i^{(i)})$ has at most one endpoint in $\bar{C}(A)$, the theorem follows. $\square$

This theorem has an important corollary.

Corollary 2.4. *Let A^u be the unfolded image of a polygon A. Then there exists a K_1 such that A^u is the image under unfolding of* at most $[n^2]^{K_1\lfloor n^{2/3}\rfloor}$ *distinct polygons, if the unfolding is done as in theorem 2.3.*

Proof. Each of the polygons which unfolds to A^u can be reconstructed by choosing pairs of vertices on A^u, and then by reflecting subwalks of A^u between these vertices through the midpoints of the line segment connecting the vertices into $C(A^u)$. A pair of vertices can be chosen in fewer than $(n+8)^2$ ways, and the reflection for a given pair is done uniquely. Finally, this must be repeated at most $K_0\lfloor n^{2/3}\rfloor$ times, giving rise to at most $(n+8)^2 + (n+8)^4 + \cdots + [(n+8)^2]^{K_0\lfloor n^{2/3}\rfloor}$ different polygons. Since there are $K_0\lfloor n^{2/3}\rfloor$ terms in this sum, and the last term is the largest, this is at most $K_0\lfloor n^{2/3}\rfloor[(n+8)^2]^{K_0\lfloor n^{2/3}\rfloor}$ polygons. Since the smallest polygon has length 4, increasing K_0 shows that a bound of the form $[n^2]^{K_1\lfloor n^{2/3}\rfloor}$ can be found. $\square$

There is a second important corollary to theorem 2.3. This corollary will allow the unfolding of a polygon to be disjoint with the closure of its convex hull.

Corollary 2.5. *Let A be a polygon, and let it be augmented to A^a. By unfolding A^a to A^u, and then augmenting and unfolding A^u to find A^{uu}, the following is obtained: $A^{uu} \cap \bar{C}(A) = \emptyset$ and $\tilde{C}(A^{uu}) \supset \bar{C}(A)$.*

Proof. Unfold A^a as in the proof of theorem 2.3 to find A^u. Every edge vw in A^u is either disjoint with $\bar{C}(A)$, in which case it will stay disjoint with $\bar{C}(A)$ if ω^u is unfolded again, or has at most one endpoint (say v) in $\bar{C}(A)$. Since its other endpoint (w) is not contained in $\bar{C}(A)$, it is the case that v is in $\tilde{C}(A^u)$, and a second unfolding will map v to be disjoint with $\bar{C}(A^u)$, and thus with $\bar{C}(A)$. $\square$

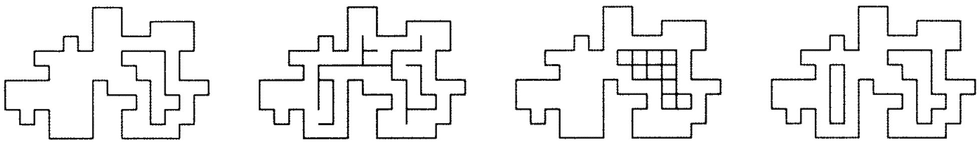

Figure 6. Composite models: (*a*)–(*c*) are examples of simple composite models. In particular, (*a*) is a polygon containing a polygon, (*b*) a polygon containing a tree and (*c*) a polygon containing a disc. The model in (*d*) is a complex composite model containing polygons.

3. Composite models of polygons

In this section an important assumption about the internal structure of composite polygons will be made. Let q_m be the number of conformations of the internal structure if it has size m and if it is connected, counted modulo translations (and with the containing polygon disregarded). For example, if the internal structure is a polygon of length m, then q_m is the number of polygons of length m, counted up to translation. I assume that q_m satisfies a generalized super-multiplicative relation of the type

$$q_{m_1} q_{m_2} \leqslant \sum_{i=-k}^{k} q_{m_1+m_2+i} \tag{3.1}$$

where k is a constant, and that q_m is bounded from above exponentially in m: $q_m \leqslant K^m$ for some value of $K > 1$. This is certainly true for internal structures which are polygon, trees or animals or discs (Hammersley 1961, Klein 1981, Janse van Rensburg and Whittington 1990). Examples of these models are illustrated in figure 6.

An immediate consequence of equation (3.1) is that the limit

$$\log \xi = \lim_{m\to\infty} \frac{1}{m} \log q_m \tag{3.2}$$

exists, where ξ is the *growth constant* of the objects which are the internal structures in our models (Wilker and Whittington 1979)†. Notice that polygons are also super-multiplicative; the number of polygons of length n will be denoted by p_n, and concatenating them similarly to the containing polygons in figure 7 gives $p_{n_1} p_{n_2} \leqslant p_{n_1+n_2}$. In other words, there exists a growth constant for polygons:

$$\log \mu_2 = \lim_{n\to\infty} \frac{1}{n} \log p_n. \tag{3.3}$$

If the internal structure is a polygon, then $\xi = \mu_2$.

3.1. Complex composite polygons

In this section I examine the limiting free energy of a complex composite polygon. The usual construction in a proof that the limiting free energy exists in a model of composite polygons is illustrated in figure 7. Place the two composite polygons such that the top edge of the first

† The proof is as follows: let k_m be that value of i which maximizes the right-hand side of equation (3.1). Then $k_n = \mathrm{o}(n)$, and $q_m q_{n-m} \leqslant (2k+1) q_{n+k_n}$. But this inequality is enough to prove the existence of ξ, provided that $q_m \leqslant K^m$ for some constant $K > 0$.

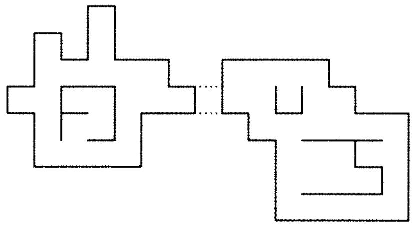

Figure 7. Concatenation of composite polygons in a complex composite model. The composite polygon on the right is translated until its primary bottom edge is parallel to the primary top edge of the composite polygon on the left, and their midpoints differ by exactly one in the X-direction (with all other coordinates equal). Delete the primary top edge of the left composite polygon, and the primary bottom edge of the right composite polygon, and paste the polygons together by inserting the dotted edges.

is one step from the bottom edge of the second in the X-direction. Delete the top and bottom edges, and join the two polygons by inserting the two edges in dotted lines. This shows that

$$\sum_{m_1=0}^{m} p^c_{n_1}(m-m_1)p^c_{n_2}(m_1) \leqslant p^c_{n_1+n_2}(m) \tag{3.4}$$

and by multiplication with z^m and summing over m, it follows that the partition function, defined by

$$p^c_n(z) = \sum_m p^c_n(m)z^m \tag{3.5}$$

satisfies a super-multiplicative inequality:

$$p^c_{n_1}(z)p^c_{n_2}(z) \leqslant p^c_{n_1+n_2}(z) \tag{3.6}$$

and therefore the limit

$$\mathcal{F}_c(z) = \lim_{n\to\infty} \frac{1}{n} \log p^c_n(z) \tag{3.7}$$

exists, but it may be infinite (Hille 1948).

Theorem 3.1. *The limiting free energy in models of complex composite polygons exists. Moreover, if $z > 0$, then $\mathcal{F}_c(z) = \infty$. In other words, there is a transition at $z = 0$ (zero temperature) to an inflated phase.*

Proof. The limiting free energy exists as in equation (3.7). I shall show that it is infinite if $z > 0$ for internal structures which are polygons; the proofs for other internal structures are similar. Consider a square polygon of side-length l. The maximum number of internal polygons that may be fit in this square is at least $\lfloor (l-2)^2/4 \rfloor$, if all these have length four edges, and are packed in the obvious densest way. Suppose that only $\lfloor \epsilon l^2 \rfloor$ polygons of length four are packed in, then they can be packed in at least $\binom{\lfloor (l-2)^2/4\rfloor}{\lfloor \epsilon l^2 \rfloor}$ ways, so that

$$\begin{aligned}\liminf_{n\to\infty} \frac{1}{n^2} \log p^c_n(z) &\geqslant \liminf_{l\to\infty} \frac{1}{16 l^2} \log \binom{\lfloor (l-2)^2/4 \rfloor}{\lfloor \epsilon l^2 \rfloor} z^{4\lfloor \epsilon l^2 \rfloor} \\ &= \frac{1}{16} \log \left(\frac{(1/4)^{1/4} z^{4\epsilon}}{\epsilon^\epsilon (1/4-\epsilon)^{1/4-\epsilon}} \right).\end{aligned}$$

This is a maximum if $\epsilon = z^4/4(1+z^4)$, in which case

$$\liminf_{n\to\infty} \frac{1}{n^2} \log p^c_n(z) \geqslant \frac{1}{16} \log(1+z^4)^{1/4}. \tag{†}$$

In other words, if $z > 0$, then $\liminf_{n\to\infty} \frac{1}{n^2} \log p_n^c(z) > 0$, so that $\mathcal{F}_c(z) = \infty$. □

The result is that models of complex composite polygons exhibits a phase transition at zero 'temperature'. It is not clear that the limit $\lim_{n\to\infty}[\log p_n^c(z)]/n^2$ exists (it exists in models of walks that cross a square (Madras 1995)). If it exists then it is non-zero and finite. In the case of polygons this may be seen as follows. Notice that the maximum combined length of internal polygons that may be put in a containing polygon of length n is $\lceil (n/4)^2 \rceil$, and that k polygons can be packed in at most $\binom{\lceil (n/4)^2\rceil}{k}$ ways into the containing polygon by choosing the location of the top vertex in each. Thus, if the lengths of the internal polygons are $\{m_1, m_2, \ldots, m_k\}$, where $\sum_i m_i = m$, then

$$p_n^c(z) \leqslant \sum_{m\geqslant 0} p_n \sum_{k\leqslant \lceil m/4\rceil} \binom{\lceil (n/4)^2\rceil}{k} \left[\sum_{\{m_i\}} \delta_{(m-\sum_i m_i)} \left[\prod_{j=1}^{k} q_{m_j} \right] \right] z^m \tag{3.8}$$

where the sum over $\{m_i\}$ is over all the possible partitions of m into $\{m_i\}$. Notice that the number of containing polygons is at most p_n, and that if there are k components in the internal structure, then $k \leqslant \lceil m/4 \rceil$. Polygons can be concatenated so that $q_{m_1} q_{m_2} \leqslant q_{m_1+m_2}$. Thus, $\prod_{j=1}^k q_{m_i} \leqslant q_m$. The combinatorial factor is a maximum when $k = \lfloor \lceil (n/4)^2 \rceil /2 \rfloor$. Then $\sum_{k\leqslant\lceil m/4\rceil} [\sum_{\{m_i\}} \delta_{(m-\sum_i m_i)}] \leqslant P(m)$, where $P(m)$ is the number of partitions of m. The outcome of equation (3.8) is then

$$p_n^c(z) \leqslant p_n \binom{\lceil (n/4)^2\rceil}{\lfloor \lceil (n/4)^2\rceil /2\rfloor} \sum_{m\geqslant 0} P(m) q_m z^m. \tag{3.9}$$

Notice that $P(m) \leqslant \mathrm{e}^{\mathrm{O}(\sqrt{m})}$, and that $m \leqslant \lceil (n/4)^2 \rceil$. Thus,

$$p_n^c(z) \leqslant \lceil (n/4)^2 \rceil p_n q_{(\lceil (n/4)^2\rceil + \kappa)} \mathrm{e}^{\mathrm{O}(n)} \binom{\lceil (n/4)^2\rceil}{\lfloor \lceil (n/4)^2\rceil /2\rfloor} \max\{1, z^{\lceil (n/4)^2\rceil}\} \tag{3.10}$$

where the fact that $q_m \leqslant q_{m+2}$ for polygons was used, and where κ is a number in $\{0, 1\}$ such that $\lceil (n/4)^2 \rceil + \kappa$ is even. Take logarithms of the above, divide by n^2 and let $n \to \infty$. This gives

$$\limsup_{n\to\infty} \frac{1}{n^2} \log p_n^c(z) \leqslant \frac{1}{16} \log[2\xi] + \frac{1}{16} \log(\max\{1, z\}). \tag{3.11}$$

A similar argument shows that this limsup is also finite if the internal structure is a forest, or a collection of animals, and so on.

3.2. Simple composite polygons

In the case of a simple composite model the proof of a super-multiplicative relation is much more complicated. The fact that the concatenation in figure 8 of two simple composite polygons will give a composite polygon containing two internal structures must be overcome by finding a construction which will concatenate the internal structures as well. It is in this part of the argument that the assumption in equation (3.1) is important.

The concatenation of simple composite polygons proceeds by the concatenation in figure 8. The next step is to concatenate the internal structures, and this can only be done with the help of the unfolding of the polygon as in section 2. I shall present a proof in the case that the internal structure is a polygon; the other models (trees, animals or discs, and so on) can be handled in a similar way, and the outcome will not differ in an important way from the case of polygons. The construction proceeds now as illustrated in figure 8.

Let A consist of a polygon containing two internal structures, where the polygon was created in the concatenation of two simple composite polygons. The obstacle to concatenating

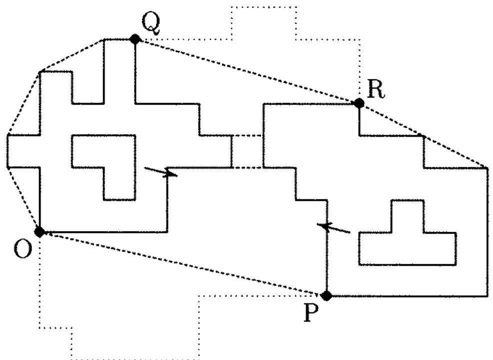

Figure 8. Concatenation in a simple composite model.

the two internal structures into one is that one of them, or both, may be entangled with the containing polygon in such a way that it is not possible to translate them into a convenient arrangement which will make the concatenation possible. To disentangle them from the containing polygon, A will be unfolded through its convex hull. The convex hull of the containing polygon A contains line segments which straddles vertices between the constituent polygons from which A was created; these are for example the line segments OP and QR in figure 8. An important point is that the internal structures in A are both disjoint with OP and QR, and are contained in the wedge formed by OP and QR.

Unfold A twice as in theorem 2.3 through its convex hull to obtain A^{uu}. Both the line segments OP and QR are in $\tilde{C}(A^{uu})$, and so the quadrangle $OPRQ$ are also contained in $\tilde{C}(A^{uu})$. By corollary 2.5 there are no vertices in the internal structures B_1 and B_2 incident with vertices in A^{uu}, and moreover, $\tilde{C}(A)$ is disjoint with A^{uu}. Since both internal structures are also contained in the convex hull of the concatenated polygons, they are untangled from A^{uu} and they can be translated (as sets in $\mathcal{R}^3$) parallel to a line confined to the wedge made by the lines OP and QR inside the convex hull. Translate them until there are two vertices (one in each) within unit distance from one another†. Since both translated internal structures are still disjoint with OP and QR, they can be pushed back onto the lattice. The result is that A^{uu} contains two internal structures such that there are two vertices, one in each internal structure, a unit distance apart.

The last step is the concatenation of the two internal structures. I shall describe the case for polygons; trees, animals or discs can be handled in a similar way. There are two vertices v and w in the two structures, (one with (say) m_1 edges, and the other with m_2 edges) which are adjacent. This is the outcome of the construction in figure 8.

The concatenation of two internal structures which are polygons proceeds by chasing through the diagrams in figure 9. Either there are two parallel edges (one in each internal structure) a unit distance apart (case (a)), or there are not (case (b)). In case (a) let va and wx be the parallel edges. Remove them and replace them with vw and ax. Then the internal polygons are concatenated and has $m_1 + m_2$ edges. Alternatively, there are no parallel edges. Then there are two vertices v and w a unit distance apart, this situation (or a rotation of it) is in case (b). There are three subcases under case (b). In the first subcase both vertices a and

† That this can always be done is seen as follows. Translate both B_1 and B_2 normal to OP until they each have a vertex in (say) OP. Then translate both or one of them parallel to OP (one can be translated towards the wider end of the wedge) towards one another until they almost intersect. Finally push them both a short distance off OP onto the lattice. Since the wedge opens in one direction, or is, at worst, a slab of constant width, this is always possible.

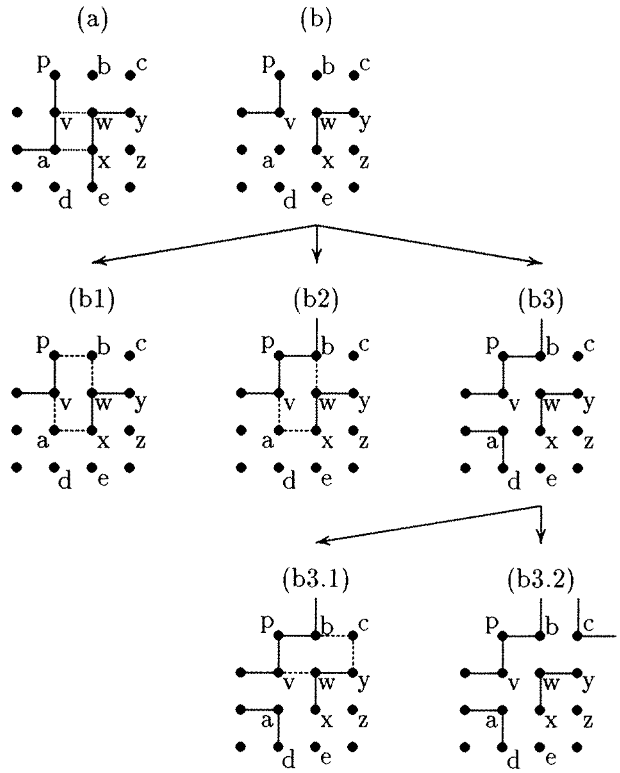

Figure 9. Two internal polygons can be concatenated by a case analysis.

b are unoccupied (case (b1)). Then proceed by deleting pv and wx, and inserting vax and pbw, this gives a polygon with $m_1 + m_2 + 2$ edges. In the second subcase (case (b2)) either a or b are occupied. Without loss of generality, suppose b is occupied, and note that bc cannot be occupied (otherwise there is a pair of parallel edges). Then the only possible case is the one in case (b2). Since a is not occupied, delete wx and vpb, and insert vax and wb to create a polygon of length $m_1 + m_2$. The third subcase is when both a and b are occupied. Since both bc and va are not present, the only possible situation is the one in case (b3). Under case (b3) there are two more subcases. If c is absent, then case (b3.1) is obtained. Delete wy and vpb, and add bcy and vw to obtain a polygon of length $m_1 + m_2$. Otherwise, both c and a are present, and subcase (b3.2) are found. Since xe is absent (there are no parallel edges), xz must be present. Similarly, yz must be present, and so this case can only arise if $m_2 = 4$. Thus, just discard the polygon of length 4 to find a polygon of length $m_1 + m_2 - 4$. This completes the case analysis. Trees, animals and discs can be handled in a similar way.

Lemma 3.2. *If $p_n^s(m)$ is the number of simple composite polygons consisting of a polygon of length n and containing an internal structure of size m, then there is a constant K_0, and a fixed integer k such that*

$$\sum_{m_1=0}^{m} p_{n_1}^s(m - m_1)p_{n_2}^s(m_1) \leqslant [(n_1 + n_2)^2]^{2+K_0(n_1+n_2)^{2/3}} \sum_{i=-k}^{k} p_{n_1+n_2+16}^s(m + i).$$

Proof. Suppose that a simple composite polygon A_1 of length n_1 and internal structure of size

$m - m_1$ is concatenated with a simple composite polygon A_2 of length n_2 and internal structure of size m_1. Then the concatenated (and unfolded) polygon has $n_1 + n_2 + 16$ edges, and the concatenated internal structure has at least $m - 4$ and at most $m + 2$ edges, thus choose $k = 4$. By corollary 2.4 there are at most $[(n_1+n_2+16)^2]^{K_0(n_1+n_2+16)^{2/3}}$ polygons which can be unfolded to the same (augmented) image. The 16 can be left away since $n_1 + n_2 \geqslant 8$ by choosing a larger K_0. In addition, the internal structures are translated before they are concatenated, so that their top vertices explore the entire area of each component polygon. Since the area of A_i is at most n_i^2, another factor of $2n_1^2 n_2^2$ is needed (the factor of 2 accounts for the fact that there are two choices for placing the internal structures). Now observe that $(n_1 + n_2)^2 \geqslant 2n_1 n_2$ to find the generalized super-multiplicative inequality as claimed. □

There is a corollary to theorem 3.1 and lemma 3.2. In particular, the super-multiplicative inequalities can be slightly weakened to get results which will be more useful for another purpose.

Corollary 3.3.

$$p^s_{n_1}(m_1)\, p^s_{n_2}(m_2) \leqslant [(n_1 + n_2)^2]^{2+K_0(n_1+n_2)^{2/3}} \sum_{i=-k}^{k} p^s_{n_1+n_2+16}(m_1 + m_2 + i).$$

The inequality in corollary 3.3 is not enough to prove that the limit $\lim_{n\to\infty} \frac{1}{n} \log p^s_n(Ln)$ exists for any integer L. I shall later show that there is a sequence of numbers $a_n = \mathrm{o}(n)$ such that the limit

$$\lim_{n\to\infty} \frac{1}{n} \log p^s_n(Ln + a_n) = \log \chi^s_L \tag{3.12}$$

exists. As a corollary of that theorem, it follows that the inequality in lemma 3.2 is enough to show existence of the limit in equation (3.12), provided that there are exponential bounds in n on $p^s_n(Ln)$ (there are such bounds, since $p^s_n(Ln) \leqslant n^2 p_n q_{Ln}$, and both p_n and q_{Ln} are bound exponentially (see equation (3.1) and the assumptions following it)). Corollary 3.3 is enough to show that there exists a free energy in this model; this is also easier to see from lemma 3.2. The existence of limiting free energies is discussed in the next section.

3.3. Free energies

The natural definition of the partition function of a model of simple composite polygons is

$$p^s_n(z) = \sum_{m\geqslant 0} p^s_n(m) z^m.$$

This partition function also satisfies some super-multiplicative inequalities; this follows from lemma 3.2.

Lemma 3.4. *The partition function of simple composite polygons satisfy the super-multiplicative relation*

$$p^s_{n_1}(z)\, p^s_{n_2}(z) \leqslant [(n_1 + n_2)^2]^{2+K_0(n_1+n_2)^{2/3}} [\phi(z)]^k\, p^s_{n_1+n_2+16}(z)$$

where $\phi(z) = z + 1 + 1/z$.

Proof. Multiply the inequality in lemma 3.2 by z^m, and sum over m. Then

$$p^s_{n_1}(z)\, p^s_{n_2}(z) \leqslant [(n_1 + n_2)^2]^{2+K_0(n_1+n_2)^{2/3}} \left[\sum_{i=-k}^{k} z^i\right] p^s_{n_1+n_2+16}(z).$$

Observe that $[\sum_{i=-k}^{k} z^i] \leqslant [\phi(z)]^k$ to find the result. □

The super-multiplicative relation in lemma 3.4 suggests the existence of a limiting free energy in these models. However, it is also the case that if $z > 1$, then the limiting free energy is infinite. To see this, note that if the containing polygon in a simple composite model is a square of side-length p, and area p^2, then it may contain an internal structure of size (say) $\lfloor p/4 \rfloor^2$ (the division by 4 gives enough unoccupied vertices to fit the structure into the square). Thus $p_n(z) \geqslant z^{\lfloor p/4 \rfloor^2}$, and so $\lim_{n\to\infty}[\log p_n(z)]/n \geqslant \lim_{p\to\infty}[\log z^{\lfloor p/4 \rfloor^2}]/4p = \infty$ if $z > 1$. In other words, the limiting free energy is infinite if $z > 1$. If $z \leqslant 1$, then the limiting free energy may be finite.

Theorem 3.5. *Suppose that ξ is defined as in equation (3.2). Then there exists a critical value of z, say z_c, in the interval $[\xi^{-1}, 1]$ such that if $z < z_c$, then there exists a finite limiting free energy in models of simple composite polygons, with an activity conjugate to the size of the internal structure:*

$$\mathcal{F}_s(z) = \lim_{n\to\infty} \frac{1}{n} \log p_n^s(z).$$

Moreover, if $z > z_c$, then this is infinite. Lastly, the free energy is a convex function of $\log z$.

Proof. That the limit exist is seen from the generalized super-multiplicative inequality of the partition function in lemma 3.4 (Hammersley 1962). If $z < z_c$, then

$$p_n^s(z) \leqslant n^2 p_n \sum_{m=0}^{\infty} q_m z^m$$

where the factor n^2 is due to the fact that the top vertex of the internal structure can explore the entire area of the containing polygon. Since $q_m = \xi^{m+o(m)}$ by equation (3.2), the sum above is finite if $z < \xi^{-1}$; thus $\lim_{n\to\infty} \frac{1}{n} \log p_n(z) < \infty$. I have already shown that the limiting free energy is infinite if $z > 1$. In other words, there exists a critical value of z in the interval $[\xi^{-1}, 1]$. Convexity follows from a standard application of the Cauchy–Schwartz inequality. □

Thus, there is a phase transition which corresponds to a divergence in the free energy. This transition occurs when the containing polygon is inflated by the internal structure, not unlike the transition in inflating vesicles (Fisher *et al* 1992). This is best illustrated by introducing the generating function of this model:

$$G_s(x, z) = \sum_{n=0}^{\infty} p_n^s(z) x^n. \tag{3.13}$$

Let the radius of convergence of $G_s(x, z)$ be $x_c(z)$. The limiting free energy of the model is related to this by

$$\mathcal{F}_s(z) = -\log x_c(z). \tag{3.14}$$

The singularity diagram of $G_s(x, z)$ is a plot of $x_c(z)$ against z, and the expected behaviour of $x_c(z)$ is illustrated in figure 10. Notice that if $z < z_c$, then $p_n^s(z) \geqslant p_n$, so that there is a critical value of x, $x_c(z) \leqslant \mu_2^{-1}$, which corresponds to a singularity in $G_s(x, z)$. In fact, it is the case that $x_c = \mu_2^{-1}$ if $z < z_c$. If $z < z_c$, then the internal structure should be small, and its interference with the containing polygon should not be important. In other words, the radius of convergence of the generating function $G_s(x, z)$ is given by $x = \mu_2^{-1}$, provided that $z < z_c$. This is seen as follows. Notice that $p_n \leqslant p_n^s(z) \leqslant n^2 p_n \sum_{m\geqslant 0} q_m z^m$, so that

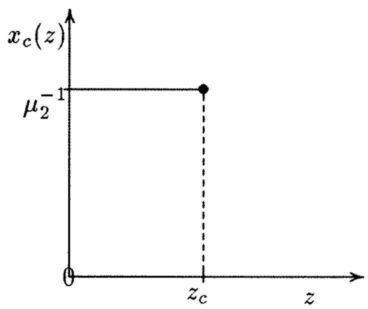

Figure 10. The conjectured singularity diagram of the generating function $G_s(x, z)$. The solid line is conjectured to be a line of branch points in $G_s(x, z)$, while the dashed line is conjectured to be a line of essential singularities in $G_s(x, z)$.

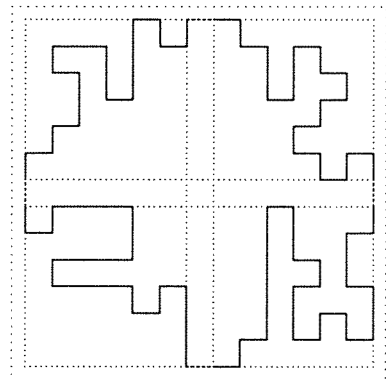

Figure 11. Four walks which cross a square of size $M \times M$ can be arranged as above and put together into a polygon contained in a $(2M + 3) \times (2M + 3)$ square.

$\sum_{n\geqslant 0} p_n x^n \leqslant G_s(x, z) \leqslant \sum_{n\geqslant 0} n^2 p_n x^n \sum_{m\geqslant 0} q_m z^m$. For every $z < z_c$ the sum over m is finite, but if $x > \mu_2^{-1}$, then $G_s(x, z)$ is infinite.

If $z > z_c$, then $x_c(z) = 0$ by theorem 3.5. The singularities in $G_s(x, z)$ for $x = \mu_2^{-1}$ seems to be a line of branch points. If, in addition, in analogy with an inflating vesicle in the Fisher–Guttmann–Whittington model (Fisher *et al* 1991) a line of essential singularities in $G(x, z)$ is encountered at $z = z_c$, then the meeting point of the critical lines in figure 10 is a tricritical point (Brak *et al* 1993). However, this fact has not been verified, and is open to further investigation.

If $z > \xi^{-1}$ then it seems natural to expect that the internal structure will inflate the containing polygon to a square conformation of maximal area. A proof that the critical point of a simple composite model containing an internal structure which is a polygon is at $z_c = \xi^{-1} = \mu_2^{-1}$ is given in figure 11. The argument is as follows. Four walks which cross a square of size $M \times M$ can be arranged as in figure 11 to find a square of size $(2M+3)\times(2M+3)$ which contains a polygon. If there are $c_M^c(m)$ walks of length m which cross an $M \times M$ square†, and if the partition function of these walks is $c_M^c(z)$, then this construction shows that $[c_M^c(z)]^4 \leqslant p_{8M+12}^s(z)$. It is a theorem that $\lim_{M\to\infty}[c_M^c(z)]^{1/M} = \infty$ if $z > \mu_2^{-1}$ (Madras 1995), and thus

$$\liminf_{M\to\infty}[p_{8M+12}^s(z)]^{1/M} = \infty \tag{3.15}$$

if $z > \mu_2^{-1}$. Thus, in the case of polygons confined to a containing polygon, $z_c = \mu_2^{-1}$ $[= \xi^{-1}]$. Trees and animals which crosses a square were also considered in Madras (1995), and if the walks in figure 11 are replaced by those, then it is found that $z_c = \xi^{-1}$ as well. An argument of this type also works if a disc is the internal structure. The result is the following theorem.

Theorem 3.6. *The critical value of z is equal to the inverse of the growth constant of the internal structure: $z_c = \xi^{-1}$.*

Theorem 3.7. *The generating function is finite in a rectangle in the xz-plane, that is, it is finite for all $z < z_c$ and $x < \mu_2^{-1}$. In other words, the radius of convergence of $G_s(x, z)$ is equal to μ_2^{-1} if $z < z_c$, and is equal to zero if $z > z_c$.*

† A walk crosses a square if it starts in the bottom vertex of the square, and terminates in the top edge of the square.

Thus, theorem 3.7 states that the divergence in the generating function as x increases and for $z < z_c$ is due to a divergence in the size of the containing polygon, while the divergence for $x < \mu_2^{-1}$ and increasing z is due to an 'inflation' of the polygon by an internal structure of size proportional to the square of the length of the containing polygon. This transition should be of first order, and should also not be unlike the transition of a walk crossing a square to its dense phase (where the walk fills the square: Whittington and Guttmann (1990), Madras (1995)).

3.4. Density functions and simple composite models

The existence of the limiting free energy in models of simple composite polygons suggest that the growth constants of simple composite polygons should be studied. The following result is a direct consequence of the existence of the free energy.

Theorem 3.8. *Suppose that the free energy $\mathcal{F}_s(z)$ exists and is finite and convex for $z \in [0, z_c)$. Then there is a function $a_n = \mathrm{o}(n)$ such that the function*

$$\mathcal{P}_s(\epsilon) = \lim_{n\to\infty} [p_n^s(\lfloor \epsilon n \rfloor + a_n)]^{1/n}$$

exists for all $0 \leqslant \epsilon < \infty$. Moreover,

$$\log \mathcal{P}_s(\epsilon) = \inf_{z>0} \{\mathcal{F}_s(z) - \epsilon \log z\}.$$

$\mathcal{P}_s(\epsilon)$ is called the density function of the model.

Proof. Let δ_n be that least value of m (dependent on z) which maximizes $p_n^s(m)z^m$. Then

$$p_n^s(\delta_n)z^{\delta_n} \leqslant p_n^s(z) \leqslant n^2 p_n^s(\delta_n)z^{\delta_n} \qquad (\dagger)$$

since there are at most n^2 terms in the partition function. This shows that if the limiting free energy exists, then the limit

$$\mathcal{F}_s(z) = \lim_{n\to\infty} \frac{1}{n} \log \left[p_n^s(\delta_n) z^{\delta_n} \right] \qquad (\ddagger)$$

also exists. If $\limsup_{n\to\infty} \delta_n/n = \infty$, then equation (†) shows that $\mathcal{F}_s(z) = -\infty$ if $z < \xi^{-1}$; this follows since $p_n^s(\delta_n) \leqslant n^2 p_n q_{\delta_n}$. This is a contradiction, so that $\limsup_{n\to\infty} \delta_n/n < \infty$ if $z < \xi^{-1}$. Substract $\epsilon \log z$ from equation (‡) to obtain the following:

$$\mathcal{F}_s(z) - \epsilon \log z = \lim_{n\to\infty} \frac{1}{n} \log p_n^s(\delta_n) + \lim_{n\to\infty} \frac{1}{n} (\delta_n - \lfloor \epsilon n \rfloor) \log z.$$

If the infimum over z is taken, then this shows that $\inf_z\{\mathcal{F}_s(z) - \epsilon \log z\} = -\infty$, *unless* $\inf_z\{\lim_{n\to\infty} \frac{1}{n}(\delta_n - \lfloor \epsilon n \rfloor) \log z\} = 0$. In other words, $\lim_{n\to\infty} \delta_n/n = \epsilon$, and this limit exists. Thus, $\delta_n = \lfloor \epsilon n \rfloor + \mathrm{o}(n)$, and the limit

$$\mathcal{P}_s(\epsilon) = \lim_{n\to\infty} [p_n^s(\lfloor \epsilon n \rfloor + a_n)]^{1/n}$$

exists so that $\log \mathcal{P}_s(\epsilon) = \inf_z\{\mathcal{F}_s(z) - \epsilon \log z\}$. □

Theorem 3.8 completes the proof that the limit in equation (3.12) exists, even if Ln is replaced by $\lfloor Ln \rfloor$, where L is a positive real number. The situation becomes more interesting if alternative definitions of the density functions is considered. For example, consider the density function of composite polygons counted by $p_n^s(\lfloor n^\epsilon \rfloor)$. Suppose that $0 \leqslant \epsilon < 1$ in the first case, and choose n so large that $n^\epsilon < n/8$. Then every conformation of the internal structure

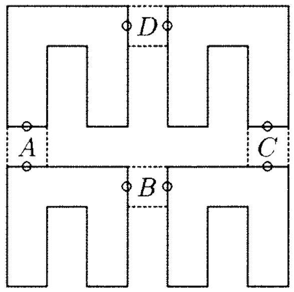

Figure 12. These four spanning polygons of a 3×3 square can be concatenated into a spanning polygon of a 7×7 square by choosing three of the four locations marked by $\{A, B, C, D\}$, deleting the marked edges and replacing them by the dotted edges. The length of any spanning polygon of a 3×3 square is 16, and the spanning polygon of the 7×7 square has $4 \times 16 = 64$ edges. If there are s_M spanning polygons in such a square, then this shows that $s_{64} \geqslant 4[s_{16}]^4$. Repetition of this construction gives $s_{4^k \times 16} \geqslant 4[4[\ldots[s_{16}]^4 \ldots]^4]^4$.

can be fit into a containing polygon which is a square or almost a square. Thus, for these large values of n,

$$q_{\lfloor n^\epsilon \rfloor} \leqslant p_n^s(\lfloor n^\epsilon \rfloor) \leqslant n^2 p_n q_{\lfloor n^\epsilon \rfloor}. \tag{3.17}$$

Thus if the $1/n$th power is taken, and $n \to \infty$, then

$$1 \leqslant \liminf_{n\to\infty} [p_n^s(\lfloor n^\epsilon \rfloor)]^{1/n} \leqslant \limsup_{n\to\infty} [p_n^s(\lfloor n^\epsilon \rfloor)]^{1/n} \leqslant \mu_2 \tag{3.18}$$

provided that $\epsilon < 1$. If $\epsilon = 1$ then $p_n^s(n) \leqslant n^2 p_n q_n$, so that

$$\limsup_{n\to\infty} [p_n^s(n)]^{1/n} \leqslant \mu_2 \xi. \tag{3.19}$$

On the other hand, if $\epsilon > 1$ and a model of composite polygons with internal structures which are polygons, trees or animals are considered, then this limit is infinite. This is seen as follows in the case of spanning polygons. Let s_m be the number of spanning polygons of a square of sidelength $N-1$; then $m = 2N^2$. The construction in figure 12 shows that $s_{4^k \times 16} \geqslant 4[4[\ldots[s_{16}]^4 \ldots]^4]^4$. Thus, $s_{4^k\times 16} \geqslant 4^{1+4+4^2+\cdots+4^k}[s_{16}]^{4^k} = 4^{(4^{k+1}-1)/3}[s_{16}]^{4^k}$. Take logarithms, divide by $4^k \times 16$, and take k to infinity. This shows that $\liminf_{k\to\infty}[\log s_{4^k\times 16}]/(4^k \times 16) \geqslant [\log 4]/48 + [\log s_{16}]/16 > 0$. Lastly, if m in s_m is not equal to $4^k \times 16$ for some k, then define $k = \lfloor \log(m/16)/\log 4 \rfloor$ so that $4^{k+1} \times 16 \geqslant m \geqslant 4^k \times 16$, and then notice that $s_m \geqslant s_{4^k\times 16}$. Thus $\liminf_{m\to\infty} \frac{1}{m} \log s_m \geqslant [\log 4]/48 + [\log s_{16}]/16$, and thus $s_m \geqslant \kappa^m$ for some $\kappa > 1$. In other words, the number of spanning polygons of a square (and thus the number of spanning trees and spanning animals) grows exponentially with its size.

Choose n large enough that $\sqrt{n^\epsilon/2} < n/8$, then all the spanning polygons of length $\lfloor n^\epsilon \rfloor$ of a square of side-length $\lfloor \sqrt{\lfloor n^\epsilon \rfloor/2} \rfloor$ can be fit into (an almost) square containing polygon of length n, provided that n is large. Thus

$$s_{\lfloor n^\epsilon \rfloor} \leqslant p_n^s(\lfloor n^\epsilon \rfloor) \leqslant n^2 p_n q_{\lfloor n^\epsilon \rfloor} \tag{3.20}$$

and by taking the power $1/n$ and letting $n \to \infty$, it follows that the limit is infinite. If the power $1/n^\epsilon$ is taken instead, then

$$1 < \limsup_{n\to\infty} [p_n^s(\lfloor n^\epsilon \rfloor)]^{1/n^\epsilon} \leqslant \xi. \tag{3.21}$$

In other words, this is finite. The existence of these limits is an outstanding issue, but from equations (3.18) and (3.21) I make the following conjecture.

Conjecture 3.9. *The following limits exist:*

$$\lim_{n\to\infty} [p_n^s(\lfloor n^\epsilon \rfloor)]^{1/n} = \mu_2 \qquad \forall \epsilon \in [0, 1)$$

$$\lim_{n\to\infty} [p_n^s(n)]^{1/n} = \mu_2 \xi$$

$$\lim_{n\to\infty} [p_n^s(\lfloor n^\epsilon \rfloor)]^{1/n^\epsilon} = \xi \qquad \forall \epsilon \in (1, 2).$$

Limits related to the above can be shown to exist. For example, if one defines

$$p_n^s(\leqslant m) = \sum_{j=0}^{m} p_n^s(j) \tag{3.22}$$

then it follows from corollary 3.3 that if $\epsilon \geqslant 1$ then

$$p_{n_1}^s(\leqslant \lfloor n_1^\epsilon \rfloor) p_{n_2}^s(\leqslant \lfloor n_2^\epsilon \rfloor) \leqslant f(n_1+n_2) p_{n_1+n_2}^s(\leqslant \lfloor (n_1+n_2)^\epsilon \rfloor + 2) \tag{3.23}$$

where $f(n) = 6n^{4+2K_0 n^{2/3}}$. In addition, the bound $p_n^s(\leqslant \lfloor n^\epsilon \rfloor) \leqslant \sum_{m \leqslant \lfloor n^\epsilon \rfloor} q_m$, is not difficult to derive, so that $p_n^s(\leqslant \lfloor n^\epsilon \rfloor) \leqslant K^{\lfloor n^\epsilon \rfloor}$ for some constant K. In other words, the limit

$$\lim_{n\to\infty} [p_n^s(\leqslant (\lfloor n^\epsilon \rfloor - 2))]^{1/n^\epsilon} \tag{3.24}$$

exists and is finite, for all $\epsilon \in [1, 2]$.

4. Interacting composite models

In this section I restrict the discussion to simple composite polygons, and an interaction between the containing polygon and the internal structure will be introduced. In particular, let $p_n^s(k, m)$ be the number of simple composite polygons with a containing polygon of size n, an internal structure of size m, and with k nearest neighbour contacts between the internal structure and the containing polygon. The partition function of this model is

$$p_n^s(y, z) = \sum_{m,k} p_n^s(k, m) y^k z^m. \tag{4.1}$$

Observe that concatenation and unfolding of these simple composite polygons gives

$$p_{n_1}^s(0, z) p_{n_2}^s(0, z) \leqslant f(n_1+n_2) p_{n_1+n_2+16}^s(0, z) \tag{4.2}$$

so that there is a limiting free energy if the interaction between the internal structure and the containing polygon is an infinite (short-ranged) repulsion.

Theorem 4.1. *The free energy of simple composite polygons exists if there is an infinite repulsion between the simple composite polygon and the internal structure:*

$$\mathcal{F}_s(0, z) = \lim_{n\to\infty} \frac{1}{n} \log p_n^s(0, z)$$

which exists, is finite and convex for all $z \in [0, z_c)$. *Arguments similar to those in the previous section show that* $z_c = \xi^{-1}$.

It is not known that the free energy exists for all values of y. Instead, if $y < 1$, then one might argue that if a polygon with an internal structure of size m and with k nearest neighbour contacts is unfolded twice, then all the nearest neighbour contacts are destroyed, and by corollaries 2.4 and 2.5,

$$p_n^s(0, m) \leqslant p_n^s(k, m) \leqslant [n^2]^{K_0 \lfloor n^{2/3} \rfloor} p_{n+16}^s(0, m). \tag{4.3}$$

Thus, multiplying the above by $y^k z^m$ and summing over m and k,

$$\frac{p_n^s(0, z)}{1-y} \leqslant p_n^s(y, z) \leqslant [n^2]^{K_0 \lfloor n^{2/3} \rfloor} \frac{p_n^s(0, z)}{1-y}. \tag{4.4}$$

Thus, by taking logarithms, dividing by n and letting $n \to \infty$, the following theorem is obtained.

Theorem 4.2. *For all values* $z \in [0, z_c)$ *and all* $y \in [0, 1]$, *the limiting free energy* $\mathcal{F}_s(y, z)$ *exists. Moreover* $\mathcal{F}_s(y, z) = \mathcal{F}_s(0, z)$ *for all* $z \in [0, \xi^{-1})$.

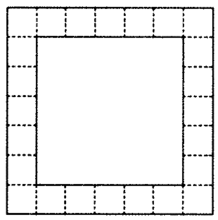

Figure 13. This polygon has length n and $n-4$ nearest neighbour contacts with an internal structure which is a polygon of length $n-8$.

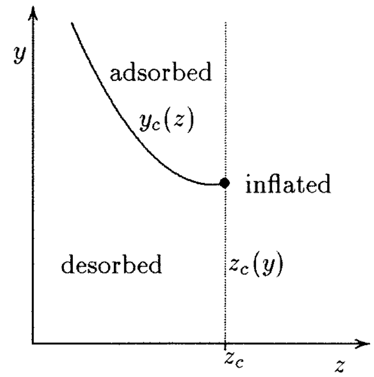

Figure 14. The phase diagram of an interacting model of complex composite polygons. There are three phases; first a desorbed phase of polygons containing internal structures of size no more than the perimeter length of the containing polygon, and then an adsorbed phase where the internal structure is adsorbed in the perimeter of the containing polygon. Finally, there is an inflated phase, where the internal structure inflates the containing polygon. These phases coexist at a triple point.

Notice that a construction similar to that of figure 11 shows that $\mathcal{F}_s(y,z) = \infty$ if $z > \xi^{-1}$, for any value of $y \geqslant 0$. If $z < \xi^{-1}$ then theorem 4.2 can be used to show that there is a non-analyticity in $\mathcal{F}_s(y,z)$ at a critical value $y_c(z)$. This may be seen by, for example, examining a situation as in figure 13. The partition function contains a term which corresponds to a square containing polygon, and an internal structure which consists of at least An edges or unit squares (for some fixed value of A), and with $n-4$ nearest neighbour contacts.

The result is that

$$p_n^s(y,z) \geqslant y^{n-4} z^{An} \tag{4.5}$$

and thus, if the free energy exists, then

$$\mathcal{F}_s(y,z) \geqslant \log y + A \log z. \tag{4.6}$$

In other words, for fixed z, there exists a $y_c(z)$ such that $\mathcal{F}_c(y,z) > \mathcal{F}_c(0,z)$ if $y > y_c(z)$. Thus, there is a second critical line $y_c(z)$ in the phase diagram. Notice that

$$\frac{\partial}{\partial y}\mathcal{F}_c(y,z) = 0 \tag{4.7}$$

and that this derivative is positive for $y > y_c(z)$ whenever it exists (and it exists almost everywhere for $z < z_c$ by the convexity properties of $\mathcal{F}_c(y,z)$. Thus, it is appropriate to interprete the critical line $y_c(z)$ as an adsorption transition of the internal structure on the containing polygon. Notice also that $y_c(0) = \infty$, since if $z = 0$, then the internal structure is empty, and no adsorption can take place. The phase diagram of this model is illustrated in figure 14.

5. Conclusions

In this paper I examined the existence of growth constants, limiting free energies and the phase diagram of a class of (interacting) composite polygon models. These models contain internal structures which satisfy a super-multiplicative relation (equation (3.2)); the methods in this paper cannot be fruitfully applied to a model of a lattice polygons containing a walk, which satisfies a sub-multiplicative relation. In that case a different idea from the methods in this paper is needed.

Two different classes of composite polygons were considered in this paper. The first case is a class of complex composite polygons, where the internal structure is not connected. These models have a transitions at zero temperature; for any positive value of the activity the limiting free energy is infinite. This means that there is an infinite free energy associated with each edge in the containing polygon, and from that perspective this model is not very interesting. However, it seems that a more appropriate normalization of the free energy would involve the area of the composite polygon, instead of its perimeter. In this context, one may define $d_n(m)$ to be the number of polygons of area n containing an internal structure(s) of size m. Concatenation shows that the limiting free energy exists, and it can also be shown that the limiting free energy (per unit area) is finite for values of z less than the inverse growth constant of the internal structure.

In the case of simple composite polygons, the limiting free energy exists and is finite for values of the activity z less than the inverse growth constant of the internal structure. The transition at the critical value of z seems to be an inflation of the containing polygon by the internal structure. Indeed, the number of edges in the internal structure is defined by the derivative of $\mathcal{F}_s(z)$, which is finite it $z < z_c$, and infinite if $z > z_c$. In the deflated phase the mean number of edges in the internal structure is $\mathrm{O}(n)$, or the number of edges in the internal structure as a fraction of the length of the containing polygon is finite in the thermodynamic limit. In the inflated phase this fraction is itself infinite. It seems that this transition resembles the inflation of a disc by its area in the thermodynamic limit (see, for example, Fisher *et al* 1991).

If there is also an interaction between the containing polygon and the internal structure, then a simple model of composite polygons may also exhibit a transition where the internal structure adsorbs on the containing polygon. In this model I was able to show that the limiting free energy $\mathcal{F}_s(y, z)$ (where y is an activity conjugate to the number of contacts between the containing polygon and the internal structure) exists for all $0 \leqslant y \leqslant y_c(z)$, (where $y_c(z)$ is the critical curve along which the adsorption transition occurs). It is not known that $\mathcal{F}_s(y, z)$ exists if $y > y_c(z)$ (and $z < 1$). This state of affairs is not unlike the case of walks with a nearest neighbour interaction (which is a model of linear polymers undergoing a θ-transition). In that model the free energy is known to exist for values of the nearest neighbour activity which corresponds to an expanded phase, but not for the collapsed phase (Tesi *et al* 1996).

Appendix

Consider M distinct points $\{(p_i, q_i)\}_{i=1}^{M}$ in the square lattice, subject to the following constraints:

(1) $0 = \frac{q_1}{p_1} < \frac{q_2}{p_2} < \cdots < \frac{q_M}{p_M} \leqslant 1$, where $q_1 = 0$, and where all pairs (p_i, q_i) are relative primes,

(2) $\sum_{i=1}^{M}(p_i + q_i) \leqslant n$.

For a given n, what is the largest number of distinct points which satisfy the constraints above? In other words, find the maximum value of M (as a function of n). Suppose that the value of M is known, and that a set $\mathcal{S}$ of M points satisfying the constaints above are given. Let the maximum value of $p_i + q_i$ in $\mathcal{S}$ be N. If a point $(p_i, q_i) \in \mathcal{S}$ with $p_i + q_i = N$ is exchanged with a new point $(p_i^*, q_i^*) \notin \mathcal{S}$ but with $p_i^* + q_i^* < N$ (suppose this is possible), then the new set of points $[\mathcal{S} \setminus \{(p_i, q_i)\}] \cup \{(p_i^*, q_i^*)\}$ satisfies the constraints above, the value of M remains unchanged, while the value of the sum $\sum_{i=1}^{M}(p_i + q_i)$ decreases. Thus, the smallest possible values of p_i and q_i should be chosen to find the maximum value of M.

If the first constraint (1) above is relaxed by abandoning the requirement that all pairs (p_i, q_i) are relative primes, then an upper bound on M will be found, since points with smaller values of $p_i + q_i$ can be chosen to satisfy condition (2). Thus, choose the p_i and q_i to be points above or on the p-axis in the pq-plane, but underneath or on the main diagonal $q = p$. Then for each p_i the values of q_i are $\{0, 1, \ldots, p_i\}$, while $p_i = 1, 2, \ldots$. If $p_i + q_i \leqslant N$, then the number of points is $1 + 2 + 2 + \cdots + \lfloor N/2 + 1 \rfloor$. Assume that N is odd, then this sums to at most

$$1 + 2 + 2 + 3 + 3 + \cdots + \lfloor N/2 + 1 \rfloor + \lfloor N/2 + 1 \rfloor = \lfloor N/2 + 1 \rfloor \lfloor N/2 + 2 \rfloor - 1 \tag{A.1}$$

so that the number of distinct points is bound from above by $M \leqslant \lfloor N/2 + 2 \rfloor^2$. On the other hand, for these choices for (p_i, q_i),

$$\begin{aligned}\sum_{i=1}^{M}(p_i + q_i) &\leqslant \sum_{i=1}^{\lceil N/2 \rceil} i(4i - 3) = \lceil N/2 + 1 \rceil (\lceil N/2 \rceil + 2)(8\lceil N/2 \rceil + 3)/6 \\ &\leqslant \tfrac{4}{3} \lceil N/2 + 2 \rceil^3. \end{aligned} \tag{A.2}$$

This is less than n if $\lceil N/2 + 2 \rceil^3 < 3n/4$, or if $\lceil N/2 + 2 \rceil \leqslant (3n/4)^{1/3}$. But then from equation (A.1), $M \leqslant \lfloor N/2 + 2 \rfloor^2$, thus, $M \leqslant (3n/4)^{2/3}$, and since M is an integer,

$$M \leqslant \lfloor (3n/4)^{2/3} \rfloor. \tag{A.3}$$

In other words, M cannot grow faster than a 2/3-power of n. So far, this is only valid if all the points $(p_i + q_i)$ with $p_i + q_i \leqslant N$ are included in the calculation. If only a subset of these are used (and some which have $p_i + q_i = N$ are discarded to minimize the sum in condition (2)), then there are $O(N)$ corrections to equations (A.1) and (A.2). But these changes will only imply a $O(n^{1/3})$ correction to equation (A.3) so that there exists a constant C_0 such that

$$M \leqslant C_0 \lfloor n^{2/3} \rfloor. \tag{A.4}$$

References

Batchelor M T 1994 *Phys. Lett.* A **184** 467

Batchelor M T and Yung C M 1994 *J. Phys. A: Math. Gen.* **27** 4055

Brak R, Owczarek A L and Prellberg T 1993 *J. Phys. A: Math. Gen.* **26** 4565

Burkhardt T W and Guim I 1991 *J. Phys. A: Math. Gen.* **24** L1221

Duplantier B and Saleur H 1987 *Nucl. Phys.* B **290** 291

Fisher M E, Guttmann A J and Whittington S G 1991 *J. Phys. A: Math. Gen.* **24** 3095

Guttmann A J 1989 *J. Phys. A: Math. Gen.* **22** 2807

Hammersley J M 1960 *Phys. Rev.* **118** 656

——1961 *Proc. Camb. Phil. Soc.* **57** 516

——1962 *Math. Proc. Camb. Phil. Soc.* **58** 235

Hammersley J M, Torrie G and Whittington S G 1982 *J. Phys. A: Math. Gen.* **15** 539

Hammersley J M and Welsh D J A 1962 *Q. J. Math. Oxford* **13** 108

Hille E 1948 *Functional Analysis and Semi-Groups* vol 31 (New York: American Mathematical Society)

Janse van Rensburg E J 1997 *J. Stat. Phys.* **88** 177

——1998a *J. Phys. A: Math. Gen.* **31** 8295

——1998b *Topology and Geometry in Polymer Science (Proc. 1995–6 IMA Program on Mathematical Methods in Material Science vol 103)* ed S G Whittington, D W Sumners and T Lodge (New York: Springer) p 193

Janse van Rensburg E J and Whittington S G 1990 *J. Phys. A: Math. Gen.* **23** 1287

Klein D J 1981 *J. Chem. Phys.* **75** 5186

Leibler S 1987 *Statistical Mechanics of Membranes and Surfaces (Jerusalem School for Theoretical Physics vol 5)* ed D Nelson, T Piran and S Weinberg (Singapore: World Scientific) p 46

Madras N 1995 *J. Phys. A: Math. Gen.* **28** 1535
Mazur J and McCrackin F L 1968 *J. Chem. Phys.* **49** 648
Nakanishi H and Moon J 1992 *Physica* A **191** 309
Orlandini E, Stella A, Einstein T L, Tesi M C, Beichl I and Sullivan F 1996 *Phys. Rev.* E **53** 5800
Orlandini E, Stella A, Tesi M C and Sullivan F 1993 *Phys. Rev.* E **48** R4203
Orlandini E and Tesi M C 1992 *Physica* A **185** 160
Orlandini E, Tesi M C, Janse van Rensburg E J and Whittington S G 1998 *J. Phys. A: Math. Gen.* **31** 5983
Prentis J J 1991 *J. Phys. A: Math. Gen.* **24** 5097
Soteros C E 1993 *J. Math. Chem.* **14** 91
——1998 *Topology and Geometry in Polymer Science (Proc. 1995–6 IMA Program on Mathematical Methods in Material Science vol 103)* ed S G Whittington, D W Sumners and T Lodge (New York: Springer) p 103
Stella A L, Orlandini E, Beichl I, Sullivan F, Tesi M C and Einstein T L 1992 *Phys. Rev. Lett.* **64** 3650
Sumners D W and Whittington S G 1988 *J. Phys. A: Math. Gen.* **21** 1689
Tesi M C, Janse van Rensburg E J, Orlandini E and Whittington S G 1996 *J. Phys. A: Math. Gen.* **29** 2451
Vrbová T and Whittington S G 1996 *J. Phys. A: Math. Gen.* **29** 6253
——1998a *J. Phys. A: Math. Gen.* **31** 3989
——1998b *J. Phys. A: Math. Gen.* **31** 7031
Welsh D 1985 *Ars Comb.* B **20** 271
Whittington S G 1993 *J. Math. Chem.* **14** 103
Whittington S G and Guttmann A J 1990 *J. Phys. A: Math. Gen.* **23** 5601
Wilker J B and Whittington S G 1979 *J. Phys. A: Math. Gen.* **12** L245