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On c-animals interacting with a surface

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Abstract. We examine the interaction of weakly embedded c-animals with an adsorbtion surface and show that such animals have the same reduced free energy as that for weakly embedded trees. By assuming the existence of $\theta_0(\omega)$, the critical exponent for trees, we show that $\theta_c(\omega)$ exists and $\theta_c(\omega)=\theta_0(\omega)-c$ for all ω.

1. Introduction

Lattice animals, as connected subgraphs of a regular lattice, are considered as a model for branched polymers in a good solvent. The influence of the cycle fugacity on the properties of lattice animals has been examined by a number of workers (Lubensky and Isaacson 1979, Family 1980, Whittington *et al* 1983, Soteroes and Whittington 1988). To study the crossover from trees to animals, Whittington *et al* (1983) introduced c-animals, which are lattice animals with a cyclomatic index c. Denoting by $a_n(c)$, the number of c-animals with n vertices, they showed that

$$\lim_{n\to\infty} n^{-1}\log a_n(c)=\log\lambda_0 \tag{1.1}$$

where λ_0 is the connective constant for lattice trees. With the assumption that $a_n(0)\sim\lambda_0^n n^{-\theta_0}$, Soteross and Whittington (1988) showed that

$$a_n(c)\sim\lambda_0^n n^{-\theta_c} \tag{1.2}$$

with

$$\theta_c=\theta_0-c. \tag{1.3}$$

Recently, De'Bell *et al* (1990) and Lookman *et al* (1990) studied the interaction of (weakly embedded) animals (trees) with an adsorption surface, which can be either penetrable or impenetrable. It has been shown that the limit

$$\lim_{n\to\infty} n^{-1}\log A_n(\omega)=\lim_{n\to\infty} n^{-1}\log\left(\sum_{i=1}^{n} a_{n,i}\,\mathrm{e}^{i\omega}\right)=\log\lambda(\omega) \tag{1.4}$$

exists for all ω, where $a_{n,i}$ is the number of n-vertex animals (trees) with i vertices in the surface (either penetrable or impenetrable), and ω is the interaction energy. By analogy, one would expect that, as $n\to\infty$,

$$A_n(\omega)\sim n^{-\theta(\omega)}\lambda^n(\omega). \tag{1.5}$$

In this paper, we consider the interaction between a penetrable or impenetrable adsorption surface and c-animals. We write $a_{n,i}(c)$ as the number of n-vertex c-animals with i vertices in the surface. By generalizing the arguments of Soteros and Whittington (1988), we show that

$$\lim_{n\to\infty} n^{-1} \log A_n(c, \omega) = \lim_{n\to\infty} n^{-1} \log\left(\sum_{i=1}^{n} a_{n,i}(c)\, \mathrm{e}^{i\omega} \right) = \log \lambda(0; \omega) \qquad (1.6)$$

where $\log \lambda(0, \omega)$ is the reduced free energy for trees. With the assumption (1.5) for trees, we show that $A_n(c, \omega)$ also has the asymptotic form of (1.5) with

$$\theta_c(\omega) = \theta_0(\omega) - c \qquad (1.7)$$

for all ω, where $\theta_0(\omega)$ is the critical exponent of trees in (1.5). In (1.6) and (1.7) we do not distinguish between the two surfaces. It is understood that the relevent $\lambda(0, \omega)$, $\theta_0(\omega)$ and $\theta_c(\omega)$ apply depending on the surface.

2. Proof of the results

Let $a_{n,i}(c)$ denote the number of n-vertex c-animals with i vertices in the surface $x_1 = 0$. Following the arguments of Whittington *et al* (1983), we obtain

$$a_{n,i}(c) \leqslant (2dn) \cdot a_{n,i}(0). \qquad (2.1)$$

Multiplying both sides by $\mathrm{e}^{i\omega}$ and summing over i yields

$$A_n(c, \omega) \leqslant (2dn) \cdot A_n(c-1, \omega). \qquad (2.2)$$

We generalize a series of theorems and lemmas given by Soteros and Whittington (1988) (SW) to the case where an adsorption surface is present.

We concentrate on c-animals embedded in the square lattice. However, the results can be generalized to the d-dimensional hypercubic lattice. In the square lattice, a vertex has coordinates (x, y). The adsorption 'surface' is $x = 0$. A vertex is a member of V_1 if it is of degree 4 and is a member of V_2, V_3, V_4 or V_5 if it is of degree 3 and is not connnected to the neighbouring vertex in south, west, north or east direction respectively (figure 1).

Theorem 1. Every n-vertex tree containing a vertex $v_0 \in V_1$, V_2, V_3, V_4 or V_5 can be converted into a 1-animal (with $n+1$ vertices) containing a 4-cycle in which v_0 is the bottom or top vertex of the 4-cycle. The resulting 1-animal can have at most three trees rooted at a vertex in V_1, V_2, V_3, V_4 and V_5 as precursors.

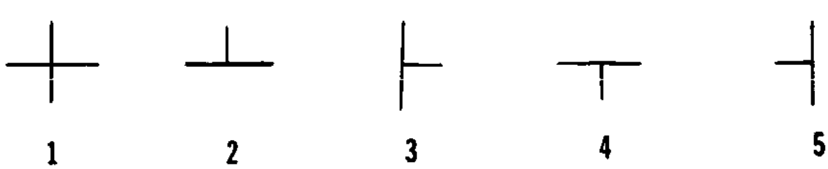

Figure 1. On the square lattice a vertex of degree greater than 2 must be one of the five types shown.

The proof of theorem 1 follows the same procedure as that given in sw except that when $v_0 = (x, y) \in V_4$ or V_5, we have to consider the vertex v_3' with coordinates $(x-1, y-1)$. We note that within the procedure, the number of vertices of a tree in the surface is unchanged. Hence, if the tree has i vertices in the surface, the resulting 1-animal can have either i or $i+1$ vertices in the surface. We denote by $b_{n,i}(\varepsilon)$ the number of n-vertex trees with i vertices in the surface containing more than εn vertices which are members of V', one of V_1, V_2, V_3, V_4 and V_5. Let $a_{n,i}(c)$ be the member of c-animals having n vertices with i of them in the surface. Following theorem 1, we have

$$a_{n+1,i}(1) + a_{n+1,i+1}(1) \geq \binom{\varepsilon n}{1} b_{n,i}(\varepsilon)/3. \tag{2.3}$$

Generally, if a tree has n vertices containing at least c vertices in V', we obtain

$$a_{n+c,i}(c) + a_{n+c,i+1}(c) + \ldots + a_{n+c,i+c}(c) \geq \binom{\varepsilon n}{c} b_{n,i}(\varepsilon)/3^c \tag{2.4}$$

for $\varepsilon n \geq c$.

Lemma 1. If $t_{n,i}(\varepsilon, >)$ is the number of n-vertex trees with i vertices in the surface and containing more than εn vertices of degree greater than 2, then, by choosing V', we have

$$b_{n,i}(\varepsilon/5) \geq t_{n,i}(\varepsilon, >)/5. \tag{2.5}$$

Proof. Let $S_{n,i}(\varepsilon, >)$ be the set of n-vertex trees with i vertices in the surface and containing more than εn vertices of degree greater than 2. We construct subsets $S^m_{n,i}(\varepsilon, >)$ such that a tree $T \in S_{n,i}(\varepsilon, >)$ is a member of $S^m_{n,i}(\varepsilon, >)$ if m is the smallest number such that the number of vertices in $V_m(T)$ is at least as large as the number in $V_k(T)$, $k = 1, \ldots, 5$, $k \neq m$. Thus T can be a member of only one subset $S^m_{n,i}(\varepsilon, >)$. Let V_m be V' such that

$$|S^m_{n,i}(\varepsilon, >)| = \max\{|S^j_{n,i}(\varepsilon, >)|, j = 1, \ldots, 5\}. \tag{2.6}$$

$|\cdot|$ denotes the cardinality of a set. From the definitions of $S_{n,i}(\varepsilon, >)$ and $S^j_{n,i}(\varepsilon, >)$, there must be more than $\varepsilon n/5$ vertices in $V' = V_m$. Hence

$$b_{n,i}(\varepsilon/5) \geq |S_{n,i}(\varepsilon, >)| \geq \sum_{j=1}^{5} |S^j_{n,i}(\varepsilon, >)|/5 = t_{n,i}(\varepsilon, >)/5. \tag{2.7}$$

From lemma 1 and (2.4), we have

$$a_{n+c,i}(c) + \ldots + a_{n+c,i+c}(c) \geq \binom{\varepsilon' n}{c} t_{n,i}(\varepsilon, >)/5 \cdot 3^c \tag{2.8}$$

with $\varepsilon' = \varepsilon/5$. Multiplying by $e^{i\omega}$ and summing over i gives

$$c \cdot (1 + e^{|\omega|} + \ldots + e^{c|\omega|}) A_{n+c}(c, \omega) \geq \binom{\varepsilon' n}{c} T_n(\varepsilon, >, \omega)/5 \cdot 3^c. \tag{2.9}$$

Lemma 2. Let $t_{n,i}(\varepsilon, \leq)$ be the number of n-vertex trees with i vertices in the surface and containing at most εn vertices of degree greater than 2. Define

$$T_n(\varepsilon, \leq, \omega) = \sum_{i=1}^{n} t_{n,i}(\varepsilon, \leq)\, e^{i\omega}. \tag{2.10}$$

Then, for any ε in $[0, 1]$, the limit

$$\lim_{n\to\infty} n^{-1} \log T_n(\varepsilon, \leqslant, \omega) = \log T(\varepsilon, \omega) < \infty \tag{2.11}$$

exists for all ω.

Proof. By using the concatenation given by Lookman *et al* (1990) and following the line of argument given by Lipson and Whittington (1983), we establish (2.9).

It is obvious that, as $\varepsilon = 0$, we have $\log T(0, \omega) = A(\omega)$, the reduced free energy for non-uniform 2-stars (see the appendix), where as if $\varepsilon = 1$, $\log T(1, \omega) = \log \lambda(0, \omega)$, the reduced free energy for trees.

Lemma 3. For given ω, $\log T(\varepsilon, \omega)$ is a concave function of ε in $[0, 1]$.

Lemma 4. For given ω, $\log T(\varepsilon, \omega)$ is a conntinuous function of ε in $[0, 1]$.

Proof. The continuity of $\log T(\varepsilon, \omega)$ for $\varepsilon \in [0, 1]$ is establshed by following the same procedure in sw exceot that we replace their equation (2.10) by

$$u_n(\omega, 4\varepsilon) \leqslant \sum_{m \leqslant 4\varepsilon n} T(n)\binom{n-2}{m-2}(n-2)\exp[nA(\omega) + o(n)] \tag{2.12}$$

where $U_n(\omega, 4\varepsilon n)$ is the generating function of the n-vertex trees with at most εn vertices of degree not equal to 2. There are a total of $m-1$ branches with length less than n-step. A branch can have either some vertices or no vertices in the surface. Following the arguments given by Zhao and Lookman (1990), we obtain the term $(n-2)\exp[nA(\omega) + o(n)]$.

Lemma 5. For given ω, there exists $\varepsilon_0(\omega) > 0$ such that for $\varepsilon < \varepsilon_0(\omega)$,

$$\lim_{n\to\infty} (T_n(\varepsilon, >, \omega)/A_n(0, \omega)) = 1. \tag{2.13}$$

Proof. Since $T(\varepsilon, \omega)$ is continuous for ε in $[0, 1]$ and $T(0, \omega) < T(1, \omega)$ (A10, A11), there exists $\varepsilon_0(\omega) > 0$ such that for all $\varepsilon < \varepsilon_0(\omega)$, $T(\varepsilon, \omega) < T(1, \omega)$. We can write

$$\begin{aligned} T_n(\varepsilon, >, \omega)/A_n(0, \omega) &= 1 - T_n(\varepsilon, \leqslant, \omega)/A_n(0, \omega) \\ &= 1 - [T(\varepsilon, \omega)/T(1, \omega)]^n \exp(o(n)) \end{aligned} \tag{2.14}$$

and letting $n \to \infty$ proves the lemma.

Equations (2.7) and (2.12) lead to lemma 6.

Lemma 6. For given ω, there exists a constant $C(\omega) > 0$ and an integer $N(\omega)$ such that for all $n > N(\omega)$

$$A_n(c, \omega) = C(\omega)\binom{\varepsilon' n}{c} A_n(0, \omega) \tag{2.15}$$

for any $\varepsilon \leqslant \varepsilon_0$, where $\varepsilon' = \varepsilon/5$.

From (2.2) and (2.13), we have theorem 2.

Theorem 2. For given ω,

$$\lim_{n\to\infty} n^{-1} \log A_n(c, \omega) = \lambda(0, \omega) \tag{2.16}$$

and, if $\lim_{n\to\infty} [\log(A_n(0, \omega)/\lambda(0, \omega)^n)/\log n] = -\theta_0(\omega)$ exists, then

$$\lim_{n\to\infty} [\log(A_n(c, \omega)/\lambda(0, \omega)^n)/\log n] = -\theta_c(\omega) \tag{2.17}$$

exists for all c and

$$\theta_c(\omega) = \theta_0(\omega) - c. \tag{2.18}$$

3. Discussion

In section 2, the results of Whittington *et al* (1983) and Soteros and Whittington (1988) for c-animals have been generalized to the case where an adsorption surface exists. We thus have an example where certain critical properties of polymer networks in the bulk are preserved when the networks interact with an adsorption surface, implying that a surface interaction is an irrelevant operator.

We also note that, if the cyclomatic index c satisfies $c = 0(n/\log n)$, from (2.2) and (2.14), all results are still valid except in this case, we have to replace (2.15) and (2.16) by the limit

$$\lim_{n\to\infty} \{[\log(A_n(c, \omega)/\lambda(0, \omega)^n)/\log n] - c(n)\} = \theta_0(\omega). \tag{3.1}$$

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Appendix

A linear polymer rooted on a surface with the root at one of the vertices in the surface can be defined as a non-uniform 2-star, and it has been shown (Zhao and Lookman 1990) that

$$\lim_{n\to\infty} n^{-1} \log S_n(2, \omega) = \lim_{n\to\infty} n^{-1} \log\left(\sum_{i=0}^{n} s_{n,i}\, e^{i\omega}\right) = A(\omega) \tag{A1}$$

and

$$\lim_{n\to\infty} n^{-1} \log S_n^+(2, \omega) = \lim_{n\to\infty} n^{-1} \log\left(\sum_{i=0}^{n} s_{n,i}^+\, e^{i\omega}\right) = A^+(\omega) \tag{A2}$$

where $s_{n,i}(s_{n,i}^+)$ is the number of non-uniform 2-stars with $(n+1)$ vertices and $(i+1)$ of them in a penetrable (impenetrable) surface, and $A(\omega)(A^+(\omega))$ is the reduced free energy of SAWs interacting with a penetrable (impenetrable) surface (Hammersley *et al* 1982).

By a translation, any n-step self-avoiding walk (SAW) in the bulk can be mapped to at least one non-uniform 2-star, which may be rooted on either a penetrable or an impenetrable surface. Such a mapping is injective. Hence we have

$$a_n \leqslant S_n^+(2,0) \leqslant S_n(2,0). \tag{A3}$$

For $\omega \geqslant 0$, we have $e^{\omega} \geqslant 1$. Consider an (n_1+n_2)-step SAW rooted on the surface with a total $(i+1)$ vertices in a penetrable surface. By cutting it at the vertex $x(n_1)$, we obtain two SAWs. By a translation until both of them have visits to the surface, we obtain two non-uniform 2-star with a total $(i'+1) \geqslant (i+1)$ vertices in the surface. Since not all 2-stars can be obtained in this way, we have

$$S_{n_1}(2,\omega) \cdot S_{n_2}(2,\omega) \geqslant A_{n_1+n_2}(\omega). \tag{A4}$$

With this inequality, we obtain that, for any n and $\omega \geqslant 0$,

$$n^{-1} \log S_n(2,\omega) \geqslant A(\omega). \tag{A5}$$

It has been shown (Lookman *et al* 1990) that

$$T_{n_1}(\omega) \cdot T_{n_2}(\omega) \leqslant T_{n_1+n_2}(\omega). \tag{A6}$$

Hence, for any n, we have

$$n^{-1} \log T_n(\omega) \leqslant \log \lambda(0,\omega). \tag{A7}$$

Since for any n,

$$S_n(2,\omega) < T_n(\omega) \tag{A8}$$

for $\omega \geqslant 0$, we have

$$A(\omega) < \lambda(0,\omega). \tag{A9}$$

For $\omega \leqslant 0$, it has been shown that $A(\omega) \equiv \kappa$ (Hammersley *et al* 1982), $\lambda(0,\omega) \equiv \lambda_0$ (Lookman *et al* 1990) and $\kappa < \lambda_0$ (Gaunt *et al* 1984). Hence for any ω, we have

$$A(\omega) < \lambda(0,\omega). \tag{A10}$$

Similarly, it can also be shown that, for any ω,

$$A^+(\omega) < \lambda^+(0,\omega). \tag{A11}$$

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