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Three-dimensional self-avoiding convex polygons

M. Bousquet-Mélou
Laboratoire Bordelais de Recherche en Informatique, Université Bordeaux 1, 351 cours de la Libération, 33405 Talence Cedex, France

A. J. Guttmann
Department of Mathematics and Statistics, The University of Melbourne Parkville, Victoria 3052, Australia

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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, the paradigm model of ring polymers. [S1063-651X(97)51206-2]

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INTRODUCTION

Three-dimensional (3D) models in statistical mechanics have proved to be exceptionally difficult to analyze, with only a very small number of solutions to nontrivial problems known. These include staircase polygons [1], directed animals [2], Zamoldchikov's model and its N-component extension [3–5] and a 3D dimer model [6]. Among these models, staircase polygons are the least intrinsically three dimensional, being generated by a concatenation argument, which is essentially one dimensional. The solution of the 3D directed animal problem is obtained by mapping it onto the 2D hard hexagon model, while Baxter's work on the Zamoldchikov solution of the tetrahedron equations (which are a genuinely 3D version of the star-triangle equations) also displays considerable two-dimensional character.

For self-avoiding walks and self-avoiding polygons [7], exact solutions have focused 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 they 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's). This solution adds to the very short list of exactly solved 3D models. The model itself contains some of the physics of ring polymers in dilute solution. It also illuminates the increase in functional complexity as one moves from a 2D to a 3D system.

Our method of solution can, in principle, be generalized to higher-dimensional SACP's, though at the cost of greatly increased algebraic complexity. The solution is long and complex, and full details will be published elsewhere [12]. In this paper we only describe the central ideas of the solution, and give an outline of its derivation.

We will study families of convex polygons *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's) can be expressed in terms of SACP's, plus CP's with loops of one, two or three dimensions. These are systematically evaluated in terms of a new class of polygon, called *unimodal polygons* (UP's), and staircase polygons, whose generating function has been previously obtained [1]. The UP's are enumerated similarly, by eliminating loops of different types by use of the inclusion-exclusion principle.

In what follows, we first carefully establish our notation, then present our results by increasing generality: staircase, unimodal, and finally convex SAP's.

I. DEFINITIONS

Let $d\geq 1$, and let us consider the lattice $\mathbb{Z}^d$, with its canonical basis $(e_1,\ldots,e_d)$. An oriented rooted polygon of perimeter $2n$ is a (not necessarily self-avoiding) walk of $2n$ steps on the lattice with coincident origin and end point. Such a walk will be encoded by a word $u=u_1u_2\cdots u_{2n}$ on the alphabet $\{1,2,\ldots,d\}\cup\{\overline{1},\overline{2},\ldots,\overline{d}\}$, meaning that, if $u_i=k$ $(\overline{k})$, then one goes from the ith vertex to the next vertex by taking a step along the unit vector e_k $(-e_k)$. Denoting the number of occurrences of k in u as $|u|_k$, rooted polygons are thus equivalent to words u satisfying $|u|_k=|u|_{\overline{k}}$ for $1\leq k\leq d$. The length $|u|$ of a word u is its number of letters. 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 nonempty SAP (rooted SAP) will also be called a loop (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 (w) is a word on $\{1,\ldots,d\}$ $(\{\overline{1},\ldots\overline{d}\})$. This implies in particular that $|v|=|w|$.

For $k\leq d$, a rooted polygon is *unimodal in direction k* if it can be written vw (where now both v and w are words on $\{1,\ldots,d\}\cup\{\overline{1},\ldots,\overline{d}\}$), with $|v|_{\overline{k}}=|w|_k=0$. 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 $I\cup\overline{I}$, with $\overline{I}=\{\overline{k}:k\in I\}$. 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 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*.

II. FIRST ENUMERATIVE RESULTS

In this subsection we first enumerate rooted *unimodal* polygons on $\mathbb{Z}^d$ *having no 1D loop.* We then obtain the corresponding result for *convex* polygons.

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

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

and the *perimeter generating function* is

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

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 $f(x_1,x_2)=\Sigma a_{n,m}x_1^n x_2^m$. Then

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

If I is the the set of all indices $\{1,\ldots,d\}$ we delete the subscript I. We denote by $\overline{f}(t)$ the series $f(t,\ldots,t)$. We define $\overline{E_I}(f(x_1,\ldots,x_d))$ to be $\overline{g}(t)$, 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 our method: the classical inclusion-exclusion principle and the use of the operator E. (We prove the first lemma. All subsequent proofs are omitted.)

Lemma I. The multiperimeter generating function for rooted unimodal polygons of $\mathbb{Z}^d$ having no 1D loop is

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

Proof. In a rooted unimodal polygon, for $k\in\{1,\ldots,d\}$, all occurrences of the letter k precede all occurrences of $\overline{k}$. 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 $k\leqslant d$. Thus their multiperimeter generating function is $E[1/(1-x_1-x_2-\cdots-x_d)]$. More generally, given a set $I\subset\{1,\ldots,d\}$, the multiperimeter generating function for rooted unimodal polygons having a factor $k\overline{k}$ for all $k\in I$ is $S_I=E[\Pi_{k\in I}x_k/(1-x_1-x_2-\cdots-x_d)]$.

For $k\leqslant d$, a unimodal rooted polygon has at most one occurrence of $k\overline{k}$. Hence the inclusion-exclusion principle implies that the multiperimeter generating function for unimodal rooted polygons having no one-dimensional loop is

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

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

Lemma II. Let $d\geqslant 2$. The multiperimeter generating function for convex polygons in $\mathbb{Z}^d$ that have no 1D loop and are of dimension exactly d is

$$E\left[(d-1)!\frac{x_1x_2\cdots x_d(1-x_1)^2(1-x_2)^2\cdots(1-x_d)^2}{(1-x_1-x_2-\cdots-x_d)^d}\right].$$

It follows that the number of d-dimensional convex polygons on $\mathbb{Z}^d$ of perimeter $2n$ having no 1D loop is asymptotically equal to

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

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

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

It is known that the number of d-dimensional convex loops is also asymptotic to $(d-1)^{2d}d^{2n}n^{d-1}/d^{3d}$ [13]. In other words, *a random d-dimensional convex polygon of large perimeter having no $1D$ loop is almost surely self-avoiding.*

III. STAIRCASE POLYGONS

The multiperimeter generating function Z_d for (self-avoiding) staircase polygons can [1] be expressed in terms of squares of the multinomial coefficients:

$$Z_d(x_1,\ldots,x_d)=\sum_{(a_1,\ldots,a_d)\in\mathbb{N}^d}\binom{a_1+\cdots+a_d}{a_1,\ldots,a_d}^2\prod_{i=1}^d x_i^{a_i}. \tag{1}$$

As shown in [1], the generating function for (oriented) staircase SAP on $\mathbb{Z}^d$ is then

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

In two dimensions we have

$$Z_2(x_1, x_2) = \sum_{(a_1, a_2) \in \mathbb{N}^2} \binom{a_1 + a_2}{a_1, a_2}^2 x_1^{a_1} x_2^{a_2}$$

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

We will also consider the series $\overline{Z_d}(t) = Z_d(t, \ldots, t)$, which is D-finite. For instance, the series $\overline{Z_3}(t)$ is characterized by $\overline{Z_3}(0) = 1$, $\overline{Z_3'}(0) = 3$, and $t(1-t)(1-9t)\overline{Z_3''}(t) + (1 - 20t + 27t^2)\overline{Z_3'}(t) - 3(1-3t)\overline{Z_3}(t) = 0$. The smallest singularity of $\overline{Z_3}$ is 1/9, and around this point, $\overline{Z_3}(t) = A + B\ln(1-9t)[1+o(1)]$.

For a further study of the series $\overline{Z_d}(t)$, including their connections with lattice Green functions, Heun functions and elliptic integrals, see [1,14,15].

IV. UNIMODAL SELF-AVOIDING POLYGONS

Next we construct the multiperimeter generating function $U_d(x_1, \ldots, x_d)$ for oriented, unimodal SAP's 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 1D loop, it factorizes uniquely as $vu'w$, where u' is a 2D USAP and vw is a staircase polygon. Combining Lemma I and Eq. (1) 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, using (2),

$$U_2(x_1, x_2) = 2\frac{x_1x_2}{\sqrt{1 - 2x_1 - 2x_2 - 2x_1x_2 + x_1^2 + x_2^2}}. \qquad (3)$$

This result was first obtained by Lin and Chang by a different method [16]. See also [17] for a third proof.

In three dimensions, if u is a rooted UP having no 1D loop, we can have either a 2D loop in one of the three orthogonal planes, or a 3D loop (but not both). In the latter case we have $u = vu'w$ where u' is a 3D 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* function of x_1, x_2 and x_3. In particular, the *perimeter* generating function $\overline{U_3}$ for 3D unimodal SAP is given by

$$\overline{Z_3}(t)\overline{U_3} = \frac{6t^2}{1-9t} - \frac{3t^2}{\sqrt{1-4t}}\{[(1-3u)(1+u)]^{-1/2} + [(1+3u)(1-u)]^{-1/2}\}, \qquad (4)$$

with $u = \sqrt{t}$. The logarithm in the asymptotic behavior of $\overline{Z_3}(t)$ shows that $1/\overline{Z_3}(t)$, and hence $\overline{U_3}$, is not D-finite. However, $\overline{Z_3}(t)\overline{U_3}$ is algebraic of degree 8. More generally, one can prove that $\overline{U_d}$ is a quotient of D-finite series [12].

V. SELF-AVOIDING CONVEX POLYGONS

To calculate the number of convex SAP's we again compute a simpler generating function, and then correct it by use of the inclusion-exclusion principle.

In two dimensions, a convex polygon u having no 1D loop is either self-avoiding, or else has two rooted unimodal loops linked by a staircase polygon. More precisely, $u = vu_1wu_2$ where u_1 and u_2 are unimodal and vw is a staircase polygon—or the symmetric case corresponding to a reflection of the entire structure. Using Lemma II and Eq. (1), this implies that the multiperimeter 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

$$C_2(x_1, x_2) = \frac{2x_1x_2[1 - 3x_1 - 3x_2 + 3x_1^2 + 3x_2^2 + 5x_1x_2 - x_1^3 - x_2^3 - x_1^2x_2 - x_1x_2^2 - x_1x_2(x_1-x_2)^2]}{\Delta^2} - \frac{8x_1^2x_2^2}{\Delta^{3/2}}$$

where $\Delta=1-2x_1-2x_2-2x_1x_2+x_1^2+x_2^2$. This result was first proved by Lin and Chang [16] (see also [18] and [17]). The perimeter generating function was previously obtained by Delest and Viennot [19]. 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 1D loop, and the algebraic part counts those that are not self-avoiding (i.e., have two loops).

In three dimensions, a convex polygon having no 1D loop is either self-avoiding, or has two 3D 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 2D loops which can be unimodal or not. One is led to study separately seven classes of polygons, the most difficult one being when there are three 2D orthogonal loops.

The seven cases are then combined to yield our main result, which is that the perimeter generating function for oriented convex SAP's of dimension 3 is, with $u=\sqrt{t}$,

$$\overline{C_3}(t)=\frac{8t^3(4-51t+198t^2-135t^3)}{(1-9t)^3}+\frac{96t^4(1-6t)}{(1-9t)(1-4t)}-\frac{24t^4(1-t)(8-60t+145t^2-120t^3+16t^4)}{(1-4t)^4}+\frac{96t^4}{\sqrt{1-4t}}\left[\frac{(1-t)(1-2t)(2-7t+4t^2)}{(1-4t)^3}-\frac{2(1-6t)}{(1-9t)^2}+\frac{2t^2}{(1+t)^2(1-4t)}\right]+\frac{24ut^4}{1-4t}\times\left[\frac{1-t-2u}{[(1-3u)(1+u)]^{3/2}}-\frac{1-t+2u}{[(1+3u)(1-u)]^{3/2}}\right]-\frac{64t^6(5-4t)}{(1+t)^2(1-4t)^{3/2}\sqrt{1-8t}}-\frac{4}{\overline{Z_3}(t)}\left[\frac{6t^2}{1-9t}-\frac{3t^2}{\sqrt{1-4t}}\{[(1-3u)(1+u)]^{-1/2}+[(1+3u)(1-u)]^{-1/2}\}\right]^2.$$

CONCLUSIONS

As the function $\overline{Z_3}(t)^{-1}$ is neither algebraic nor D-finite, it follows that $\overline{C_3}$ is neither algebraic nor D-finite. However, $\overline{Z_3}(t)\overline{C_3}$ is D-finite (but not algebraic). If we write $\overline{C_3}=A(t)+B(t)/\overline{Z_3}(t)$, 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 $\overline{Z_3}(t)\overline{C_3}$ must be large.

The singularities of $\overline{C_3}$ 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 $\overline{U_3}$ for 3D unimodal loops [see (4)].

The expansion of $\overline{C_3}$ provides the following asymptotic form for the number of 3D oriented self-avoiding convex polygons of perimeter $2n$ (see [20]):

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

The generating function for oriented convex SAP's *lying* in $\mathbb{Z}^3$ (but possibly having a smaller dimension) is $\overline{C_3}+3\overline{C_2}+3\overline{C_1}$ where $\overline{C_1}=t$ is the generating function for 1D convex loops.

The generating function for the number of 3D *nonoriented* convex SAP's is $\overline{C_3}/2$. The above expression for $\overline{C_3}(t)$ can be readily expanded in t, which allowed us to confirm our result by comparing it with the known, unpublished data obtained previously by Enting and Guttmann.

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