Three dimensional self-avoiding convex polygons

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We calculate the generating function of three-dimensional self-avoiding convex polygons. This both adds to the very short list of exactly solved three-dimensional statistical mechanics systems, and illuminates the properties of self-avoiding polygons.

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Solutions of three-dimensional models in statistical mechanics have proved to be exceptionally difficult, with only a very small number of solutions to non-trivial problems known. These include staircase polygons [1], directed animals [2] and Zamoldchikov's model and its N-component extension [3–5] and recently a 3-dimensional dimer model [6].

For self-avoiding walks and in particular their proper subset, self-avoiding polygons [7], exact solutions have focussed on simpler models [8,9], such as staircase, convex, row convex and three-choice polygons [10]. The aim of studying these simpler models is twofold. While they have intrinsic combinatorial interest, to physicists they appear to capture many of the important features of self-avoiding polygons, and additionally can be generalized to model collapse transitions [11] observed in vesicles and the like.

In this paper we obtain the perimeter generating function for *three-dimensional* self-avoiding convex polygons (SACP). This solution adds to the short list of exactly solved three-dimensional models, and also illuminates the increase in functional complexity as one moves from a two-dimensional to a three-dimensional system.

Of the previously solved three-dimensional systems, staircase polygons [1] are the least intrinsically three-dimensional, being generated by a concatenation argument, which is essentially one-dimensional. The solution of the three-dimensional directed animal problem [2] is obtained by mapping it onto the two-dimensional hard hexagon model, so the solution is essentially that of a two-dimensional model, while Baxter's work on the Zamoldchikov solution of the tetrahedron equations (which are a genuinely three-dimensional version of the star-triangle equations), also displays considerable two-dimensional character.

We find that while the solution of two-dimensional convex polygons [12,13] is algebraic, the three-dimensional solution is neither algebraic, nor even D-finite (expressible as a linear o.d.e. with polynomial coefficients), but is mostly simply given as the quotient of two D-finite functions.

The method of solution can, in principle, be generalised to higher dimensional SACP, though at the cost of greatly increased algebraic complexity. The solution is long and complex, and full details will be published elsewhere [14]. In this paper we only describe the central ideas of the solution, and give an outline of its derivation.

We will study families of polygons of increasing complexity *without imposing the condition of self-avoidance.* We then consider the different types of self-intersection, and systematically remove these by an inclusion-exclusion argument.

Proceeding backwards from our final result, we find that convex polygons (CP) can be expressed in terms of SACP, plus CP with loops of one, two or three dimensions. These are systematically evaluated in terms of a new class of polygon, called *unimodal polygons* (UP) defined below, and staircase polygons, whose generating functions have been previously obtained [1].

The UP are evaluated similarly, by eliminating loops of different types by use of the inclusion-exclusion principle. In this paper we first carefully establish our notation, then illustrate our technique with the simplest kind of UP, then develop other UP needed, then show how this method first gives two-dimensional SACP, then finally three-dimensional SACP.

I. DEFINITIONS

Let $d \geq 1$, and let us consider the lattice $\mathbb{Z}^d$, with its basis $(e_1, \ldots, e_d)$. An *oriented rooted polygon* of perimeter $2n$ is a (not necessarily self-avoiding) walk on the lattice of $2n$ steps with coincident origin and end-point. Such a walk will be encoded by a word $u = u_1 u_2 \ldots u_{2n}$ on the alphabet $\mathcal{A} = \{1, 2, \ldots, d\} \cup \{\bar{1}, \bar{2}, \ldots, \bar{d}\}$, meaning that, if $u_i = k$ (resp. $\bar{k}$), then one goes from the i^{th} vertex to the next vertex by taking a step along the unit vector e_k (resp. $-e_k$). Denoting the number of occurrences of k in u as $|u|_k$, rooted polygons are equivalent to words satisfying $|u|_k = |u|_{\bar{k}}$

for $1 \leq k \leq d$. The *length* $|u|$ of a word u is its number of letters. The *dimension* of a polygon u is the dimension of its convex hull. An *oriented polygon* is an oriented rooted polygon defined up to a cyclic permutation of its vertices. (All the polygons we consider are oriented; hence the word "oriented" will often be omitted). A (rooted or unrooted) polygon is *self-avoiding* if no vertex (except the origin(is revisited. A non-empty SAP (resp. rooted SAP) will also be called a *loop* (resp. *rooted loop*).

We now define three important classes of polygons: the *staircase, unimodal*, and *convex* polygons.

A rooted polygon is a rooted *staircase* polygon if it factors as vw, where v (resp. w) is a word on $\{1,\ldots,d\}$ (resp. $\{\bar{1},\ldots\bar{d}\}$). This implies in particular that $|v| = |w|$.

Let $k \leq d$. A rooted polygon is *unimodal in direction* k if it can be written vw (where now both v and w are words on $\{1,\ldots,d\} \cup \{\bar{1},\ldots,\bar{d}\}$), with $|v|_{\bar{k}} = |w|_k = 0$. It is *unimodal* if it is unimodal in all directions. A polygon is unimodal if it can be represented by a unimodal rooted polygon (which is unique when it exists.)

A polygon is *convex in direction* k if it can be represented by a rooted polygon that is unimodal in direction k. It is *convex* if it is convex in all directions: for each k, there exists a rooted version of the polygon (usually depending on k) that is unimodal in direction k (for unimodal polygons, the *same* rooted polygon works for all directions). Equivalently, its perimeter is exactly twice the sum of the side lengths of its smallest bounding hyper-rectangle (its *box*). A unimodal polygon is naturally convex. More precisely, a unimodal polygon is a convex polygon that contains the vertex of minimal coordinates of its *box*. Similarly, a staircase polygon is a unimodal polygon that contains the vertex of maximal coordinates of its *box*.

Let $I \subset \{1,2,\ldots,d\}$, and let ℓ be a rooted loop of dimension $|I|$ on the alphabet $I \cup \bar{I}$, with $\bar{I} = \{\bar{k} : k \in I\}$. Let u be a (rooted or unrooted) polygon. If there exist two words v and w such that $u = v\ell w$, we say that ℓ is a *loop* of u, and that u *has a loop* in I. Our method for counting convex SAP relies on the fact that, if $\ell_1,\ldots,\ell_i$ are i loops of a convex polygon u, then removing all the letters of u occurring in these i loops leaves another polygon. This is only true because two loops of a convex polygon never *overlap*.

A. First enumerative results

In this subsection we first enumerate rooted *unimodal* polygons on $\mathbb{Z}^d$ *having no* 1*-dimensional loop.* This illustrates our general technique. We then obtain the corresponding result for *convex* polygons. From this, we derive an asymptotic expression for the number of such polygons, which gives an upper bound on the number of convex SAP.

Let $\mathcal{P}$ be a set of (rooted or unrooted) polygons. The *multi-perimeter generating function* for the elements of $\mathcal{P}$ is

$$\sum_{u\in\mathcal{P}} x_1^{|u|_1}\ldots x_d^{|u|_d},$$

and the *perimeter generating function* is

$$\sum_{u\in\mathcal{P}} t^{|u|_1+\cdot+|u|_d} = \sum_{u\in\mathcal{P}} t^{|u|/2}.$$

We will have frequent occasion to perform a particular operation on a Laurent series, so we define an operator for this purpose. For $I \subset \{1,\ldots,d\}$, we define an operator E_I that acts on Laurent series in the variables $x_1,\ldots,x_d$ with real coefficients. Its action can be described as retaining only terms of even powers in the subscripted subset I, which are then replaced with their respective square roots. For example, let $f(x_1,x_2) = \sum a_{n,m}x_1^n x_2^m$. Then

$$E_{\{1\}}(f(x_1,\ldots,x_d)) = \sum a_{2n,m}x_1^n x_2^m.$$

If I is the the set of all indices $\{1,\cdots,d\}$ we delete the subscript.

We denote by $\bar{f}(t)$ the series $f(t,\ldots,t)$. We define $\bar{E}_I(f(x_1,\ldots,x_d))$ to be $\bar{g}(t)$, where $g(x_1,\ldots,x_d) = E_I(f(x_1,\ldots,x_d))$.

We now give two lemmas, which illustrate two ingredients of this paper: the classical inclusion-exclusion principle and the use of the operator E. (We prove the first lemma. All subsequent proofs are omitted). The second lemma provides a very good asymptotic upper bound on the number of convex loops.

Lemma I.1 — *The multi-perimeter generating function for rooted unimodal polygons of* $\mathbb{Z}^d$ *having no one-dimensional loop is*

$$E\left[\frac{(1-x_1)(1-x_2)\ldots(1-x_d)}{1-x_1-x_2-\cdots-x_d}\right].$$

Proof. In a rooted unimodal polygon, for $k \in \{1, \ldots, d\}$, all occurrences of the letter k precede all occurrences of $\bar{k}$. Hence, the rooted unimodal polygons (including the empty polygon) are in one-to-one correspondence with the words u on the alphabet $\{1, 2, \ldots, d\}$ such that $|u|_k$ is even for all $k \le d$. Thus their multi-perimeter generating function is

$$E\left[\frac{1}{1 - x_1 - x_2 - \cdots - x_d}\right].$$

More generally, given a set $I \subset [1, \ldots, d]$, the multi-perimeter generating function for rooted unimodal polygons having a factor $k\bar{k}$ for all $k \in I$ is

$$S_I = E\left[\frac{\prod_{k \in I} x_k}{1 - x_1 - x_2 - \cdots - x_d}\right].$$

For $k \le d$, a unimodal rooted polygon has at most one occurrence of $k\bar{k}$. Hence the inclusion-exclusion principle implies that the multi-perimeter gf for unimodal rooted polygons having no one-dimensional loop is

$$\sum_{I \subset [1,d]} (-1)^{|I|} S_I,$$

which concludes the proof.

■

By a similar, but more complicated argument we can prove the following result for convex polygons:

Lemma I.2 *Let $d \ge 2$. The multi-perimeter generating function for convex polygons of $\mathbb{Z}^d$ that have no one-dimensional loop and are of dimension exactly d is*

$$E\left[(d-1)! \frac{x_1 x_2 \ldots x_d (1-x_1)^2 (1-x_2)^2 \ldots (1-x_d)^2}{(1 - x_1 - x_2 - \cdots - x_d)^d}\right].$$

An asymptotic result can be derived from the above exact result:

Corollary I.3 *The number of d-dimensional convex polygons on $\mathbb{Z}^d$ of perimeter $2n$ having no 1-dimensional loop is asymptotically equal to*

$$\frac{(d-1)^{2d}}{d^{3d}} d^{2n} n^{d-1} \left(1 + O(1/n)\right).$$

This gives an asymptotic upper bound for the number $c_n^{(d)}$ of d-dimensional convex loops of perimeter $2n$:

$$\limsup_{n \to \infty} \frac{c_n^{(d)} d^{3d}}{(d-1)^{2d} d^{2n} n^{d-1}} \le 1.$$

We remark that the number of d-dimensional convex loops is also asymptotic to $(d-1)^{2d} d^{2n} n^{d-1} / d^{3d}$. This can be proved [38] via a probablistic argument similar to that used in [19]. In other words, *a random d-dimensional convex polygon of large perimeter having no 1-dimensional loop is almost surely self-avoiding.*

B. Staircase polygons

As shown in [1], the generating function for self-avoiding staircase polygons can be derived from the generating function of the square of the multinomial coefficient. In particular, let

$$Z_n(x_1, \ldots, x_n) = \sum_{(a_1, \ldots, a_n) \in \mathbb{N}^n} \binom{a_1 + \cdots + a_n}{a_1, \ldots, a_n}^2 \prod_{i=1}^{n} x_i^{a_i}.$$

Then the multi-perimeter generating function for (oriented) staircase loops on $\mathbb{Z}^d$ is

$$S_d(x_1, \ldots, x_d) = 1 - \frac{1}{Z_d(x_1, \ldots, x_d)}.$$

In two dimensions we have

$$Z_2(x_1,x_2) = \sum_{(a_1,a_2)\in\mathbb{N}^2} \binom{a_1+a_2}{a_1,a_2}^2 x_1^{a_1}x_2^{a_2} = \frac{1}{\sqrt{1-2x_1-2x_2-2x_1x_2+x_1^2+x_2^2}}. \qquad (1)$$

We will also consider the series $\bar{Z}_d(t) = Z_d(t,\ldots,t)$, which is D-finite. For instance, $\bar{Z}_2(t)$ is, according to (1), equal to $(1-4t)^{-1/2}$, but it can alternatively be characterized by the initial condition $\bar{Z}_2(0) = 1$ and the differential equation

$$(1-4t)\bar{Z}_2'(t) - 2\bar{Z}_2(t) = 0.$$

Similarly, the series $\bar{Z}_3(t)$ is characterized by $\bar{Z}_3(0) = 1$, $\bar{Z}_3'(0) = 3$ and

$$t(1-t)(1-9t)\bar{Z}_3''(t) + (1-20t+27t^2)\bar{Z}_3'(t) - 3(1-3t)\bar{Z}_3(t) = 0.$$

The smallest singularity of $\bar{Z}_3$ is $1/9$, and around this point, $\bar{Z}_d(t) = A + B\ln(1-9t)(1+o(1))$.

For a further study of the series $\bar{Z}_d(t)$, including their connections with lattice Green functions, Heun functions and elliptic integrals, see [18,1,31].

C. Unimodal self-avoiding polygons

Next we construct the multi-perimeter generating function $U_d(x_1,\ldots,x_d)$ for oriented, unimodal self-avoiding polygons on $\mathbb{Z}^d$. This can be computed for arbitrary d by induction, but here we give the results for $d=2$ and $d=3$ only.

As a unimodal polygon is represented by a *unique* unimodal *rooted* polygon, we only need to handle rooted polygons, i.e., words. Our method is based on the following two observations: (i) a loop ℓ of a rooted unimodal polygon $u\ell v$ is unimodal; (ii) if a rooted unimodal polygon has a loop in $I \subset [1,\ldots,d]$ and a loop in J, then $I\cap J = \emptyset$. That is, the two loops occupy orthogonal subspaces.

In two dimensions, if u is a rooted UP having no one-dimensional loop, it factorizes uniquely as $vu'w$, where U' is a two-dimensional USAP and vw is a staircase polygon. Combining lemma 1.1 and * gives

$$E\left[\frac{(1-x_1)(1-x_2)}{1-x_1-x_2}\right] = U_2(x_1,x_2)Z_2(x_1,x_2).$$

Hence

$$U_2(x_1,x_2) = 2\frac{x_1x_2}{\sqrt{1-2x_1-2x_2-2x_1x_2+x_1^2+x_2^2}}. \qquad (2)$$

This result was first obtained by Lin and Chang by a different method [13]. See also [46] for a third proof.

In three dimensions, if u is a rooted UP having no one-dimensional loop, we can have either a two-dimensional loop in one of 3 orthogonal planes, or a three-dimensional loop (but not both). In the latter case we have $u = vu'w$ where u' is a three-dimensional loop and vw is a staircase polygon. This gives a contribution $U_3(x_1,x_2,x_3)Z_3(x_1,x_2,x_3)$.

In the former case, when the loop is in the (x_1,x_2) plane, it can be proved that the corresponding generating function is

$$E_{\{3\}}\left[\frac{1}{1-x_3}Z_2\left(\frac{x_1}{(1-x_3)^2},\frac{x_2}{(1-x_3)^2}\right)\right]U_2(x_1,x_2).$$

Using Lemma I and the above results, the series Z_3U_3 can be expressed as an *algebraic* series in x_1, x_2 and x_3. However we only need the *perimeter* generating function $\bar{U}_3$, for three-dimensional unimodal loops, which is given by

$$\bar{Z}_3(t)\bar{U}_3 = \frac{6t^2}{1-9t} - \frac{3t^2}{\sqrt{1-4t}}\left[[(1-3u)(1+u)]^{-1/2} + [(1+3u)(1-u)]^{-1/2}\right]. \qquad (3)$$

with $u=\sqrt{t}$. The logarithm in the asymptotic behaviour of $\bar{Z}_3(t)$ shows that $1/\bar{Z}_3(t)$, and hence $\bar{U}_3$, is not D-finite. However, $\bar{Z}_3(t)\bar{U}_3$ is algebraic of degree 8. More generally, one can prove that $\bar{U}_d$ is a quotient of D-finite series [14].

D. Convex polygons

We now use all the above results to calculate the number of CSAP. Again we construct a simpler generating function which overcounts, and then we correct by use of the inclusion-exclusion principle. The situation is now more complicated, as (i) a loop of a convex polygon is convex, but not necessarily unimodal, and (ii)1 a convex polygon $u\ell_1 v\ell_2 w$ may have a loop in I and a loop in J with $I\cap J\neq\emptyset$.

For two-dimensional CP, there is either no one-dimensional loop, in which case the CP is a SACP, or there are two rooted unimodal loops linked by a staircase polygon. More precisely, in this case we have $u = vu_1wu_2$ where u_1 and u_2 are unimodal and vw is a staircase polygon - and the symmetric case corresponding to a reflection of the entire structure. These considerations taken together imply that the multi-perimeter generating function for oriented convex self-avoiding polygons of dimension 2 is

$$C_2(x_1,x_2) = E_{[1,2]}\left[\frac{x_1x_2(1-x_1)^2(1-x_2)^2}{(1-x_1-x_2)^2}\right] - 2Z_2(x_1,x_2)(U_2(x_1,x_2))^2,$$

that is

$$\frac{2x_1x_2\left[1-3x_1-3x_2+3x_1^2+3x_2^2+5x_1x_2-x_1^3-x_2^3-x_1^2x_2-x_1x_2^2-x_1x_2(x_1-x_2)^2\right]}{\Delta^2} - \frac{8x_1^2x_2^2}{\Delta^{3/2}}$$

where $\Delta = 1-2x_1-2x_2-2x_1x_2+x_1^2+x_2^2$.

We remark that this result was first proved by Lin and Chang [13]. It is a refinement of the perimeter generating function, previously obtained by Delest and Viennot [12]. See also [46] and [32] for alternative proofs of these two results, as well as [26] or [46] for the expansion of the series $C_2(x_1,x_2)$. Our proof provides a nice combinatorial interpretation of each of the two parts of the expression of $C_2(x_1,x_2)$: the rational part counts convex polygons having no one-dimensional loop, and the algebraic part counts those that are not self-avoiding (i.e., have two loops).

For three dimensional CP we can perform the same type of construction. We note that a three-dimensional CP having no one-dimensional loop is either a SACP, or has two three-dimensional loops separated by a staircase polygon - giving rise to a term $4Z_3(x_1,x_2,x_3)(U_3(x_1,x_2,x_3))^2$, or has one, two or at most three two-dimensional loops which can be unimodal or not. Careful consideration of the number of distinct ways such polygons can occur reveals that there are seven distinct types. The most difficult case being when there are three two-dimensional orthogonal loops.

These ingredients are then combined, as in the two-dimensional case, to yield our main result, which is that the perimeter generating function for 3-dimensional oriented convex self-avoiding polygons is, with $u=\sqrt{t}$,

$$\bar{C}_3 = \frac{8t^3(4-51t+198t^2-135t^3)}{(1-9t)^3} + \frac{96t^4(1-6t)}{(1-9t)(1-4t)} - \frac{24t^4(1-t)(8-60t+145t^2-120t^3+16t^4)}{(1-4t)^4}$$

$$+\frac{96t^4}{\sqrt{1-4t}}\left[\frac{(1-t)(1-2t)(2-7t+4t^2)}{(1-4t)^3} - \frac{2(1-6t)}{(1-9t)^2} + \frac{2t^2}{(1+t)^2(1-4t)}\right]$$

$$+\frac{24ut^4}{1-4t}\left[\frac{1-t-2u}{[(1-3u)(1+u)]^{3/2}} - \frac{1-t+2u}{[(1+3u)(1-u)]^{3/2}}\right] - \frac{64t^6(5-4t)}{(1+t)^2(1-4t)^{3/2}\sqrt{1-8t}}$$

$$-\frac{4}{\bar{Z}_3(t)}\left[\frac{6t^2}{1-9t} - \frac{3t^2}{\sqrt{1-4t}}\left[[(1-3u)(1+u)]^{-1/2} + [(1+3u)(1-u)]^{-1/2}\right]\right]^2.$$

E. Conclusion

Note that the generating function for oriented convex self-avoiding polygons *lying* in $\mathbb{Z}^3$ (but possibly having a smaller dimension) is naturally $\bar{C}_3+3\bar{C}_2+3\bar{C}_1$ where $\bar{C}_1=t$ is the generating function for 1-dimensional convex loops.

We note that the series $\bar{C}_3$ is of the same nature as $\bar{Z}_3(t)^{-1}$, and in particular, is not D-finite. However, $\bar{Z}_3(t)\bar{C}_3$ is D-finite (but not algebraic). If we write $\bar{C}_3 = A(t)+B(t)/\bar{Z}_3(t)$, where $A(t)$ and $B(t)$ are algebraic series, then $A(t)$ is algebraic of degree 16 and $B(t)$ is algebraic of degree 8. This indicates that the order of the differential equation satisfied by $\bar{Z}_3(t)\bar{C}_3$ must be large.

The singularities of $\bar{C}_3$ are at $t = 1/9, 1/8, 1/4, 1$ and -1. The singularities at $1/8$ and -1 are unexpected, for they are not singularities of the generating function $\bar{U}_3$ for three-dimensio nal unimodal loops. Both singularities come from polygons having three 2-dimensional loops.

The expression of $\bar{C}_3$ provides the following asymptotic form for the number of three-dimensional oriented self-avoiding convex polygons of perimeter $2n$ (see [24]):

$$2^6 3^{2n-9} n^2 \left\{ 1 + \frac{c}{n} + \frac{c_1}{n \ln n} + \frac{c_2}{n(\ln n)^2} + \cdots + \frac{c_k}{n(\ln n)^k} + o\left(\frac{1}{n(\ln n)^k}\right) \right\}.$$

The generating function for the number of three-dimensional *non-oriented* self-avoiding convex polygons is naturally $\bar{C}_3/2$. The above expression for $\bar{C}_3(t)$ can be readily expanded in t, which allowed us to confirm our results by comparing them with the known, unpublished data obtained previously by Enting and Guttmann.

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