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Interaction of loops with a surface

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Abstract. We consider the interaction of k-loops with an adsorption surface and prove that the polymer model of k-loops has exactly the same reduced free energy as that for self-avoiding walks interacting with a surface.

1. Introduction

The influence of topology on the critical properties of polymers has been the subject of recent interest (Gaunt *et al* 1984, Duplantier 1986). For a general polymer network attached to a surface and in a number of restricted geometries, Duplantier and Saleur (1986) have conjectured the dependence of the critical exponent γ on polymer topology. Ohno and Binder (1988) have derived a scaling theory for a polymer network by using the equivalence between the generating function for the number of configurations and the correlation function for the classical n-spin Heisenberg model in the limit $n \to 0$. It is of interest to examine the effects of an interaction between an adsorption surface and such polymer networks. A rigorous treatment for the linear chain was provided by Hammersley *et al* (1982), who proved that a self-avoiding walk (SAW) interacting with a surface with energy ω undergoes a phase transition with a crossover from d- to $(d-1)$-dimensional behaviour. In this paper we consider the interaction of k-loops with a surface, which can be either penetrable or impenetrable, and where $d \geqslant 3$ and $k \leqslant 2d$. A k-loop consists of k self-avoiding walks (or branches) in which the initial vertices of the k walks are joined together at a single vertex, hereafter referred to as a branch point. Similarly, the terminal vertices of the k walks are joined together at the other branch point. The initial and terminal vertices of a walk cannot be the same. A k-loop can be considered as a special case of a polymer network with a specified topology in which $n_k = 2$, $k > 2$ and $n_i = 0$, $i \neq k$, where n_k is the number of vertices (branch points) with degree k (Duplantier 1986).

In a d-dimensional hypercubic lattice, a vertex is a point in d-dimensional Euclidean space with integer coordinates $x = (x_1, \ldots, x_d)$ and an n-step SAW is a sequence of vertices $\{x(0), \ldots, x(n)\}$ with $|x(i) - x(i+1)| = 1$. We define the unit vectors $e_1 = (1, 0, \ldots, 0)$, $e_2 = (0, 1, \ldots, 0), \ldots, e_d = (0, 0, \ldots, 1)$ and the unordered pair $[x_1, x_2]$ as the edge joining the two vertices x_1 and x_2. The interaction surface is the hyperplane $x_1 = 0$. The k-loop may be attached at the surface in two ways: the attachment can be at the branch point or at a vertex other than a branch point. We will refer to the point of attachment of a k-loop to a surface as the 'root'. The k walks of the k-loop may have equal numbers of monomers (uniform k-loop) or different numbers of monomers (non-uniform k-loop).

In this paper, we mainly concentrate on uniform k-loops, which interact with the penetrable surface $x_1 = 0$, with the root at one of the branch points. Let $\mathscr{L}_{n,m}(k)$ denote the set of such k-loops with k n-step walks joining the two branch points and a total of m edges in the surface and $l_{kn,m}$ denote the number of loops in $\mathscr{L}_{n,m}(k)$. We define the generating function

$$L_n(k, \omega) = \sum_{m=0}^{kn} l_{kn,m} \, \mathrm{e}^{m\omega} \tag{1.1}$$

where ω is the energy of interaction of the monomers of the walks with the surface. By using the 'squeeze law', we establish that

$$\lim_{n\to\infty} (kn)^{-1} \log L_n(k, \omega) = A(\omega) \tag{1.2}$$

where $A(\omega)$ is the reduced free energy for a SAW in terms of the number of edges of the SAW in the penetrable surface. Hammersley *et al* (1982) obtained the reduced free energy for SAWs by considering numbers of vertices of a SAW, rather than edges, in the surface. In this paper, we shall refer to such results that have been obtained by counting in terms of numbers of vertices (Hammersley *et al* 1982, Whittington and Soteros 1990). We note that by following the same arguments and procedures that have been used to obtain results by vertex counting, one can obtain corresponding results if the counting is in terms of numbers of edges.

2. Uniform k-loop with the root at a branch point

We first derive an upper bound for the function (1.1). A k-loop in $\mathscr{L}_{n,m}$ consists of k branches, each of which is an n-step SAW. By treating each branch independently, we obtain

$$l_{kn,m} \leqslant \sum_{m_1+\ldots+m_k=m} \prod_{i=1}^{k} a_{n,m_i} \tag{2.1}$$

and

$$L_n(k, \omega) = \sum_{m=0}^{kn} l_{kn,m} \, \mathrm{e}^{m\omega} \leqslant \left(\sum_{m=0}^{n} a_{n,m} \, \mathrm{e}^{m\omega} \right)^k = (A_n(\omega))^k \tag{2.2}$$

where $a_{n,m}$ is the number of n-step SAWs with m edges in the surface and $A_n(\omega)$ is the generating function (1.1) for SAWs.

Definition. $f_{i,j}$ and g_i are maps such that, for any $\boldsymbol{x} = (x_1, \ldots, x_i, \ldots, x_j, \ldots, x_d)$,

$$f_{i,j}(\boldsymbol{x}) = (x_1, \ldots, x_j, \ldots, x_i, \ldots, x_d) \qquad i, j \geqslant 2 \tag{2.3}$$

$$g_i(\boldsymbol{x}) = (x_1, \ldots, -x_i, \ldots, x_j, \ldots, x_d) \qquad \forall i. \tag{2.4}$$

For a sequence of vertices $w = \{\boldsymbol{x}(0), \boldsymbol{x}(1), \ldots, \boldsymbol{x}(n)\}$,

$$f_{i,j}(w) = \{f_{i,j}(\boldsymbol{x}(0)), f_{i,j}(\boldsymbol{x}(1)), \ldots, f_{i,j}(\boldsymbol{x}(n))\} \tag{2.5}$$

$$g_i(w) = \{g_i(\boldsymbol{x}(0)), g_i(\boldsymbol{x}(1)), \ldots, g_i(\boldsymbol{x}(n))\}. \tag{2.6}$$

The map $f_{i,j}$ interchanges the coordinates x_i, x_j and g_i replaces x_i with $-x_i$. These lead to lemma 1 in a straightforward manner.

Lemma 1. (a) The map $f_{i,j}$ and g_i are injective. (b) If w is a given SAW, the image w' of w under these mappings is still a SAW and w' and w have the same number of edges (vertices) in the surface $x_1 = 0$.

We define a wedge by

$$\boldsymbol{W}: \quad 1 \leqslant x_2, \ldots, 1 \leqslant x_{d-1} \leqslant x_d \tag{2.7}$$

and consider a SAW w which is confined in $\boldsymbol{W}$ and satisfies

(i) $$\boldsymbol{x}(0) = \boldsymbol{e}_2 + \boldsymbol{e}_3 + \ldots + \boldsymbol{e}_{d-1} + 4\boldsymbol{e}_d \tag{2.8}$$

(ii) for $\boldsymbol{x}(i)$, $1 \leqslant i \leqslant n-1$

$$x_d(0) < x_d(i) \leqslant x_d(n) \tag{2.9}$$

and

$$x_{d-1}(i) < x_d(i) \tag{2.10}$$

(iii) for $\boldsymbol{x}(n)$,

$$x_d(n) = x_{d-1}(n). \tag{2.11}$$

An example of such a walk is given in figure 1.

Lemma 2. Let $\mathscr{B}_n$ be the set of all such n-step walks and $\mathscr{B}_{n,m}$ the subset of $\mathscr{B}_n$ that have m edges in the surface. We denote by $b_{n,m}$ the number of walks in $\mathscr{B}_{n,m}$ and define

$$B_n(\omega) = \sum_{m=0}^{n} b_{n,m}\, \mathrm{e}^{m\omega} \tag{2.12}$$

then

$$\lim_{n\to\infty} n^{-1} \log B_n(\omega) = A(\omega). \tag{2.13}$$

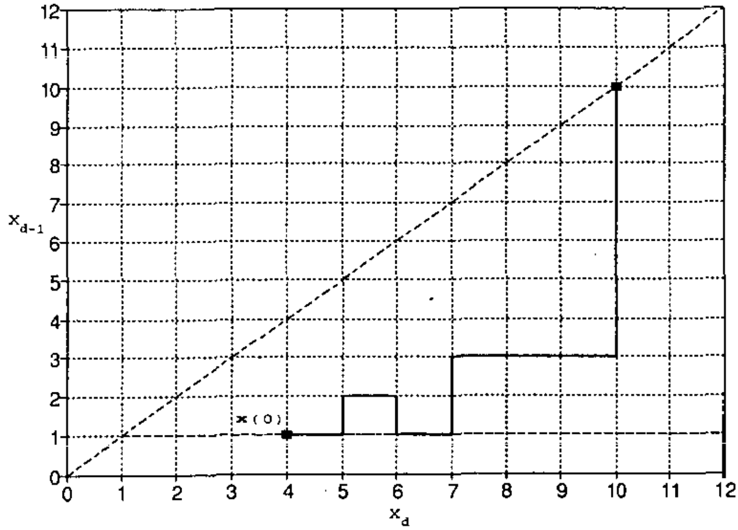

Figure 1. Example of a SAW (heavy full line) defined in (2.8)–(2.11) confined to the wedge defined in (2.7). The broken lines represent the hyperplane $x_{d-1} = x_d$ and $x_{d-1} = 1$.

Proof. It has been shown (Whittington and Soteros 1990) that SAWs confined to a wedge and interacting with a surface have the same reduced free energy $A(\omega)$ as a SAW interacting with a surface. With this result and following the line of argument in Hammersley *et al* (1982), other than replacing their reflection hyperplane by the hyperplane $x_{d-1}+x_d=\text{constant}$, we obtain (2.13).

Let L_1 and L_2 be two fixed $(d+4)$-step SAWs defined by

$$L_1: \quad \{\mathbf{0}, \mathbf{e}_1, \mathbf{e}_1+\mathbf{e}_d, \mathbf{e}_1+2\mathbf{e}_d, \mathbf{e}_1+3\mathbf{e}_d, \mathbf{e}_1+4\mathbf{e}_d, \mathbf{e}_1+\mathbf{e}_{d-1}+4\mathbf{e}_d, \ldots, \mathbf{e}_1+\mathbf{e}_2+\ldots+\mathbf{e}_{d-1}+4\mathbf{e}_d, \mathbf{e}_2+\ldots+\mathbf{e}_{d-1}+4\mathbf{e}_d\} \tag{2.14}$$

$$L_2: \quad \{\mathbf{0}, \mathbf{e}_d, 2\mathbf{e}_d, \mathbf{e}_{d-1}+2\mathbf{e}_d, \mathbf{e}_{d-1}+3\mathbf{e}_d, 3\mathbf{e}_d, 4\mathbf{e}_d, \mathbf{e}_{d-1}+4\mathbf{e}_d, \ldots, \mathbf{e}_2+\ldots+\mathbf{e}_{d-2}+\mathbf{e}_{d-1}+4\mathbf{e}_d\} \tag{2.15}$$

(figure 2). L_1 has no edges in the surface $x_1=0$, while L_2 is totally embedded in the surface. These two walks intersect only at the points $\mathbf{0}$ and $\mathbf{x}(0)=\mathbf{e}_2+\ldots+\mathbf{e}_{d-1}+4\mathbf{e}_d$. Concatenating L_1 (or L_2) with one walk in $\mathscr{B}_{n,m}$ results in an $(n+d+4)$-step walk with m (or $m+d+4$) edges in the surface and the edge $[\mathbf{0}, \mathbf{e}_1]$ (or $[\mathbf{0}, \mathbf{e}_d]$) as its first step.

We partition $\mathscr{B}_n$ into subclasses by placing two walks in the same subclass if they have the same last vertex. With the definition of $\mathscr{B}_n$, there are, at most, $I=(n+1)^{d-1}(2n+1)$ subclasses. In the ith subclass B_n^i, we denote by

$$\mathbf{x}(n)=(x_1(n), x_2(n), \ldots, x_d(n)) \tag{2.16}$$

the end vertex of all the walks. By using any two walks w_1 and w_2 from $\mathscr{B}_n^i$, we describe two constructions, which form the basis to form a k-loop.

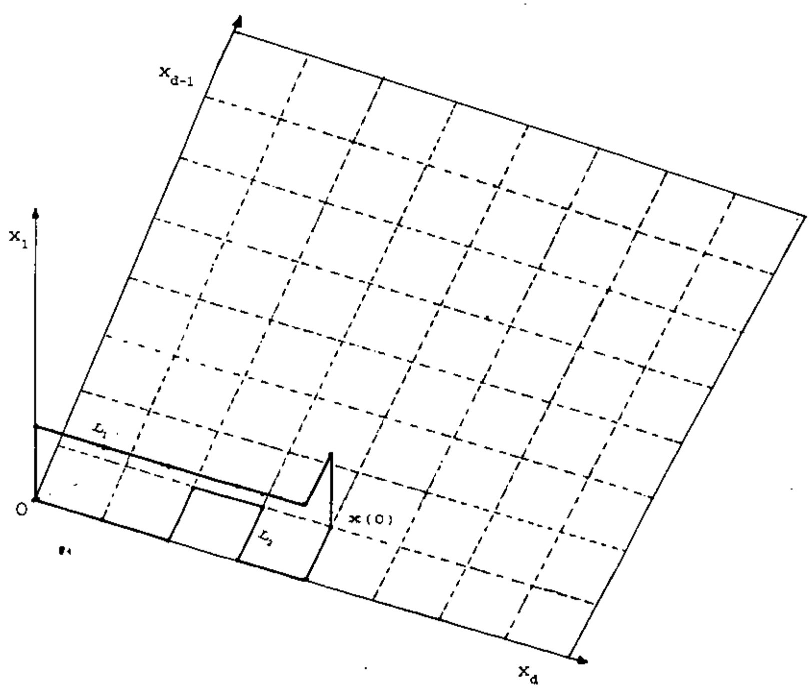

Figure 2. Heavy full lines represent the finite walks L_1 and L_2 defined in (2.14) and (2.15).

Construction 1. We concatenate both w_1 and w_2 by the same L_i ($i=1$ or 2) and, without confusion, we still denote the new walks by w_1 and w_2. We reflect w_2 in the hyperplane $x_d=x_d(n)$ to get a new walk w_2' such that its first (last) vertex is the reflection of the last (first) vertex of w_2. We delete the last edge from w_1 and the first edge from w_2' and body shift w_2' in the $\boldsymbol{e}_d$ direction by J steps, where J is equal to 3 or 4 so that each new walk obtained below can have an odd or even number of edges. By joining the two walks with a $(J+2)$-step walk: $\{\boldsymbol{x}(n-1), \boldsymbol{x}(n-1)+\boldsymbol{e}_d, \boldsymbol{x}(n-1)+\boldsymbol{e}_d-\boldsymbol{e}_{d-1}, \boldsymbol{x}(n-1)+2\boldsymbol{e}_d-\boldsymbol{e}_{d-1}, \ldots, \boldsymbol{x}(n-1)+(J-1)\boldsymbol{e}_d-\boldsymbol{e}_{d-1}, \boldsymbol{x}(n-1)+(J-1)\boldsymbol{e}_d, \boldsymbol{x}_2'(2)\}$, we obtain a $2(n+d+4)+J$-step walk w^1 (figure 3).

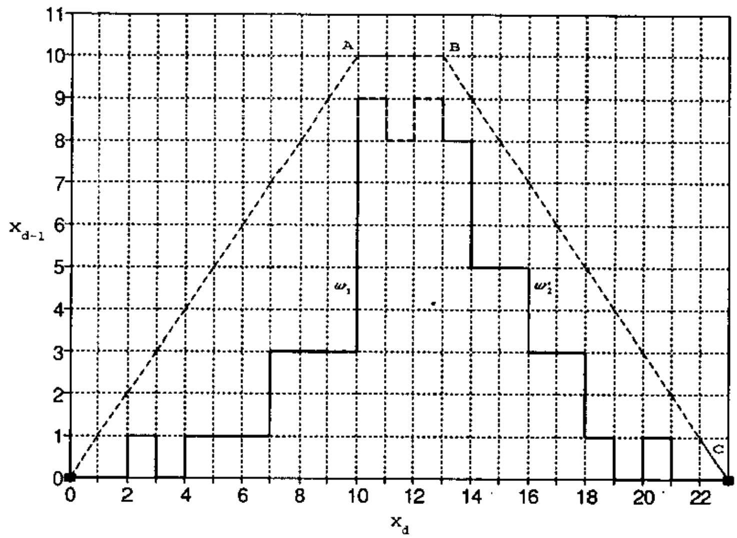

Figure 3. Example of the two walks w_1 and w_2' (heavy full lines) joined together by a 5-step walk (heavy broken lines) to form a new walk w^1 in construction 1. $0ABC$ encloses the region $\boldsymbol{R}$ in (2.18). $0A$ is the hyperplane $x_{d-1}=x_d$, AB is the hyperplane $x_{d-1}=x_d(n)$ and BC is the hyperplane $x_{d-1}+x_d=2x_d(n)+J$.

Construction 2. We concatenate w_1 and w_2 by L_2 and similarly write them as w_1 and w_2. We define two new walks by

$$w_i'=f_{d-1,d}(w_i) \qquad \text{for } i=1 \text{ and } 2. \tag{2.17}$$

The new walks are confined to the wedge $\{x_2\geqslant 0,\ldots,x_d\geqslant 0, x_{d-1}\geqslant x_d\}$ and have $\boldsymbol{x}(n)$ as their end vertices since $x_{d-1}(n)=x_d(n)$ for $\boldsymbol{x}(n)$. We reflect w_2' in the hyperplane $x_d=x_d(n)$ to get w_2'' and body shift it by J steps in the $\boldsymbol{e}_d$ direction. Finally, we join the two walks by a J-step walk: $\{\boldsymbol{x}(n), \boldsymbol{x}(n)+\boldsymbol{e}_d, \ldots, \boldsymbol{x}(n)+(J-1)\boldsymbol{e}_d, \boldsymbol{x}_2''(0)\}$ to obtain another $(2(n+d+4)+J)$-step walk w^2 (figure 4).

Both w^1 and w^2 start at the origin $\boldsymbol{0}$ and end at the point $\boldsymbol{E}=(0,\ldots,0,2x_d(n)+J)$. The walk w^1 is confined to the region

$$\boldsymbol{R}:\quad 0\leqslant x_2,\ldots,0\leqslant x_{d-1}<x_d(n), x_{d-1}\leqslant x_d\leqslant 2x_d(n)+J-x_{d-1} \tag{2.18}$$

while w^2 is confined outside of $\boldsymbol{R}$ and they only intersect at their start and end vertices (figures 3 and 4).

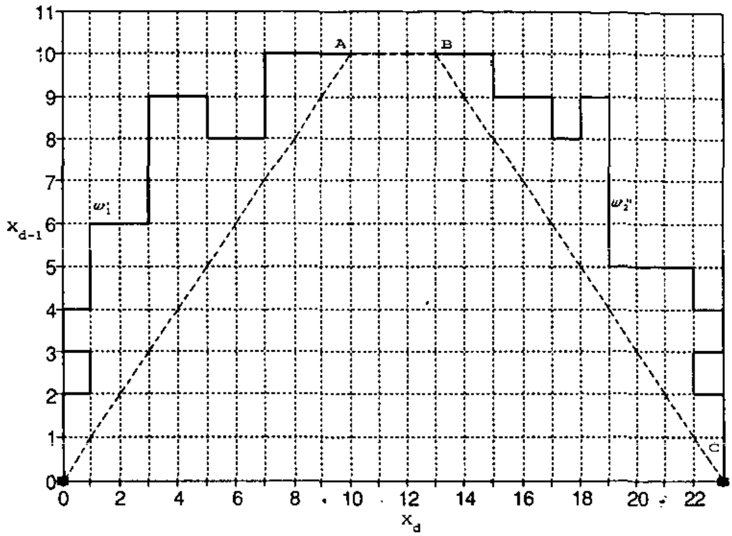

Figure 4. Example showing the joining of the two walks w_1' and w_2'' (heavy full lines) by a 3-step walk (heavy broken lines) to form a new walk w^2 in construction 2.

Now we take $2k$ walks $w_1, w_2, \ldots, w_{2k}$ from $\mathscr{B}_n^i$ and concatenate w_1 and w_2 by L_1 and the other $2(k-1)$ walks by L_2. We write these $2k$ walks in pairs by

$$\boldsymbol{W}_j = [w_{2j-1}, w_{2j}] \qquad (j=1,\ldots,k). \tag{2.19}$$

We obtain w_1^1, w_2^1 from $\boldsymbol{W}_1$, $\boldsymbol{W}_2$ by construction 1 and $w_3^2, \ldots, w_k^2$ from the other $k-2$ pairs by construction 2. The k walks $w_1^1, w_2^1, w_3^2, \ldots, w_k^2$ start at the origin $\mathbf{0}$ and terminate at the point $\boldsymbol{E}$, and all of them are totally confined to the subsection:

$$\boldsymbol{S}_1: \quad x_2 \geq 0, \ldots, x_{d-1} \geq 0, x_d \geq 0. \tag{2.20}$$

We leave w_1^1 and w_3^2 in S_1 and use $g_{d-1} \circ f_{d-2,d-1}$ to map w_2^1 and w_4^2 into the subsection

$$\boldsymbol{S}_2: \quad x_2 \geq 0, \ldots, x_{d-2} \geq 0, x_{d-1} \leq 0, x_d \geq 0. \tag{2.21}$$

Then, by properly choosing k'' numbers $i_{1.} < i_{2.} < \ldots < i_{k.}$ and another number j from the set $\{2, 3, \ldots, d-1\}$ $(1 \leq k'' \leq d-2)$, we construct a composite map by

$$F(i_{1.}, \ldots, i_{k.}, j, d-1) = g_{i_{1.}} \circ \ldots \circ g_{i_{k.}} \circ f_{j,d-1} \tag{2.22}$$

which maps one of the $k-4$ walks $w_5^2, \ldots, w_k^2$ into the subsection

$$\boldsymbol{S}': \quad x_2 \geq 0, \ldots, x_{i_{1.}} \leq 0, \ldots, x_{i_{k.}} \leq 0, \ldots, x_d \geq 0. \tag{2.23}$$

The new walk has $[\mathbf{0}, \boldsymbol{e}_j]$ (or $[\mathbf{0}, -\boldsymbol{e}_j]$) and $[\boldsymbol{E}, \boldsymbol{E}+\boldsymbol{e}_j]$ (or $[\boldsymbol{E}, \boldsymbol{E}-\boldsymbol{e}_j]$) as its first and last steps respectively. The last vertex of the new walk remains at the point $(0, 0, \ldots, 2x_d(n)+J)$ since its coordinates are unchanged under the defined composite map (2.18). The total number of subsections defined in (2.23) is $2^{(d-1)}-2$, which is not less than $2(d-1)-4(\geq k-4)$ for $d \geq 3$. Each of the walks $w_5^2, \ldots, w_k^2$ can be mapped into one individual subsection. In this way, all of k $2(n+d+4)+J$-step walks intersect only at their first and last vertices and form a member ℓ of $\mathscr{L}_{2(n+d+4)+J}(k)$ (figure 5). Let w_i $(1 \leq i \leq 2k)$ have m_i edges in the surface, then ℓ will have either $m_1 + \ldots + m_{2k} + 2(k-1)(d+4)$ or $m_1 + \ldots + m_{2k} + 2(k-1)(d+4) + Jk$ edges in the surface, depending on the position of $x(n)$.

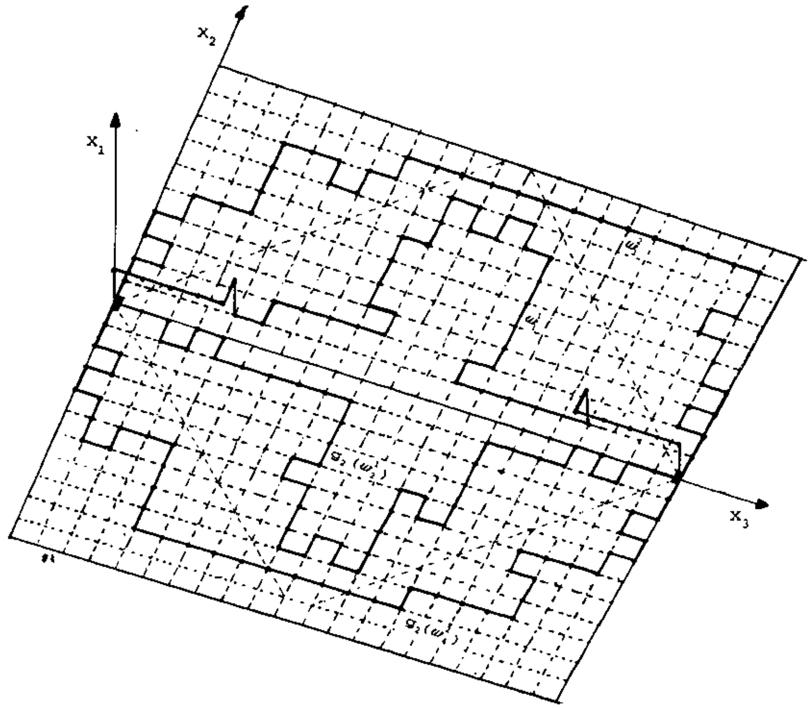

Figure 5. An example of a 4-loop formed by joining the walks w_1^1, w_3^2, $g_2(w_2^1)$ and $g_2(w_4^2)$ in a simple cubic lattice.

We consider the procedure to construct ℓ from the walks $w_1, w_2, \ldots, w_{2k}$ as a standard procedure which has to be followed whenever a group of $2k$ walks from $\mathscr{B}_n^i$ are used to construct a k-loop. Hence, a distinct group of $2k$ walks will give a distinct k-loop. We denote by $b_{n,m}^i$ the number of walks in $\mathscr{B}_n^i$ with m edges in the surface, we then have

$$\prod_{j=1}^{2k} b_{n,m_j}^i \leqslant l_{2k(n+d+4)+Jk,m'} + l_{2k(n+d+4)+Jk,\, m'+Jk} \tag{2.24}$$

with $m' = m_1 + \ldots + m_{2k} + 2(k-1)(d+4)$. We write

$$B_n(\omega, i) = \sum_{m=0}^{n} b_{n,m}^i \, \mathrm{e}^{m\omega}. \tag{2.25}$$

From (2.24), we have

$$\begin{aligned}
[B_n(\omega, i)]^{2k} &= \left(\sum_{m=0}^{n} b_{n,m}^i \, \mathrm{e}^{m\omega} \right)^{2k} \\
&= \sum_{m=0}^{2kn} \sum_{m_1+\ldots+m_k=m} \prod_{j=1}^{2k} b_{n,m_j}^i \, \mathrm{e}^{m\omega} \\
&\leqslant (2kn) \sum_{m=0}^{2kn} (l_{2k(n+d+4)+Jk,m'} + l_{2k(n+d+4)+Jk,m'+Jk}) \, \mathrm{e}^{m\omega} \\
&\leqslant (2kn)^{2k} f(\omega) L_{2(n+d+4)+J}(k, \omega)
\end{aligned} \tag{2.26}$$

where $f(\omega)=1+e^{Jk|\omega|})\,e^{2(k-1)(d+4)|\omega|}$. We let $p=2k$ and $q=2k(2k-1)^{-1}$, then $p^{-1}+q^{-1}=2k^{-1}+(2k-1)2k^{-1}=1$. By Holder's inequality, we have

$$[B_n(\omega)]^{2k}=\left(\sum_{i=1}^{I} B_n(\omega,i)\right)^{2k}\leqslant\left(\sum_{i=1}^{I} 1^{2k/(2k-1)}\right)^{(2k-1)}\sum_{i=1}^{I}(B_n(\omega,i))^{2k}$$
$$\leqslant I^{2k}(2kn)^{2k}f(\omega)L_{2(n+d+4)+J}(k,\omega) \tag{2.27}$$

which, combining with (2.2) and (2.13), gives (1.2) for any $k\leqslant 2(d-1)$.

The above construction gives a special polymer network, where for any vertex $\boldsymbol{x}$ on the loop, the coordinate x_d is between 0 and $2x_d(n)+J$, the x_d coordinates of the two branch points. Such a polymer network is termed a 'watermelon' and the two branch points are referred to as the extremes (Duplantier 1986). We shall henceforth refer to such a k-loop as a k-watermelon ($k\leqslant 2(d-1)$).

For $k>2(d-1)$, a k-loop can be constructed by joining watermelons together. We give an example for $d=3$ and $k=2d=6$. By following the above procedure, we can obtain a 3-watermelon ℓ with two of its branches confined to $x_2\geqslant 0$ and another confined in the closed region

$$\boldsymbol{R}_1:\quad -x_3(n)<x_2\leqslant 0 \qquad -x_2<x_3<2x_3(n)+J+x_2. \tag{2.28}$$

These three branches are joined together at $\mathbf{0}$ by the edges $[\mathbf{0},\boldsymbol{e}_1]$, $[\mathbf{0},\boldsymbol{e}_2]$ and $[\mathbf{0},\boldsymbol{e}_3]$, respectively, and at $\boldsymbol{E}=(0,0,2x_3(n)+J)$ by the edges $[\boldsymbol{E},\boldsymbol{E}+\boldsymbol{e}_1]$, $[\boldsymbol{E},\boldsymbol{E}+\boldsymbol{e}_2]$ and $[\boldsymbol{E},\boldsymbol{E}-\boldsymbol{e}_3]$. We denote it by $\ell(\boldsymbol{e}_3,\boldsymbol{e}_1,\boldsymbol{e}_2)$, where we put $\boldsymbol{e}_3$ at the first position to indicate that the two extremes are on the positive x_3-axis. Now we construct four 3-watermelons $\ell_1(\boldsymbol{e}_3,\boldsymbol{e}_1,\boldsymbol{e}_2)$, $\ell_2(\boldsymbol{e}_3,\boldsymbol{e}_1,\boldsymbol{e}_2)$, $\ell_3(\boldsymbol{e}_3,\boldsymbol{e}_1,\boldsymbol{e}_2)$ and $\ell_4(\boldsymbol{e}_3,\boldsymbol{e}_1,\boldsymbol{e}_2)$ such that ℓ_1 and ℓ_2 have their two extremes at $\mathbf{0}$ and $(0,0,2x_d(n)+J)$ with a uniform $(2(n+d+4)+J)$-step length for each branch, while l_3 and l_4 have their two extremes at $\mathbf{0}$ and $(0,0,2x_d(n)+J')$ with a uniform $(2(n+d+4)+J')$-step length for each branch. For l_3 and ℓ_4, the closed region $\boldsymbol{R}_1$ is replaced by

$$\boldsymbol{R}_1':\quad -x_3(n)<x_2\leqslant 0 \qquad -x_2<x_3<2x_3(n)+J'+x_2. \tag{2.29}$$

We define:

(i) $\ell_2'(\boldsymbol{e}_3,\boldsymbol{e}_1,-\boldsymbol{e}_2)=g_2(\ell_2)$, which has two branches confined to $x_2\leqslant 0$ and one branch confined in the closed region

$$\boldsymbol{R}_2:\quad 0\leqslant x_2<x_3(n) \qquad x_2<x_3<2x_3(n)+J-x_2. \tag{2.30}$$

(ii) $\ell_3'(-\boldsymbol{e}_2,-\boldsymbol{e}_1,\boldsymbol{e}_3)=g_1\circ g_2\circ f_{2,3}(\ell_2)$, which has its two extremes at $\mathbf{0}$ and $(0,-2x_d(n)+J',0)$ with two branches confined to $x_3\geqslant 0$ and another confined in

$$\boldsymbol{R}_3:\quad -2x_3(n)-J'-x_3<x_2<x_3 \qquad -x_3(n)<x_3\leqslant 0. \tag{2.31}$$

(iii) $\ell_4'(-\boldsymbol{e}_2,-\boldsymbol{e}_1,-\boldsymbol{e}_3)=g_1\circ g_2\circ g_3\circ f_{2,3}(\ell_4)$, which has its two extremes at $\mathbf{0}$ and $(0,-2x_d(n)+J',0)$ with two branches confined to $x_3\leqslant 0$ and another confined in

$$\boldsymbol{R}_4:\quad -2x_3(n)-J'+x_3<x_2<-x_3 \qquad 0\leqslant x_3<x_3(n). \tag{2.32}$$

We body shift ℓ_2' in the $-\boldsymbol{e}_2$ direction by $2x_d(n)+J'$ steps and ℓ_3' in the $\boldsymbol{e}_3$ direction by $2x_d(n)+J$ steps. The four watermelons are joined together at their branch points to form a network with four branch points of degree 6 at $\boldsymbol{A}=(0,0,0)$, $\boldsymbol{B}=(0,0,2x_d(n)+J)$, $\boldsymbol{C}=(0,-2x_d(n)-J',2x_d(n)+J)$ and $\boldsymbol{D}=(0,-2x_d(n)-J',0)$. At the branch point $\boldsymbol{B}$, we delete the edges $[\boldsymbol{B},\boldsymbol{B}+\boldsymbol{e}_2]$, $[\boldsymbol{B},\boldsymbol{B}-\boldsymbol{e}_2]$, $[\boldsymbol{B},\boldsymbol{B}+\boldsymbol{e}_3]$ and $[\boldsymbol{B},\boldsymbol{B}+\boldsymbol{e}_3]$. We then join the vertices $\boldsymbol{B}+\boldsymbol{e}_2$ and $\boldsymbol{B}+\boldsymbol{e}_3$ by the edges $[\boldsymbol{B}+\boldsymbol{e}_2,\boldsymbol{B}+\boldsymbol{e}_2+\boldsymbol{e}_3]$ and

$[\boldsymbol{B}+e_2+e_3, \boldsymbol{B}+e_3]$, the vertices $\boldsymbol{B}-e_2$ and $\boldsymbol{B}-e_3$ by the edges $[\boldsymbol{B}-e_2, \boldsymbol{B}-e_2-e_3]$ and $[\boldsymbol{B}-e_2-e_3, \boldsymbol{B}-e_3]$. We also make the same modifications at the branch point $\boldsymbol{D}$. On completion, we obtain a 6-loop with its two branch points at the points $\boldsymbol{A}$ and $\boldsymbol{C}$ and a uniform length of $4(n+d+4)+J+J'$ step, which can be either odd or even by taking certain values for J and J'.

For $d>3$, we note that the construction of a d-watermelon is not unique and the number of subsections satisfying $x_{d-1}\geqslant 0$ and $x_d\geqslant 0$ is $2^{d-3}\geqslant d-2$ for $d>3$ (we can embed two branches independently in the same subsection). We can construct a d-watermelon $\ell(e_d, e_1, \ldots, e_{d-1})$, which has all of its branches confined to $x_{d-1}\geqslant 0$. By using four such d-watermelons and following the same procedure for $d=3$, we obtain a $2d$-loop.

3. Other cases

In section 2, the proof of (1.2) is specifically for uniform k-loops with the root at one of the branch points and interacting with a penetrable surface. As mentioned previously, we can also consider other cases.

3.1. *k-loop with the root at a vertex other than a branch point*

In this case, a k-loop has its root at one of its vertices other than a branch point. We denote by

$$L'_n(k,\omega)=\sum_{m=0}^{kn} l'_{kn,m}\,\mathrm{e}^{m\omega} \tag{3.1}$$

the generating function for such k-loops. We note that in the previous construction there is a vertex with coordinates $(0, 1, \ldots, 1, 4)$, i.e. the start vertex of a walk w in $\mathscr{B}_n$, which is not the branch point of the k-loop. By changing the origin to this point, we obtain a lower bound for $L'_n(k,\omega)$.

We derive an upper bound for $L'_n(k,\omega)$. Since the branch points of such a k-loop may not be in the surface, some of the k branches may have no vertices in the surface. We classify all such k-loops by the number of branches which have at least one vertex in the surface. There are k such classes. In each class, for any k-loop, if a branch of the k-loop has vertices in the surface, we choose one of them and consider this branch as a non-uniform 2-star rooted on the surface at the chosen vertex (see the appendix). For a branch without any vertex in the surface, we consider it as a SAW in the bulk. By treating each branch independently and summing over all k classes, we obtain

$$L'_n(k,\omega)\leqslant\sum_{i=1}^{k}(S'_n(2,\omega))^i a_n^{k-i} \tag{3.2}$$

where a_n is the number of n-step walks in the bulk and $S'_n(2,\omega)$ is defined by (A7). As $n\to\infty$, we have, for a given ω,

$$S'_n(2,\omega)\leqslant\exp(nA(\omega)+\mathrm{o}(n)) \tag{3.3}$$

(A11) and

$$a_n\leqslant\exp(n\kappa+\mathrm{o}(n))\leqslant\exp(nA^+(\omega)+\mathrm{o}(n))\leqslant\exp(nA(\omega)+\mathrm{o}(n)) \tag{3.4}$$

where κ is the connective constant of walks in the bulk and $A^{+}(\omega)$ is the reduced free energy of walks interacting with an impenetrable surface. We have used the result that, for any ω, $\kappa \leqslant A^{+}(\omega) \leqslant A(\omega)$ (Hammersley *et al* 1982). Hence, we have, for a given ω,

$$L'_n(k, \omega) \leqslant k \exp(knA(\omega) + o(n)). \tag{3.5}$$

Combining (2.27) and (3.5) gives

$$\lim_{n \to \infty} (kn)^{-1} \log L'_n(k\omega) = A(\omega). \tag{3.6}$$

3.2. *k-loop interacting with an impenetrable surface*

When the interaction surface is impenetrable, a k-loop is totally confined to one side of the surface, say $x_1 \geqslant 0$. In this case, we consider the subset $\mathscr{B}_n^{+}$ of $\mathscr{B}_n$, which is the set of all n-SAWs that belong to $\mathscr{B}_n$ and satisfy

$$x_1(i) \geqslant 0 \qquad \text{for all } i = 0, \ldots, n. \tag{3.7}$$

By following the steps in lemma 2, we can show that such walks have the same reduced free energy $A^{+}(\omega)$ as that in (3.4). We also restrict g_i to $i \geqslant 2$. For $k \leqslant 2d-1$, by following exactly the procedures in sections 2 and 3.1, we can show that k-loops interacting with an impenetrable surface have the reduced free energy $A^{+}(\omega)$.

For $k = 2d$, a k-loop can only have its root at one vertex other than a branch point. We define three new uniform finite-step walks L'_1, L'_2 and L'_3 to replace L_1 and L_2:

$$L'_1 = \{3e_1, 2e_1, 2e_1 + e_d, e_1 + e_d, e_1, \mathbf{0}, e_d, 2e_d, 3e_d, e_{d-1} + 3e_d, \ldots, e_2 + \ldots + e_{d-1} + 3e_d, e_2 + \ldots + e_{d-1} + 4e_d\} \tag{3.8}$$

$$L'_2 = \{3e_1, 3e_1 + e_d, 3e_1 + 2e_d, 2e_1 + 2e_d, 2e_1 + 3e_d, 3e_1 + 3e_d, 3e_1 + 4e_d, 2e_1 + 4e_d, e_1 + 4e_d, 4e_d, e_{d-1} + 4e_d, \ldots, e_2 + \ldots + e_{d-1} + 4e_d\} \tag{3.9}$$

$$L'_3 = \{3e_1, 4e_1, 4e_1 + e_d, \ldots, 4e_1 + 4e_d, 4e_1 + e_{d-1} + 4e_d, \ldots, 4e_1 + e_2 + \ldots + e_{d-1} + 4e_d, 3e_1 + e_2 + \ldots + e_{d-1} + 4e_d, \ldots, e_2 + \ldots + e_{d-1} + 4e_d\} \tag{3.10}$$

(figure 6). L'_1, L'_2 and L'_3 only intersect at the points $(3, 0, \ldots, 0)$ and $x(0)$. By following the procedure in section 2 for $k > 2(d-1)$, we obtain a k-loop which is totally confined to the side $x_1 \geqslant 0$ with the two branch points at $(3, 0, \ldots, 0)$ and $(3, 0, \ldots, -2x_d(n) - J', 2x_d(n) + J)$.

3.3. *Non-uniform k-loops*

For $k = 2$, a k-loop is reduced to a polygon with two branches intersecting at $\mathbf{0} = (0, 0, \ldots, 0)$ and $\boldsymbol{E} = (0, 0, \ldots, 2x_d(n) + J)$. By choosing one of the two vertices and following the construction given by Gaunt *et al* (1984), one can obtain a lower bound for non-uniform k-loops with either one of the two attachments. An upper bound can be obtained by following the procedure in section 3.1.

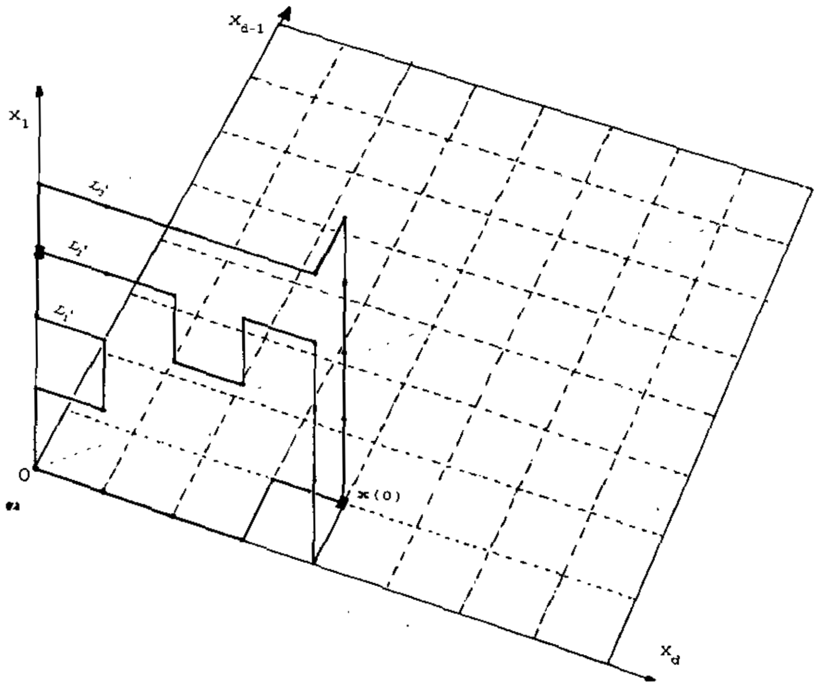

Figure 6. Three new finite walks L_1', L_2' and L_3' defined in (3.9)–(3.11).

4. Summary

We have considered the interaction between a surface and the polymer topology defined as k-loops, which consists of k SAWs connected together at their initial and terminal vertices. The k-loops may be uniform or non-uniform and may be attached to the surface at a branch point or at any other vertex. We have shown that the reduced free energy per step of the k-loops is identical to that for SAWs interacting with a surface. It thus follows that the critical point and crossover properties of the k-loops are identical to those for SAWs adsorbed to a surface.

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Appendix. Non-uniform 2-star

We define a non-uniform 2-star and prove that it has the same reduced free energy as that for a SAW interacting with a surface. In the following, we do not distinguish the surfaces. However, the appropriate results apply, depending on whether the surface is penetrable or impenetrable.

We denote by $\mathscr{A}_n$ the set of n-step SAWs starting at $\mathbf{0}$ and interacting with the surface. $\mathscr{C}_n$ is the subset of $\mathscr{A}_n$ that satisfies the additional conditions

$$0 = x_1(0) = x_1(n) \tag{A1}$$

and

$$0 = x_d(0) \leqslant x_d(i) < x_d(n) \qquad (i = 1, \ldots, n-1). \tag{A2}$$

We define

$$C_n(\omega) = \sum_{m=0}^{n} c_{n,m}\, \mathrm{e}^{m\omega} \qquad \text{and} \qquad A_n(\omega) = \sum_{m=0}^{n} a_{n,m}\, \mathrm{e}^{m\omega} \tag{A3}$$

the generating functions fc: $\mathscr{C}_n$ and $\mathscr{A}_n$ respectively. It has been shown (Hammersley *et al* 1982) that

(i) $$C_n(\omega)C_{n'}(\omega) \leqslant (n+n'+1)C_{n+n'}(\omega) \tag{A4}$$

(ii) $$A_n(\omega) \leqslant (2n+5)^{d+1/2} \exp(cn^{1/2} + 2|\omega|)C_{2n+4}^{1/2}(\omega) \tag{A5}$$

(iii) $$\lim_{n\to\infty} (1/n) \log C_n(\omega) = \lim_{n\to\infty} (1/n) \log A_n(\omega) = A(\omega). \tag{A6}$$

We consider an n-step SAW interacting with the surface. The SAW has one of its vertices at $\mathbf{0}$, which may not be any of the end vertices. We call such a SAW a non-uniform 2-star with n edges and the vertex at $\mathbf{0}$ as its branch point. Each of the two branches of a non-uniform 2-star is an n_i-step SAW ($n_i \geqslant 0$) with $n_1 + n_2 = n$. Thus, a SAW starting at $\mathbf{0}$ is a special case of a non-uniform 2-star with only one branch. We define

$$S'_n(2, \omega) = \sum_{m=0}^{n} s'_{n,m}\, \mathrm{e}^{m\omega} \tag{A7}$$

as the generating function for such 2-stars interacting with the surface. Then, we have

$$A_n(\omega) \leqslant S'_n(2, \omega). \tag{A8}$$

By treating each branch independently, we obtain

$$S'_n(2, \omega) \leqslant \sum_{n_1+n_2=n} A_{n_1}(\omega)A_{n_2}(\omega). \tag{A9}$$

From (A4) and (A5), (A9) is replaced by

$$\begin{aligned} S'_n(2, \omega) &\leqslant (n+1)[(2n_1+5)^{d+1/2} \exp(cn_1^{1/2} + 2|\omega|)C_{2n_1+4}^{1/2}(\omega)] \\ &\quad \times [(2n_2+5)^{d+1/2} \exp(cn_2^{1/2} + 2|\omega|)C_{2n_2+4}^{1/2}(\omega)] \\ &\leqslant (n+1)(2n+5)^{2d+1}(2n+9) \exp(c'n^{1/2} + 4|\omega|)C_{2n+8}^{1/2}(\omega). \end{aligned} \tag{A10}$$

Combining (A6), (A8) and (A10), we obtain

$$\lim_{n\to\infty} (1/n) \log S'_n(2, \omega) = A(\omega). \tag{A11}$$

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