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Note

On fully extended self-avoiding polygons

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Abstract

The paper gives recurrence relations on the number of $2n$ step fully extended (i.e., full-dimensional) self-avoiding polygons in n- and $(n-1)$-dimensional integer lattices.

1. Introduction

We define a *walk* in the d-dimensional integer lattice $\boldsymbol{Z}^d$ as a sequence $W = \{x_0, e_1, x_1, e_2, \ldots, x_{\ell-1}, e_\ell, x_\ell\}$ where x_i's are points of the integer lattice, $x_i - x_{i-1} = e_i$ for all $i = 1, 2, \ldots, \ell$ and the vectors e_i are unit vectors (of positive or negative orientation). ℓ is called the length of the walk. A walk is *self-avoiding* (SAW) if $x_i \neq x_j$ for any $0 \leqslant i \neq j \leqslant \ell$. In other words self-avoiding property means that there is no repetition in the sequence of visited sites. *Self-avoiding polygons* (SAP) are walks of length $2n$ where for all pairs $0 \leqslant i \neq j \leqslant 2n$, $x_i \neq x_j$ except that $x_0 = x_{2n}$. To find the number of SAWs and SAPs and several other questions in this topic are unsolved problems; the mathematical community consider them as problems having no exact solutions (closed formulae) and so raised several related but easier models. Rossi [1] studied the number of so-called fully extended and almost fully extended self-avoiding polygons. This note gives somewhat simpler proofs to the recurrence relations — found by Rossi — on the number of these particular sets of polygons. The reader can find an extensive introduction of SAWs and SAPs in [2].

2. The results

Definition 1. A self-avoiding polygon $P = \{x_0, e_1, x_1, e_2, \ldots, x_{2n-1}, e_{2n}, x_{2n}\}$ in $\boldsymbol{Z}^n$ is called fully extended if the vectors $e_1, e_2, \ldots, 2_{2n}$ span $\boldsymbol{Z}^n$. Note that for $n = 1$ the SAP

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$x_0, e_1, x_1, -e_1, x_0$ is a fully extended SAP. We denote by $S_n = S_{2n,n}$ the number of fully extended SAPs of length $2n$.

We mention here that in a fully extended polygon every direction of the underlying lattice is represented by two unit vectors among the vectors $e_1, e_2, \ldots, e_{2n}$, once for both of the possible orientations.

A SAP of length $2n$ in $\boldsymbol{Z}^n$ is called almost fully extended if its unit vectors $e_1, e_2, \ldots, 2_{2n}$ span a hyperplane of dimension $n-1$ in $\boldsymbol{Z}^n$.

Theorem 1. $S_n = (n-1)\sum_{i=1}^{n-1} \binom{n}{i} S_i S_{n-i}$.

Before giving our second theorem we need some additional definitions.

We say that a self-avoiding polygon $P = \{x_0, e_1, x_1, e_2, \ldots, x_{2n-1}, e_{2n}, x_{2n}\}$ is *collapsible* with respect to a pair of vectors e_i, e_j, $i < j$ if $e_i = -e_j$ and if we remove this pair from the vector sequence above, the remaining polygon is still self-avoiding. We call this pair of vectors *removable*. Let $S_{a,b}$ denote the number of SAPs of length a spanning $\boldsymbol{Z}^b$ and $\widehat{S}^{(v)}_{a,b}$ denote the number of these SAPs having at least v pair of (not necessarily simultaneously) removable vectors. With this terminology one can easily prove that

$$\widehat{S}^{(1)}_{2(n+1),n+1} = 2n(2n-1)S_{2n,n}. \tag{1}$$

Our main result is the following set of multiple recurrence relations for the number of almost fully extended SAPs of length $2n$.

Theorem 2.

$$S_{2n,n-1} = \widehat{S}^{(1)}_{2n,n-1} + \sum_{i=3}^{n-3} \frac{1}{2i}\binom{n-1}{i-1}\widehat{S}^{(1)}_{2i,i-1}S_{2(n-i),n-i} + \sum_{i=3}^{n-3} \frac{1}{2i}\binom{n-1}{i-1}\widehat{S}^{(1)}_{2i,i}S_{2(n-i),n-i-1},$$

where

$$\widehat{S}^{(1)}_{2n,n-1} = \widehat{S}^{(2)}_{2n,n-1} + \sum_{i=3}^{n-3} \frac{1}{2i}\binom{n-1}{i-1}\widehat{S}^{(2)}_{2i,i-1}S_{2(n-i),n-i} + \sum_{i=3}^{n-3} \frac{1}{2i}\binom{n-1}{i-1}\widehat{S}^{(1)}_{2i,i}\widehat{S}^{(1)}_{2(n-i),n-i-1},$$

$$\widehat{S}^{(2)}_{2n,n-1} = \widehat{S}^{(4)}_{2n,n-1} + \sum_{i=3}^{n-3} \frac{1}{2i}\binom{n-1}{i-1}\widehat{S}^{(4)}_{2i,i-1}S_{2(n-i),n-i} + \sum_{i=3}^{n-3} \frac{1}{2i}\binom{n-1}{i-1}\widehat{S}^{(1)}_{2i,i}\widehat{S}^{(1)}_{2(n-i),n-i-1},$$

$$\widehat{S}^{(4)}_{2n,n-1} = \left(\binom{2(n-2)}{4} + \binom{2(n-2)}{4} + 2\binom{2(n-2)}{3} + \binom{2(n-2)}{2}\right) S_{2(n-2),n-2}.$$

Proof of Theorem 1. Let $P = \{x_0, e_1, x_1, e_2, \ldots, x_{2n-1}, e_{2n}, x_{2n}\}$ be any fully extended SAP and $(\alpha, \beta) = (e_i, e_j)$, $i < j$ be the two occurrences of the first unit vector in the sequence of P, that is $e_i = -e_j = \pm(1, 0, \ldots, 0)$. Let k be the first index such that $i < k$ and $x_k - \alpha = x_l$ for some $k < l$. Since $i < j$ and $x_{j-1} + \beta = x_{j-1} - \alpha = x_j$ we have that $k \leqslant j - 1$ (k being equal to $j - 1$ only if (α, β) is a removable pair of vectors). The vector $x_l - x_k$ is by the definition $-\alpha$, that is β. Let us subdivide the SAP P into three parts: $C_1 = \{x_0, e_1, \ldots, x_k\}$, $C_2 = \{x_k, e_{k+1}, \ldots, x_l\}$, and $C_3 = \{x_l, e_{l+1}, \ldots, x_{2n}\}$, and form two new SAPs out of these parts: $P_1 = C_1 \cup \{\beta\} \cup C_3$ and $P_2 = \{x_k, e_{k+1} \ldots, x_l\}$. It is easy to see that both P_1 and P_2 will be fully extended SAPs; moreover, P_1 will have the removable pair (α, β). Now if P_1 has length $2(i + 1)$ then P_2 has length $2(n - i)$ and so the number of fully extended SAPs of length $2n$ with P_1 of length $2(i + 1)$ is $\widehat{S}^{(1)}_{2(i+1),i+1} \times S_{n-i}$ where $\widehat{S}^{(1)}_{2(i+1),i+1}$ is the number of fully extended SAPs having at least one vector pair which is removable (in our case of the first direction, the pair (α, β)). Thus, by a similar argument that gives (1) we have

$$\widehat{S}^{(1)}_{2(i+1),i+1} = 2i(2i - 1)S_{2i,i}/2i.$$

Now putting all this together we have

$$S_n = \sum_{i=1}^{n-1} (2i - 1)\binom{n}{i} S_i S_{n-i},$$

which is easily equivalent to the statement of the theorem due to symmetry reasons. □

Proof of Theorem 2. Let $P = \{x_0, e_1, x_1, e_2, \ldots, x_{2n-1}, e_{2n}, x_{2n}\}$ be an almost fully extended SAP in which all directions occur exactly twice except the dth, $1 \leqslant d \leqslant n$ which occurs four times. This direction will be called the doubled direction. Again, let $(\alpha, \beta) = (e_i, e_j)$ denote one of the pairs of the oppositely oriented vectors of the doubled direction. Define again $k > i$ as the first index such that $x_k - \alpha = x_l$ for an $l > k$ and $\beta = x_l - x_l$. If (α, β) is a removable pair the problem will be reduced to the enumeration of SAPs with at least one removable pair of vectors; this will be given by first term in the equation, that is by $\widehat{S}^{(1)}_{2n,n-1}$. In the other case the SAP can be decomposed as above into P_1, P_2. The only novelty in this case is that either P_1 or P_2 will contain the doubled direction and both will have smaller length than the original polygon. Depending on which of them will contain the doubled direction we will get the last two terms in (2):

$$S_{2n,n-1} = \widehat{S}^{(1)}_{2n,n-1} + \sum_{i=3}^{n-3} \frac{1}{2i}\binom{n-1}{i-1}\widehat{S}^{(1)}_{2i,i-1}S_{2(n-i),n-i} + \sum_{i=3}^{n-3} \frac{1}{2i}\binom{n-1}{i-1}\widehat{S}^{(1)}_{2i,i}S_{2(n-i),n-i-1}. \tag{2}$$

To make the recurrence complete and calculable we need other recurrences for $\widehat{S}^{(1)}_{2n,n}$ and $\widehat{S}^{(1)}_{2n,n-1}$. For $\widehat{S}^{(1)}_{2n,n}$ the recurrence is given above by (1). For $\widehat{S}^{(1)}_{2n,n-1}$ it comes from a decomposition very similar to the previous cases. Let us pick the pair of vertices of the doubled direction $\{\alpha',\beta'\}$ (disjoint as a set from $\{\alpha,\beta\}$). Removing this pair similar subcases can be distinguished as above and we have the recurrence

$$\widehat{S}^{(1)}_{2n,n-1} = \widehat{S}^{(2)}_{2n,n-1} + \sum_{i=3}^{n-3} \frac{1}{2i}\binom{n-1}{i-1}\widehat{S}^{(2)}_{2i,i-1}S_{2(n-i),n-i} + \sum_{i=3}^{n-3} \frac{1}{2i}\binom{n-1}{i-1}\widehat{S}^{(1)}_{2i,i}\widehat{S}^{(1)}_{2(n-i),n-i-1}. \tag{3}$$

The next recurrence we need is for $S^{(2)}_{2n,n-1}$. It is worth to mention that if in a SAP there are three removable pairs then there must be further a fourth one as well. This fact and a similar argument to the previous ones gives us

$$\widehat{S}^{(2)}_{2n,n-1} = \widehat{S}^{(4)}_{2n,n-1} + \sum_{i=3}^{n-3} \frac{1}{2i}\binom{n-1}{i-1}\widehat{S}^{(4)}_{2i,i-1}S_{2(n-i),n-i} + \sum_{i=3}^{n-3} \frac{1}{2i}\binom{n-1}{i-1}\widehat{S}^{(1)}_{2i,i}\widehat{S}^{(1)}_{2(n-i),n-i-1}. \tag{4}$$

The last equation of Theorem 2 is straightforward which together with the Eqs (2)–(4) give the required statement. □

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