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Self-avoiding walks interacting with a surface

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Abstract. We discuss two models of polymer adsorption. In one model a self-avoiding walk on a D-dimensional lattice interacts with a $(D-1)$-dimensional hyperplane; in the other model, this walk must also lie in or on one side of this hyperplane. Both models exhibit non-analytic behaviour corresponding to a phase transition, but these phase transitions do not occur at the same point. We give numerical estimates of the locations of these transitions.

1. Introduction

Self-avoiding walks on a three-dimensional lattice, interacting with a plane and restricted to lie on one side of (or in) the plane have been studied as a model of excluded volume effects in the adsorption of polymers at a solid–liquid interface. Silberberg (1967) developed a mean field treatment of this model, and some early Monte Carlo work was carried out by Clayfield and Lumb (1966) and McCrackin (1967). Several groups of workers have enumerated short walks exactly, and obtained information on longer walks by extrapolation techniques (e.g. Lax 1974a, b, Ma *et al* 1978). Also there are a few results on bounds and the existence of limits for the partition function (Whittington 1975). One can also make contact with surface magnetism through the $D_S \to 0$ limit of D_S-component spin systems where, in this limit, the coefficients in high-temperature expansions of the layer and surface susceptibilities turn out to be related to the numbers of self-avoiding walks, confined to a half-space, having respectively one or both of their ends in the bounding plane (Barber *et al* 1978).

In this paper we deal with the relationship between the foregoing model and one in which the walk, while interacting with the plane, is not confined to lie on one side of that plane. Adsorption of a polymer at a liquid–liquid interface probably lies somewhere between these two models.

We consider the D-dimensional hypercubic lattice ($D \geq 2$), whose vertices are points in D-dimensional Euclidean space with integer coordinates $z = (x, \ldots, y)$. An n-step walk on the lattice is a sequence of vertices $w = \{z_0, z_1, \ldots, z_n\}$ such that z_i and z_{i+1} differ by unity in exactly one of their coordinates. The walk is self-avoiding if no two of the z_i are identical; and, for brevity, we call it an n-SAW. Let $\mathscr{A}_{nv}$ be the set of n-SAWS with $z_0 = \mathbf{0}$ (i.e. which start at the origin) and with exactly $v+1$ vertices in the hyperplane $x = 0$. We say that the walk *visits* the hyperplane $v+1$ times. Let $\mathscr{A}^+_{nv}$ be the subset of $\mathscr{A}_{nv}$ such that $x_i \geq 0$ for all $i = 0, 1, \ldots, n$ (i.e. the x component of every vertex on the walk is non-negative). We shall call these walks *positive*. We write a_{nv} and

a_{nv}^{+} for the number of n-SAWs in $\mathscr{A}_{nv}$ and $\mathscr{A}_{nv}^{+}$ respectively, and we define the generating functions

$$A_n(\omega)=\sum_{v=0}^{n} a_{nv}\,\mathrm{e}^{v\omega}, \tag{1.1}$$

$$A_n^{+}(\omega)=\sum_{v=0}^{n} a_{nv}^{+}\,\mathrm{e}^{v\omega}. \tag{1.2}$$

We shall prove in § 2 the following rigorous results.

(i) The limits

$$A(\omega)=\lim_{n\to\infty} n^{-1}\log A_n(\omega), \tag{1.3}$$

$$A^{+}(\omega)=\lim_{n\to\infty} n^{-1}\log A_n^{+}(\omega), \tag{1.4}$$

exist for all ω.

(ii) These limits are convex non-decreasing continuous functions of ω satisfying the inequalities

$$\max(\kappa,\kappa'+\omega)\leqslant A^{+}(\omega)\leqslant A(\omega)\leqslant\max(\kappa,\kappa+\omega), \tag{1.5}$$

where κ is the connective constant of the D-dimensional lattice and κ' is the connective constant of the corresponding (D-1)-dimensional lattice (for a definition of the connective constant, see Hammersley (1957)).

(iii) There exist critical values ω_0 and ω_0^{+} defined by

$$\omega_0=\sup\{\omega: A(\omega)=\kappa\},\qquad \omega_0^{+}=\sup\{\omega: A^{+}(\omega)=\kappa\} \tag{1.6}$$

and

$$A(\omega)>A^{+}(\omega)\qquad \text{if } \omega>\omega_0. \tag{1.7}$$

(iv) These critical values satisfy

$$0\leqslant\omega_0\leqslant\omega_0^{+}\leqslant\kappa-\kappa', \tag{1.8}$$

$$\omega_0^{+}-\omega_0\geqslant\frac{[\log(1+\mathrm{e}^{-2\kappa})]\log 2}{4\kappa+4\log(1+\mathrm{e}^{-2\kappa})}. \tag{1.9}$$

It follows from these results that $A(\omega)=A^{+}(\omega)=\kappa$ for $\omega\leqslant 0$ and so remain constant in that range, while $A(\omega)$ and $A^{+}(\omega)$ are strictly increasing functions of ω for $\omega>\omega_0$ and $\omega>\omega_0^{+}$ respectively. Hence $A(\omega)$ and $A^{+}(\omega)$ must be non-analytic at $\omega=\omega_0$ and $\omega=\omega_0^{+}$ respectively. The foregoing results may be compared with previous work (Whittington 1975): namely that (for $D=3$)

$$\max(\kappa,\kappa'+\omega)\leqslant\liminf_{n\to\infty} n^{-1}\log A_n^{+}(\omega)$$
$$\leqslant\limsup_{n\to\infty} n^{-1}\log A_n^{+}(\omega)\leqslant\max(\kappa,\kappa+\omega), \tag{1.10}$$

which, of course, implied the existence and constancy of $A^{+}(\omega)=\kappa$ for $\omega\leqslant 0$.

The inequality (1.9) is sufficient to prove rigorously that the two models have different phase transition points. But numerically, it is a weak result: the best numerical estimates of κ inserted into (1.9) yield

$$\omega_0^+ - \omega_0 \geq \begin{array}{ll} 0.0211 & \text{when } D=2, \\ 0.0049 & \text{when } D=3, \end{array} \tag{1.11}$$

which may be contrasted with the computer estimates of ω_0 and ω_0^+ given below. We may also note from (1.8) that ω_0 and ω_0^+ must converge to zero as $D \to \infty$, because $\kappa - \kappa' \to 0$ as $D \to \infty$. We believe that $\omega_0 = 0$ for all values of $D \geq 2$, but we have been unable to prove this.

The upper bounds for ω_0 and ω_0^+ given in (1.8) can be strengthened slightly to

$$\omega_0^+ \leq 2\kappa - \kappa' - \sinh^{-1}(\tfrac{1}{2}e^\kappa), \tag{1.12}$$

$$\omega_0 \leq 2\kappa - \kappa' - \sinh^{-1}\cosh\kappa. \tag{1.13}$$

Numerically, (1.12) gives

$$\omega_0^+ \leq 0.8503 \quad \text{for } D=2, \qquad \omega_0^+ \leq 0.5311 \quad \text{for } D=3, \tag{1.14}$$

and (1.13) gives

$$\omega_0 \leq 0.7407 \quad \text{for } D=2, \qquad \omega_0 \leq 0.4900 \quad \text{for } D=3. \tag{1.15}$$

These may be compared with (1.8), which yields

$$\omega_0^+ \leq 0.9702 \quad \text{for } D=2, \qquad \omega_0^+ \leq 0.5738 \quad \text{for } D=3, \tag{1.16}$$

or with (1.8) and (1.9) combined, which yield

$$\omega_0 \leq 0.9491 \quad \text{for } D=2, \qquad \omega_0 \leq 0.5689 \quad \text{for } D=3. \tag{1.17}$$

The corresponding theory for walks that are not necessarily self-avoiding is much simpler and exact results can be found (Hammersley 1982). If bars are used to denote the corresponding expressions for Pólya random walks, then $\bar{\omega}_0 = 0$ and $\bar{\omega}_0^+ = \log[2D/(2D-1)]$.

There have been a number of attempts to estimate ω_0^+ and how $A^+(\omega)$ depends on ω, using series analysis techniques (e.g. Ma *et al* 1978 and references therein). In § 3 we report exact values of a_{nv} and a_{nv}^+ for $n \leq 21$ on the square lattice ($D = 2$) and for $n \leq 14$ for the simple cubic lattice ($D = 3$). We use standard ratio techniques (see e.g. Gaunt and Guttmann 1974) to estimate $A(\omega)$ and $A^+(\omega)$ and thence ω_0 and ω_0^+. These estimates suggest that $\omega_0 < 0.04$ for $D = 2$ and $\omega_0 < 0.03$ for $D = 3$. The numerical data are consistent with the conjecture $\omega_0 = 0$ in both cases. We estimate that ω_0^+ lies between 0.5 and 0.6 for $D = 2$ (cf $\omega_0^+ \simeq 0.37$ for $D = 3$ (Ma *et al* 1978)).

2. Proof of results

The sets $\mathcal{A}_{nv}$ and $\mathcal{A}_{nv}^+$ are difficult to handle directly. Instead we approach them indirectly through the more tractable sets $\mathcal{B}_{nv}$ and $\mathcal{B}_{nv}^+$ defined below. We recall, in these definitions, that an n-SAW is a sequence of distinct points $w = \{z_0, z_1, \ldots, z_n\}$ with $z_0 = \mathbf{0}$, and that x_i and y_i respectively denote the first and last coordinates of the point z_i.

Let $\mathcal{C}_n$ denote the set of n-SAWs that satisfy

$$0 = y_0 \leq y_i < y_n \qquad (i = 0, 1, \ldots, n-1) \tag{2.1}$$

and let $\mathscr{B}_n$ denote the set of n-SAWS that satisfy (2.1) and the additional condition

$$0 = x_0 = x_n. \tag{2.2}$$

Let $\mathscr{B}_n^+$ be the set of n-SAWS that belong to $\mathscr{B}_n$ and also satisfy

$$0 = x_0 \leq x_i \qquad (i = 1, 2, \ldots, n). \tag{2.3}$$

Then define $\mathscr{B}_{nv}$ and $\mathscr{B}_{nv}^+$ to be the subsets of $\mathscr{B}_n$ and $\mathscr{B}_n^+$ respectively that have precisely $v+1$ visits. We write b_{nv} and b_{nv}^+ for the number of n-SAWS in $\mathscr{B}_{nv}$ and $\mathscr{B}_{nv}^+$ respectively. Finally define the generating functions

$$B_n(\omega) = \sum_{v=0}^{n} b_{nv}\, e^{v\omega}, \qquad B_n^+(\omega) = \sum_{v=0}^{n} b_{nv}^+\, e^{v\omega}. \tag{2.4}$$

2.1.

We first establish the existence of the limits

$$B(\omega) = \lim_{n\to\infty} n^{-1} \log B_n(\omega), \qquad B^+(\omega) = \lim_{n\to\infty} n^{-1} \log B_n^+(\omega). \tag{2.5}$$

The proof is the same for both limits, so we deal only with $B(\omega)$.

Let $w = \{z_0, z_1, \ldots, z_n\}$ be a given n-SAW belonging to $\mathscr{B}_{nv}$, and let $w' = \{z'_0, z'_1, \ldots, z'_{n'}\}$ be a given n'-SAW belonging to $\mathscr{B}_{n'v'}$, where n' and v' are any other values of n and v. Remembering that $z'_0 = \mathbf{0}$, consider the walk

$$w \oplus w' = \{z_0, z_1, \ldots, z_n, z_n + z'_1, z_n + z'_2, \ldots, z_n + z'_{n'}\}. \tag{2.6}$$

The notation $w \oplus w'$, which we shall use hereafter without further explicit mention, indicates that the walk w' has been shifted bodily without rotation so that its first point coincides with the last point of w. The two walks combined in this way form an $(n+n')$-SAW, because (2.1) ensures that w cannot intersect the shifted w'. Moreover (2.2) ensures that $w \oplus w'$ has precisely $v + v' + 1$ visits. Hence $w \oplus w'$ is a member of $\mathscr{B}_{n+n',v+v'}$. Each given pair of walks w and w' leads to a distinct $w \oplus w'$ in $\mathscr{B}_{n+n',v+v'}$, and therefore

$$b_{nv} b_{n'v'} \leq b_{n+n',v+v'}. \tag{2.7}$$

Hence from (2.4)

$$B_n(\omega) B_{n'}(\omega) \leq \sum_{v=0}^{n+n'} (v+1) b_{n+n',v}\, e^{v\omega} \leq (n + n' + 1) B_{n+n'}(\omega), \tag{2.8}$$

and therefore

$$\log B_n(\omega) + \log B_{n'}(\omega) \leq \log B_{n+n'}(\omega) + \log(n + n' + 1). \tag{2.9}$$

Also, there are at most $2D$ possible choices for the direction of any step in a SAW. So $b_{nv} \leq (2D)^n$, and thus

$$B_n(\omega) \leq \sum_{v=0}^{n} (2D)^n\, e^{v\omega} \leq (n+1)(2D\, e^{|\omega|})^n \leq (4D\, e^{|\omega|})^n. \tag{2.10}$$

So

$$\log B_n(\omega) \leq n \log(4D\, e^{|\omega|}). \tag{2.11}$$

Now (2.11) shows that, for each fixed ω, $-\log B_n(\omega)$ is bounded below by a linear function of n; and (2.9) shows that $-\log B_n(\omega)$ is a generalised subadditive function of n, because $\Sigma_{n=1}^{\infty} n^{-2}\log(n+1)$ is a convergent series. So we can now apply the theory of generalised subadditive functions (Hammersley 1962). This establishes the existence of the limit $B(\omega)$ in (2.5).

2.2.

The next step is to prove that

$$\lim_{n\to\infty} n^{-1}\log A_n(\omega) = \lim_{n\to\infty} n^{-1}\log B_n(\omega) \tag{2.12}$$

with a similar relation for A_n^+ and B_n^+. Since $\mathscr{B}_{nv}$ is a subset of $\mathscr{A}_{nv}$, we have $a_{nv} \geqslant b_{nv}$; and therefore (2.12) will be proved as soon as we establish that

$$\limsup_{n\to\infty} n^{-1}\log A_n(\omega) \leqslant \lim_{n\to\infty} n^{-1}\log B_n(\omega). \tag{2.13}$$

Consider any given member of $\mathscr{A}_{nv}$, say $w=\{z_0, z_1, \ldots, z_n\}$. The hyperplane $y=\max_i y_i$ is called the upper tangent of w, and the hyperplane $y=\min_i y_i$ is the lower tangent of w. Let j be the smallest integer such that $y_j=\min_i y_i$, and let k be the largest integer such that $y_k=\max_i y_i$. We call the initial segment $\{z_0, z_1, \ldots, z_j\}$ the *head* of w, and the final segment $\{z_k, z_{k+1}, \ldots, z_n\}$ the *tail* of w. We now employ a technique (Hammersley and Welsh 1962) for converting w into a member of the set $\mathscr{C}_{n+1}$ defined in (2.1). We reflect the head of w in the lower tangent of w and the tail of w in the upper tangent of w. This gives a new walk w'. We then repeat the process on w' (i.e. we reflect the head of w' in the lower tangent of w' and the tail of w' in the upper tangent of w'); and we continue in this fashion until eventually we obtain a walk w'' which is unchanged by the operation, because the first point of w'' lies on the lower tangent of w'' and the last point of w'' lies on the upper tangent of w''. Thus w'' satisfies $y_0'' \leqslant y_i'' \leqslant y_n''$. It is easy to see that w'' has the same number of visits as the original walk w (because reflections do not change any x coordinate), and that w'' is a SAW. The point z_0'' may no longer be at the origin, but it must lie on the hyperplane $x=0$, and so, by a bodily shift of the whole of w'' in the direction of the y axis, we can bring the first point of w'' to the origin without altering the number of visits on w''. Finally we add an extra step in the direction of the y axis to the end of w''. The resulting walk, denoted by w^*, will be a member of $\mathscr{C}_{n+1}$; and w^* will have either $v+1$ or $v+2$ visits, the latter possibility only arising if the extra step at the end of w'' created an extra visit.

In general, starting from two different members of $\mathscr{A}_{nv}$, we may get the same walk w^*; but it can be shown (Hammersley and Welsh 1962) that at most $e^{c\sqrt{n}}$ different members of $\mathscr{A}_{nv}$ can lead to the same w^* in $\mathscr{C}_{n+1}$, where c is some absolute constant. Hence

$$a_{nv} \leqslant e^{c\sqrt{n}} \max(c_{n+1,v}, c_{n+1,v+1}), \tag{2.14}$$

where $c_{n+1,v}$ is the number of members of $\mathscr{C}_{n+1}$ having precisely $v+1$ visits. Hence

$$A_n(\omega) \leqslant e^{c\sqrt{n}+|\omega|} C_{n+1}(\omega) \tag{2.15}$$

where

$$C_{n+1}(\omega) = \sum_{v=0}^{n} c_{n+1,v}\, e^{v\omega}. \tag{2.16}$$

The next step is to partition $\mathscr{C}_n$ into subclasses, placing two walks in the same subclass if they have the same final point. Since an n-SAW, starting from the origin, must be entirely enclosed in a hypercube of side $2n$ centred at the origin, there will be at most $(2n+1)^D$ subclasses. Let c_{nvk} denote the number of n-SAWS with $v+1$ visits in the kth subclass, where $k=1, 2, \ldots, K \leq (2n+1)^D$. For given k, consider two walks w_1 and w_2 both belonging to the kth subclass of $\mathscr{C}_n$ and having v_1+1 and v_2+1 visits respectively. Let w_2' denote the reflection of w_2 in the upper tangent of w_2. We regard w_2' as being read backwards, i.e. the first point of w_2' is the reflection of the last point of w_2 and the last point of w_2' is the reflection of the first point of w_2. Let w_3 be the walk obtained by following first w_1 and then w_2'. This will be a $2n$-SAW with either v_1+v_2+1 visits or v_1+v_2+2 visits (according as the last point of w_1 is or is not on the hyperplane $x=0$). Moreover, the last point of w_3 will be on the hyperplane $x=0$; and so, if we add an extra step in the direction of the y axis to the end of w_3, we shall obtain a member of $\mathscr{B}_{2n+1}$ with v_1+v_2+2 or v_1+v_2+3 visits. Each distinct pair of walks w_1 and w_2 will yield a distinct member of $\mathscr{B}_{2n+1}$ in this way. So

$$c_{nv_1k}c_{nv_2k} \leq \max(b_{2n+1,v_1+v_2+1}, b_{2n+1,v_1+v_2+2}). \tag{2.17}$$

Write

$$C_n(\omega, k) = \sum_{v=0}^{n} c_{nvk}\, e^{v\omega}. \tag{2.18}$$

From (2.17) we obtain

$$\begin{aligned} C_n^2(\omega, k) &\leq \sum_{v_1=0}^{n} \sum_{v_2=0}^{n} \max(b_{2n+1,v_1+v_2+1}, b_{2n+1,v_1+v_2+2}) \exp[(v_1+v_2)\omega] \\ &\leq e^{2|\omega|} \sum_{v=0}^{2n+2} (v+1) b_{2n+1,v}\, e^{v\omega} \\ &\leq (2n+3) e^{2|\omega|} B_{2n+2}(\omega); \end{aligned} \tag{2.19}$$

and hence, by Cauchy's inequality,

$$\begin{aligned} C_n^2(\omega) &= \left(\sum_{k=1}^{K} C_n(\omega, k)\right)^2 \leq \sum_{k=1}^{K} 1^2 \sum_{k=1}^{K} C_n^2(\omega, k) \\ &\leq K^2(2n+3)\, e^{2|\omega|} B_{2n+2}(\omega) \\ &\leq (2n+3)^{2D+1}\, e^{2|\omega|} B_{2n+2}(\omega). \end{aligned} \tag{2.20}$$

From (2.15) and (2.20)

$$A_n(\omega) \leq (2n+5)^{D+1/2} \exp(c\sqrt{n} + 2|\omega|) B_{2n+4}^{1/2}(\omega), \tag{2.21}$$

and hence

$$\limsup_{n\to\infty} n^{-1} \log A_n(\omega) \leq \limsup_{n\to\infty} (2n)^{-1} \log B_{2n+4}(\omega) = \lim_{n\to\infty} n^{-1} \log B_n(\omega), \tag{2.22}$$

because the limit on the right-hand side of (2.22) exists. This proves (2.13) and hence (2.12). The proof of the analogous relation for $A_n^+(\omega)$ is exactly similar, because the foregoing argument does not affect any inequality of the type $x_i \geq 0$. Thus we may define the limit functions

$$\begin{aligned} A(\omega) &= \lim_{n\to\infty} n^{-1} \log A_n(\omega) = \lim_{n\to\infty} n^{-1} \log B_n(\omega), \\ A^+(\omega) &= \lim_{n\to\infty} n^{-1} \log A_n^+(\omega) = \lim_{n\to\infty} n^{-1} \log B_n^+(\omega). \end{aligned} \tag{2.23}$$

2.3.

It is obvious from the definition of $A_n(\omega)$ in (1.1) that $A_n(\omega)$ is a non-decreasing function of ω, and, for fixed n, $A_n(\omega)$ is a polynomial in e^{ω} and so bounded in any fixed closed interval of values of ω. Consequently (Hardy *et al* 1934), to establish that $\log A_n(\omega)$ is a convex function of ω, it is enough to prove that

$$\tfrac{1}{2} \log A_n(\omega_1) + \tfrac{1}{2} \log A_n(\omega_2) \geqslant \log A_n(\tfrac{1}{2}\omega_1 + \tfrac{1}{2}\omega_2) \tag{2.24}$$

for all real ω_1 and ω_2. But, by Cauchy's inequality

$$\begin{aligned} A_n(\omega_1)A_n(\omega_2) &= \sum_{v=0}^{n} a_{nv} \exp(v\omega_1) \sum_{v=0}^{n} a_{nv} \exp(v\omega_2) \\ &\geqslant \left(\sum_{v=0}^{n} a_{nv} \exp[\tfrac{1}{2}v(\omega_1 + \omega_2)] \right)^2 = A_n^2(\tfrac{1}{2}\omega_1 + \tfrac{1}{2}\omega_2), \end{aligned} \tag{2.25}$$

which proves (2.24). Now, if the limit of a sequence of convex functions exists, that limit is also a convex function. Hence $A(\omega)$, and similarly $A^+(\omega)$, defined by (2.23) are both non-decreasing convex functions of ω for all real ω.

2.4.

In this section we shall establish the inequalities (1.5). Consider the set $\mathcal{P}_n$ of n-SAWS $w = \{z_0, z_1, \ldots, z_n\}$ that satisfy $|z_0 - z_n| = 1$, which implies that n must be odd; and let p_n be the number of members of $\mathcal{P}_n$. It is known (Hammersley 1961) that

$$\lim_{n\to\infty} n^{-1} \log p_n = \kappa \qquad (n \text{ odd}). \tag{2.26}$$

Suppose w belongs to $\mathcal{P}_n$, and let z_j be the first point of w such that $x_j = \min_i x_i$. Write $\zeta = -z_j + (1, 0, \ldots, 0)$ and consider

$$w' = \{\mathbf{0}, z_j + \zeta, z_{j+1} + \zeta, \ldots, z_n + \zeta, z_0 + \zeta, z_1 + \zeta, \ldots, z_{j-1} + \zeta, z_{j-1} - z_j\}. \tag{2.27}$$

It is easy to verify that $w' \in \mathcal{A}_{n+2,1}^+$. Moreover, distinct $w \in \mathcal{P}_n$ yield distinct $w' \in \mathcal{A}_{n+2,1}^+$. Suppose $\omega \leqslant 0$. Then, if n is odd,

$$p_{n-2}\, e^{\omega} \leqslant a_{n1}^+\, e^{\omega} \leqslant A_n^+(\omega) \leqslant A_n(\omega) \leqslant A_n(0) = s_n, \tag{2.28}$$

where s_n is the number of n-SAWS. Since

$$\lim_{n\to\infty} n^{-1} \log s_n = \kappa \tag{2.29}$$

by the definition of the connective constant κ, we have

$$\kappa \leqslant A^+(\omega) \leqslant A(\omega) \leqslant \kappa \qquad (\omega \leqslant 0) \tag{2.30}$$

on taking logarithms of (2.28), dividing by n, and letting $n \to \infty$ through odd values of n.

Suppose, on the other hand, that $\omega \geqslant 0$. Let s'_n denote the number of n-SAWS wholly confined to the $(D-1)$-dimensional hyperplane $x=0$. Then, again by the definition of κ',

$$\lim_{n\to\infty} n^{-1} \log s'_n = \kappa'. \tag{2.31}$$

But $s'_n = a^+_{nn}$. Hence

$$s'_n\, e^{n\omega} = a^+_{nn}\, e^{n\omega} \leqslant A^+_n(\omega) \leqslant A_n(\omega) \leqslant s_n\, e^{n\omega}. \tag{2.32}$$

Take logarithms of (2.32), divide by n, and let $n\to\infty$. We obtain

$$\kappa' + \omega \leqslant A^+(\omega) \leqslant A(\omega) \leqslant \kappa + \omega \qquad (\omega \geqslant 0) \tag{2.33}$$

and now (1.5) follows from (2.30) and (2.33) combined.

Further, (1.5) shows that $A^+(\omega)$ and $A(\omega)$ are bounded in any closed interval of values of ω. It follows from the convexity of these bounded functions that they are actually continuous convex functions of ω, possessing left-hand and right-hand derivatives for all finite ω (Hardy *et al* 1934).

2.5.

We now return to a consideration of the sets $\mathcal{B}_{nv}$ and $\mathcal{B}^+_{nv}$. Consider an n-SAW $w \in \mathcal{B}_{nv}$. We classify the points of w as either visits, denoted by V, or non-visits, denoted by N. Under this classification the sequence $w=\{z_0, z_1, \ldots, z_n\}$ can be written as an ordered sequence of symbols V or N, in which we may bracket together like symbols into runs: for example, $w = (\mathrm{VVV})(\mathrm{NN})(\mathrm{V})(\mathrm{NNN})\ldots(\mathrm{VV}) = \mathrm{V}^3\mathrm{N}^2\mathrm{V}\mathrm{N}^3\ldots\mathrm{V}^2$. Each bracketed run of V-symbols will be called an *incursion* and each bracketed run of N-symbols will be called an *excursion*. Since z_0 and z_n are necessarily both visits, the first and last symbols in w must both be V. Hence w is an alternating sequence of incursions and excursions, beginning and ending with an incursion. So, if w has $u \geqslant 0$ excursions it will have $u+1$ incursions and *vice versa*. We write $\mathcal{B}_{nvu}$ for the subset of $\mathcal{B}_{nv}$ consisting of n-SAWS with exactly $v+1$ visits and $u+1$ incursions. Reference to the argument used to prove (2.7) also shows that

$$b_{nvu} b_{n'v'u'} \leqslant b_{n+n',v+v',u+u'} \tag{2.34}$$

where b_{nvu} is the number of members of $\mathcal{B}_{nvu}$. Similarly, writing b^+_{nvu} for the number of members of $\mathcal{B}^+_{nvu}$, the subset of $\mathcal{B}_{nvu}$ satisfying $x_i \geqslant 0$, we have

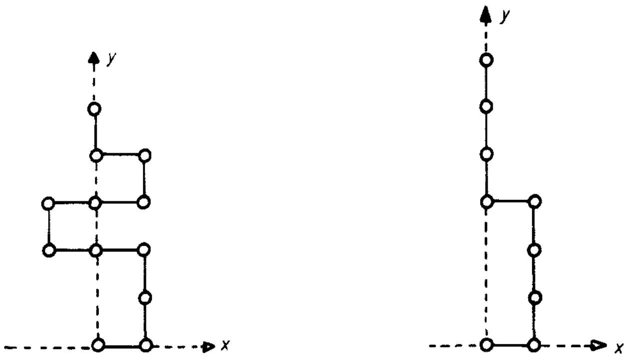
$$b^+_{nvu} b^+_{n'v'u'} \leqslant b^+_{n+n',v+v',u+u'}. \tag{2.35}$$

We shall now establish the necessary and sufficient conditions that $\mathcal{B}_{nvu}$ shall not be empty. Since $x_0=0$, $y_{n-1}<y_n$ by (2.1) and (2.2), and $|z_n - z_{n-1}|=1$, we must have $x_{n-1}=0$. So z_{n-1} is also a visit, and the final incursion of w must contain at least two visits. The remaining incursions each contain at least one visit. Hence w has at least $u+2$ visits. Thus $v+1 \geqslant u+2$ is necessary. If any excursion contained only one non-visit, the walk could not be self-avoiding because it would have to return upon its track in leaving and entering the hyperplane $x=0$. Hence each excursion contains at least two non-visits; and the total number of points on w must therefore satisfy $n+1 \geqslant v+1+2u$, which is another necessary condition. If $u=0$, there are no excur-

sions so $n+1=v+1$. Hence

$$\begin{aligned} &\textit{either } u=0 \text{ and } v=n \\ &\textit{or} \quad 1\leqslant u<v\leqslant n-2u \end{aligned} \tag{2.36}$$

are necessary conditions for $\mathscr{B}_{nvu}$ to be non-empty. We shall show that the conditions (2.36) are also sufficient. Since we can always find, trivially, an n-SAW lying wholly in the hyperplane $x=0$ and satisfying (2.1) and (2.2), the first alternative in (2.36) is a sufficient condition. So let n, v, u be any integers satisfying the second alternative in (2.36). Then there exist non-negative integers k, l, m such that $u=l+1$, $v=u+1+m$, $n=2u+v+k$. The walk $w=\mathrm{VN}^{k+2}(\mathrm{VN}^2)^l\mathrm{V}^{m+2}$ has the required values of n, v, u; and it can be realised as a member of $\mathscr{B}_{nvu}$ by taking its steps in the directions of the x and y axes only, as illustrated for two particular cases in the diagrams below.



$k=1$, $l=2$, $m=0$, $k=2$, $l=0$, $m=2$.

In the case of $\mathscr{B}^+_{nvu}$, each incursion (except perhaps the first) must contain at least two visits, for otherwise the walk would not be self-avoiding. So $v+1\geqslant 2(u+1)-1$ is necessary. The remaining conditions in (2.36) also hold because $\mathscr{B}^+_{nvu}$ is a subset of $\mathscr{B}_{nvu}$. We find by the methods used above that the necessary and sufficient conditions for $\mathscr{B}^+_{nvu}$ to be not empty are

$$\begin{aligned} &\textit{either } u=0 \text{ and } v=n \\ &\textit{or} \quad 2\leqslant 2u\leqslant v\leqslant n-2u. \end{aligned} \tag{2.37}$$

2.6.

Now let ∇ denote the set of pairs of real numbers (α, β) such that

$$0\leqslant\alpha\leqslant 1, \qquad 0\leqslant\beta\leqslant 1, \qquad \alpha+\beta=1; \tag{2.38}$$

let Δ be the set of pairs of real numbers (p, q) such that

$$\textit{either } (p,q)=(0,1) \qquad \textit{or } 0<p<q\leqslant 1-2p; \tag{2.39}$$

and let Δ^+ be the set of pairs of real numbers (p, q) such that

$$\textit{either } (p,q)=(0,1) \qquad \textit{or } 0<2p\leqslant q\leqslant 1-2p. \tag{2.40}$$

Thus, in terms of the points $\Delta_0=(0,0)$, $\Delta_1=(0,1)$, $\Delta_2=(\frac{1}{3},\frac{1}{3})$, $\Delta_3=(\frac{1}{4},\frac{1}{2})$ in the (p,q) plane,

(i) Δ consists of the interior of the triangle $\Delta_0\Delta_1\Delta_2$ together with the interior of the side $\Delta_1\Delta_2$ and the point Δ_1;

(ii) Δ^+ consists of the interior of the triangle $\Delta_0\Delta_1\Delta_3$ together with the interiors of the sides $\Delta_1\Delta_3$ and $\Delta_0\Delta_3$ and the points Δ_1 and Δ_3.

Comparison of (2.36) and (2.39) shows that $b_{nvu}>0$ or $b_{nvu}=0$ according as $(u/n, v/n)$ does or does not belong to Δ. Similarly $b^+_{nvu}>0$ or $b^+_{nvu}=0$ according as $(u/n, v/n)$ does or does not belong to Δ^+.

Let p, q be rational numbers such that $(p,q)\in\Delta$, and write I_{pq} for the set of integers n such that np and nq are both integers. Evidently I_{pq} is a principal ideal in the set of all integers. Suppose that n and n' are positive integers belonging to I_{pq}. From (2.34) we have

$$\begin{aligned}0 &\leq \log b_{n,nq,np}+\log b_{n',n'q,n'p}\\ &\leq \log b_{(n+n'),(n+n')q,(n+n')p}\leq \log s_{n+n'}.\end{aligned} \tag{2.41}$$

This asserts that $\log b_{n,nq,np}$ is a superadditive function of n for positive $n\in I_{pq}$. Hence there exists a number $\theta(q,p)$ such that

$$0\leq \theta(q,p)=\lim n^{-1}\log b_{n,nq,np}\leq \kappa, \tag{2.42}$$

where the limit in (2.42) is taken as $n\to\infty$ through positive integers belonging to I_{pq}.

Moreover, if p', q' are rational numbers such that $(p',q')\in\Delta$, and n is a positive integer belonging to both I_{pq} and $I_{p'q'}$, then by (2.34)

$$\log b_{n,nq,np}+\log b_{n,nq',np'}\leq \log b_{2n,n(p+p'),n(q+q')}. \tag{2.43}$$

Divide (2.43) by $2n$ and let $n\to\infty$ through positive integers belonging to the intersection of I_{pq} and $I_{p'q'}$ and $I_{(p+p')/2,(q+q')/2}$. From (2.42) we obtain

$$0\leq \tfrac{1}{2}\theta(q,p)+\tfrac{1}{2}\theta(q',p')\leq \theta(\tfrac{1}{2}q+\tfrac{1}{2}q', \tfrac{1}{2}p+\tfrac{1}{2}p')\leq \kappa. \tag{2.44}$$

It follows (Hardy *et al* 1934) that

$$0\leq \alpha\theta(q,p)+\beta\theta(q',p')\leq \theta(\alpha q+\beta q', \alpha p+\beta p')\leq \kappa \tag{2.45}$$

for all rational $(\alpha,\beta)\in\nabla$ and all rational $(p,q)\in\Delta$ and all rational $(p',q')\in\Delta$. We can now extend the definition of $\theta(q,p)$ to all real $(p,q)\in\Delta$ by continuity: namely, in the interior of Δ, it is the continuous concave function of p, q (concave in both variables considered as a two-dimensional vector) that agrees with the previously defined values of θ at rational p, q; while, on the interior of the side $\Delta_1\Delta_2$, it is the continuous concave function of $q=1-2p$ (concave in the single variable q) that agrees with the previously defined values of $\theta(q, \frac{1}{2}-\frac{1}{2}q)$ at rational q satisfying $\frac{1}{3}<q<1$.

If (p,q) does not belong to Δ, we have $b_{n,nq,np}=0$, either in accordance with the case $b_{nvu}=0$ or by definition for other (e.g. irrational) values of p, q; and hence we define $\theta(q,p)=-\infty$ for (p,q) not belonging to Δ.

So now $\theta(q,p)$ is defined for all p, q, and it is a concave function of these two variables considered as a two-dimensional vector. Also $\theta(q,p)$ is finite on the whole of Δ, and continuous in the interior of Δ. But it is not continuous on the boundary of Δ.

Similarly we can define a concave function

$$\theta^+(q,p)=\lim n^{-1}\log b^+_{n,nq,np} \tag{2.46}$$

which satisfies $0 \leqslant \theta^+(q, p) \leqslant \kappa$ for $(p, q) \in \Delta^+$ and $\theta^+(q, p) = -\infty$ for (p, q) not belonging to Δ^+; and $\theta^+(q, p)$ has similar properties of continuity with respect to Δ^+ instead of Δ.

2.7.

Next we define

$$\theta(q) = \sup_p \theta(q, p), \qquad \theta^+(q) = \sup_p \theta^+(q, p). \tag{2.47}$$

Suppose we are given $(\alpha, \beta) \in \nabla$ and any prescribed $\varepsilon > 0$. Then for given q, q' we can find p, p' depending on q, q' respectively, such that

$$\theta(q) \leqslant \theta(q, p) + \varepsilon, \qquad \theta(q') \leqslant \theta(q', p') + \varepsilon. \tag{2.48}$$

Hence, by (2.45) and the fact that $\alpha + \beta = 1$,

$$\begin{aligned}\alpha\theta(q) + \beta\theta(q') &\leqslant \alpha\theta(q, p) + \beta\theta(q', p') + \varepsilon \\ &\leqslant \theta(\alpha q + \beta q', \alpha p + \beta p') + \varepsilon \leqslant \theta(\alpha q + \beta q') + \varepsilon;\end{aligned} \tag{2.49}$$

and since $\varepsilon > 0$ is arbitrary in (2.49) we conclude that $\theta(q)$ is a concave function of q, namely

$$\alpha\theta(q) + \beta\theta(q') \leqslant \theta(\alpha q + \beta q'). \tag{2.50}$$

Moreover, if $0 < q \leqslant 1$, there exists a value of p such that $(p, q) \in \Delta$ by virtue of (2.39). Hence, by (2.42), we have

$$0 \leqslant \theta(q) \leqslant \kappa \qquad (0 < q \leqslant 1). \tag{2.51}$$

If either $q \leqslant 0$ or $q > 1$, no (p, q) can lie in Δ, and so $\theta(q) = -\infty$ when $q \leqslant 0$ or $q > 1$. The boundedness of $\theta(q)$ in $0 < q \leqslant 1$ and the concavity in (2.50) ensures that $\theta(q)$ is a continuous function of q for $0 < q < 1$.

Similarly $\theta^+(q)$ is a concave function for all q; it is continuous for $0 < q < 1$ and bounded for $0 < q \leqslant 1$; and $\theta^+(q) = -\infty$ when $q \leqslant 0$ or $q > 1$.

2.8.

We shall next prove that

$$A(\omega) = \sup_q \{\theta(q) + q\omega\}, \qquad A^+(\omega) = \sup_q \{\theta^+(q) + q\omega\}; \tag{2.52}$$

that is to say, A and A^+ are the so-called *maximum transforms* of θ and θ^+ respectively.

Prescribe an arbitrary $\varepsilon > 0$, and consider any given rational $(p, q) \in \Delta$. Then, for all sufficiently large positive $n \in I_{pq}$ we have by (2.42)

$$\exp[n\theta(q, p) - n\varepsilon] \leqslant b_{n,nq,np} \leqslant b_{n,nq}. \tag{2.53}$$

Hence

$$B_n(\omega) = \sum_{v=0}^{n} b_{nv}\, e^{n\omega} \geqslant b_{n,nq}\, e^{nq\omega} \geqslant \exp[n\theta(q, p) - n\varepsilon + nq\omega]. \tag{2.54}$$

Take logarithms of (2.54), divide by n, let $n \to \infty$ through values of I_{pq}, and use (2.23) to obtain

$$A(\omega) \geqslant \theta(q, p) + q\omega - \varepsilon. \tag{2.55}$$

Then let $\varepsilon \to 0$, so that

$$A(\omega) \geqslant \theta(q, p) + q\omega. \tag{2.56}$$

Now (2.56) is true for all rational $(p, q) \in \Delta$, and hence it is true for all real $(p, q) \in \Delta$ by continuity, in view of the manner used in § 2.6 to define $\theta(q, p)$ for irrational $(p, q) \in \Delta$. Since (2.56) thus holds for all (p, q) when ω is fixed, we obtain

$$A(\omega) \geqslant \sup_{(p,q)} \{\theta(q, p) + q\omega\} = \sup_{q} \{\theta(q) + q\omega\}. \tag{2.57}$$

To establish the opposite inequality, we recall that superadditive functions approach their limit from below (Hammersley 1961). Hence, if n, v, u are any positive integers such that $b_{nvu} > 0$, we have $(u/n, v/n) = (p, q) \in \Delta$; and from (2.42)

$$n^{-1} \log b_{nvu} = n^{-1} \log b_{n,nq,np} \leqslant \theta(q, p) \leqslant \theta(q) = \theta(v/n). \tag{2.58}$$

Hence

$$b_{nvu} \leqslant \exp[n\theta(v/n)]. \tag{2.59}$$

This is also trivially true if $b_{nvu} = 0$. Hence

$$\begin{aligned} B_n(\omega) &= \sum_{v=0}^{n} \sum_{u=0}^{n} b_{nvu}\, \mathrm{e}^{v\omega} \\ &\leqslant (n+1)^2 \exp\left(n \max_{0 \leqslant v \leqslant n} \left\{\theta\left(\frac{v}{n}\right) + \frac{v}{n}\omega\right\}\right) \\ &\leqslant (n+1)^2 \exp\left(n \sup_{q} \{\theta(q) + q\omega\}\right). \end{aligned} \tag{2.60}$$

Taking logarithms of (2.60), dividing by n, and letting $n \to \infty$, we deduce from (2.23) that

$$A(\omega) \leqslant \sup_{q} \{\theta(q) + q\omega\}. \tag{2.61}$$

Thereupon (2.57) and (2.61) yield the first equation in (2.52). The other equation in (2.52) follows in the same way from a consideration of b^{+}_{nvu}, θ^{+} and Δ^{+}.

2.9.

In § 2.7 we showed that $\theta(q) = -\infty$ if either $q \leqslant 0$ or $q > 1$. Hence we can write (2.52) in the form

$$\begin{aligned} A(\omega) &= \sup_{0<q\leqslant 1} \{\theta(q) + q\omega\} \\ &= \max\left(\sup_{0<q\leqslant\varepsilon} \{\theta(q) + q\omega\},\ \sup_{\varepsilon\leqslant q\leqslant 1} \{\theta(q) + q\omega\}\right) \end{aligned} \tag{2.62}$$

for any $0 < \varepsilon < 1$. In (2.62) we take $\omega < 0$, and use (2.30) and (2.51) to obtain

$$\begin{aligned} \kappa &= \max\left(\sup_{0<q\leqslant\varepsilon} \{\theta(q) + q\omega\},\ \kappa + \varepsilon\omega\right) \\ &= \sup_{0<q\leqslant\varepsilon} \{\theta(q) + q\omega\} \leqslant \sup_{0<q\leqslant\varepsilon} \theta(q) \leqslant \kappa, \end{aligned} \tag{2.63}$$

because $\kappa+\varepsilon\omega<\kappa$ and $q\omega<0$. Since $\theta(q)$ is concave and continuous for $0<q\leq\varepsilon$ and $\varepsilon>0$ is arbitrary, (2.63) implies that

$$\lim_{q\to0+}\theta(q)=\kappa. \tag{2.64}$$

Similarly, from $A^+(\omega)$ and $\theta^+(q)$, we can show that

$$\lim_{q\to0+}\theta^+(q)=\kappa. \tag{2.65}$$

2.10.

Next define

$$\theta^*(q)=\begin{matrix}\kappa & \text{if } q=0,\\ \theta(q) & \text{if } q\neq0.\end{matrix} \tag{2.66}$$

Also define

$$A^*(\omega)=\sup_q\{\theta^*(q)+q\omega\}. \tag{2.67}$$

From (2.51) and (2.66) we have $\theta(q)\leq\theta^*(q)$, and hence (2.52) and (2.67) yield

$$A(\omega)\leq A^*(\omega). \tag{2.68}$$

On the other hand, by (2.66), (2.67), (2.52) and (1.5)

$$A^*(\omega)=\max\left(\sup_{q\neq0}\{\theta(q)+q\omega\},\kappa\right)\leq\max\left(\sup_q\{\theta(q)+q\omega\},A(\omega)\right)=A(\omega). \tag{2.69}$$

From (2.68) and (2.69) we deduce

$$A(\omega)=\sup_q\{\theta^*(q)+q\omega\}. \tag{2.70}$$

2.11.

Since $\theta(q)$ is concave for all q and continuous for $0<q<1$, we see from (2.64) and (2.66) that $\theta^*(q)$ is concave for all q and continuous for $0\leq q<1$. Hence (Hardy *et al* 1934) $\theta^*(q)$ possesses a right-hand derivative at $q=0$, namely

$$\theta_0=\lim_{q\to0+}q^{-1}\{\theta^*(q)-\kappa\}, \tag{2.71}$$

and

$$\theta^*(q)\leq\kappa+q\theta_0 \tag{2.72}$$

for all q. Now $A(\omega)$ is continuous for all ω; so, by the definition of ω_0 in (1.6),

$$\kappa=A(\omega_0)=\sup_q\{\theta^*(q)+q\omega_0\}. \tag{2.73}$$

Consider any $\theta_1<\theta_0$. According to (2.71) there exists some $q_1>0$ such that

$$\theta^*(q_1)>\kappa+q_1\theta_1. \tag{2.74}$$

Hence, by (2.73),

$$\kappa\geq\theta^*(q_1)+q_1\omega_0>\kappa+q_1(\theta_1+\omega_0), \tag{2.75}$$

which implies

$$\theta_1+\omega_0<0. \tag{2.76}$$

Since this is true for arbitrary $\theta_1<\theta_0$, we conclude that

$$\omega_0\leqslant-\theta_0. \tag{2.77}$$

On the other hand, $\theta^*(q)=-\infty$ for $q<0$ and $q>1$; so (2.70) yields

$$A(\omega)=\sup_{0\leqslant q\leqslant 1}\{\theta^*(q)+q\omega\}\leqslant\sup_{0\leqslant q\leqslant 1}\{\kappa+q(\theta_0+\omega)\}\leqslant\kappa+\theta_0+\omega \tag{2.78}$$

by (2.72). If $\omega>\omega_0$, the left-hand side of (2.78) is strictly greater than κ. Hence $\theta_0+\omega>0$ for any $\omega>\omega_0$, and therefore

$$\omega_0\geqslant-\theta_0. \tag{2.79}$$

From (2.77) and (2.79) and the fact that $\theta^*(q)=\theta(q)$ for $q>0$, we obtain

$$\omega_0=\lim_{q\to0+}q^{-1}(\kappa-\theta(q)). \tag{2.80}$$

Similarly, with only trivial and obvious changes of notation, we have

$$\omega_0^+=\lim_{q\to0+}q^{-1}(\kappa-\theta^+(q)), \tag{2.81}$$

and therefore

$$\omega_0^+-\omega_0=\lim_{q\to0+}q^{-1}(\theta(q)-\theta^+(q)). \tag{2.82}$$

2.12.

To prove (1.9), we need to find a positive lower bound for the right-hand side of (2.82). As a first step towards this end, we return to a study of the function $\theta^+(q,p)$. We begin by considering rational numbers p, q such that

$$0<q<1 \tag{2.83}$$

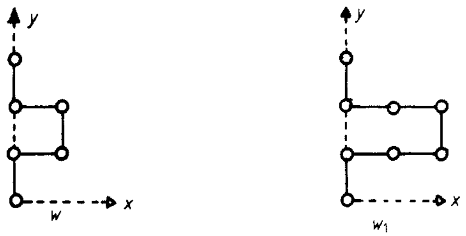
and

$$0<p<\min(\tfrac{1}{4}q,\tfrac{1}{2}-\tfrac{1}{2}q). \tag{2.84}$$

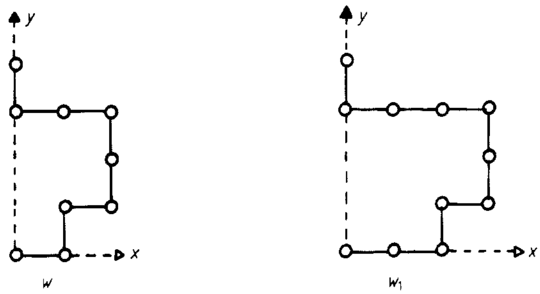
Since (2.84) is stronger than (2.40), we see that $(p,q)\in\Delta^+$. Suppose that n is a positive integer belonging to I_{pq}, and consider any given n-SAW w belonging to $\mathscr{B}^+_{n,nq,np}$. Then w has $n+1$ points, $nq+1$ visits, and $np+1$ incursions. We are going to modify w in two stages: in the first stage we shall replace w by another SAW w_1, and in the second stage we shall replace w_1 by a second new SAW w_2.

2.13.

To deal with the first stage from w to w_1, let the points of w be $w=\{z_0,z_1,\ldots,z_n\}$. We replace each z_i by $z_i+(1,0,\ldots,0)$ whenever z_i is not a visit, while those z_i that are visits are left unchanged. This breaks the SAW w; and to restore the property that successive points of a SAW are unit distance apart, we must interpolate some extra points $z_i+(1,0,\ldots,0)$ for all those values of $i<n$ such that z_i is either the first or the last point of an incursion of w, with the exception that $i=0$ is not to be treated in this way unless z_0 is the *last* point of an incursion. This gives the SAW w_1. The diagrams below illustrate the relationship between w and w_1.



Relationship between w and w_1 when z_0 is not the last point of an incursion.

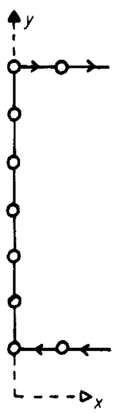


Relationship between w and w_1 when z_0 is the last point of an incursion.

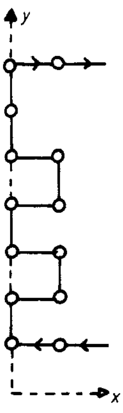
The number of extra points interpolated is twice the number of excursions in w; so w_1 has $n+2np+1$ points. It also has $nq+1$ visits and $np+1$ incursions because the number of visits and the number of incursions are both unchanged. Clearly w_1 is a SAW, because w is a SAW; and also w_1 satisfies all the conditions (2.1), (2.2) and (2.3). Hence $w_1 \in \mathscr{B}^{+}_{n+2np,nq,np}$.

2.14.

For the second stage of modification, we shall interpolate some further points in w_1 to obtain w_2. Consider any particular incursion in w_1 that has $k \geq 4$ visits in that incursion. Then we could insert $[\frac{1}{2}k]-1$ excursions into that incursion, given that each such extra excursion has exactly three steps, of which the first and third are parallel to the x axis and the second lies in the hyperplane $x=1$. The following diagram shows the situation for an incursion of w_1 in the particular case $k=7$.



Incursion of w_1 with $k=7$



Two possible excursions in w_1

These inserted excursions cannot destroy the self-avoidance of the new walk w_2, because in the construction of w_1 we shifted out of the way any points that might have interfered with these new excursions. We speak of *possible* new excursions because, as we shall see presently, in constructing w_2 from w_1 we shall only utilise some of these possibilities. Thus it is best to think in terms of the places where new excursions *might* be placed. If $k \geq 4$ is even, these places are fixed in the incursion, if the incursion is not the last incursion. On the other hand, if $k \geq 4$ is odd, we take these places to be as early on the incursion as possible (as in the diagram above). This ensures that the places are fixed when w_1 is given. The last incursion of w_1 requires an additional gloss, namely that the places are taken as early as possible on the last incursion whether or not $k \geq 4$ is even. This gloss ensures that, however many of the places we utilise for extra excursions, the resulting walk w_2 will still satisfy conditions (2.1), (2.2) and (2.3).

Suppose that w_1 has exactly e_k incursions with k visits each. The case $k = 1$ can only arise if z_0 is the last point of an incursion, so $e_1 = 0$ or 1. Counting up the number of visits and incursions on w_1, we have

$$\sum_{k\geq 1} ke_k = nq + 1, \qquad \sum_{k\geq 1} e_k = np + 1, \tag{2.85}$$

and hence

$$\sum_{k\geq 2} ke_k \geq nq, \qquad \sum_{k\geq 2} e_k \leq np + 1. \tag{2.86}$$

The number of places for possible extra excursions, in deriving w_2 from w_1, is therefore

$$\sum_{k\geq 4} ([\tfrac{1}{2}k]-1)e_k = \sum_{k\geq 2} ([\tfrac{1}{2}k]-1)e_k \geq \sum_{k\geq 2} (\tfrac{1}{2}k-2)e_k \geq \tfrac{1}{2}nq - 2np - 2. \tag{2.87}$$

Now let f and g be rational numbers such that

$$0 < f < g < \tfrac{1}{2}q - 2p, \tag{2.88}$$

this being possible in view of (2.84). Then, provided n is any sufficiently large positive integer belonging to the intersection of I_{pq} and I_{fg}, we can by virtue of (2.87) and (2.88) find ng fixed places on w_1 at which extra excursions could be placed; and we can choose any nf of these fixed places for the actual places at which extra excursions are to be inserted in deriving w_2 from w_1.

The walk w_2 obtained in this fashion will have the same number of visits as w_1, $2nf$ more points than w_1 and nf more excursions than w_1; and $w_2 \in \mathscr{B}^+_{n+2np+2nf,nq,np+nf}$. Further, each distinct choice of the nf places and each distinct member of $w \in \mathscr{B}^+_{n,nq,np}$, from which we originally started in § 2.12, will lead to a distinct $w_2 \in \mathscr{B}^+_{n+2np+2nf,nq,np+nf}$. Hence

$$\binom{ng}{nf} b^+_{n,nq,np} \leq b^+_{n+2np+2nf,\,nq,\,np+nf}, \tag{2.89}$$

because $\binom{ng}{nf}$ is the number of ways in which we could choose the nf places from amongst the ng available places. A straightforward calculation, based upon Stirling's formula for the factorial function, reveals

$$\lim_{n\to\infty} n^{-1} \log\binom{ng}{nf} = g[-\rho \log \rho - (1-\rho)\log(1-\rho)] \tag{2.90}$$

where

$$0 < \rho = f/g < 1. \tag{2.91}$$

Take logarithms of (2.89), divide by n, and let $n\to\infty$ through members of the intersection of I_{pq} and I_{fg}. From (2.46) we obtain

$$\theta^+(q,p)+g[-\rho\log\rho-(1-\rho)\log(1-\rho)]$$
$$\leqslant(1+2p+2f)\theta^+\left(\frac{q}{1+2p+2f},\frac{p+f}{1+2p+2f}\right). \quad (2.92)$$

For brevity write

$$q_1=q/(1+2p+2f),\qquad p_1=(p+f)/(1+2p+2f). \quad (2.93)$$

Suppose that p, q, f, g are any real numbers satisfying (2.83), (2.84) and (2.88). Then

$$0<\frac{2p+2f}{1+2p+2f}=2p_1<\frac{2p+q-4p}{1+2p+2f}<\frac{q}{1+2p+2f}=q_1<\frac{1}{1+2p+2f}=1-2p_1. \quad (2.94)$$

Reference to (2.40) shows that (p_1,q_1) lies strictly in the interior of Δ^+. Since $\theta^+(q,p)$ is continuous in the interior of Δ^+, we see that (2.92), previously established for rational p, q, f, g, remains true for all real p, q, f, g satisfying (2.83), (2.84) and (2.88). Further, by continuity, we may let $g\to\frac{1}{2}q-2p$ in (2.88). Hence

$$\theta^+(q,p)+(\tfrac{1}{2}q-2p)[-\rho\log\rho-(1-\rho)\log(1-\rho)]\leqslant(1+2p+2f)\theta^+(q_1,p_1) \quad (2.95)$$

for any real p, q satisfying (2.83) and (2.84), and any real f such that

$$0<f<\tfrac{1}{2}q-2p=f/\rho. \quad (2.96)$$

It is also clear from (2.93) and (2.94) that

$$0<q_1<q<1 \quad (2.97)$$

because $p+f>0$ and $p_1>0$. By virtue of (2.97), there exists $(\alpha,\beta)\in\nabla$ such that

$$\alpha q_1+\beta 1=q,\qquad \alpha+\beta=1. \quad (2.98)$$

Hence

$$\alpha=\frac{(1-q)(1+2p+2f)}{1-q+2p+2f},\qquad \beta=\frac{2q(p+f)}{1-q+2p+2f} \quad (2.99)$$

and also

$$\alpha p_1+\beta 0=\frac{(1-q)(p+f)}{1-q+2p+2f}=p_2, \quad (2.100)$$

where p_2 is defined by (2.100).

Since $\theta^+(q,p)$ is concave, (2.98) and (2.100) yield

$$\alpha\theta^+(q,p_1)+\beta\theta^+(1,0)\leqslant\theta^+(q,p_2)\leqslant\theta^+(q). \quad (2.101)$$

From (2.95), (2.99) and (2.101) we obtain

$$\theta^+(q,p)+(\tfrac{1}{2}q-2p)[-\rho\log\rho-(1-\rho)\log(1-\rho)]$$
$$\leqslant\theta^+(q)+\frac{2(p+f)}{1-q}[\theta^+(q)-q\theta^+(1,0)]. \quad (2.102)$$

Also (2.46) gives

$$\theta^+(1,0)=\lim_{n\to\infty}n^{-1}\log b^+_{nn0}=\kappa', \quad (2.103)$$

because b^+_{nn0} is the number of n-SAWs that are entirely confined to the $(D-1)$-dimensional hyperplane $x=0$. Define the function

$$\psi=\psi(q)=2(\theta^+(q)-q\kappa')/(1-q), \tag{2.104}$$

and note that $f=(\frac{1}{2}q-2p)\rho$ according to (2.96). Then (2.102) becomes

$$\theta^+(q,p)+(\tfrac{1}{2}q-2p)[-\rho\log\rho-(1-\rho)\log(1-\rho)-\rho\psi]-p\psi\leq\theta^+(q). \tag{2.105}$$

In this we put

$$\rho=(1+e^{\psi})^{-1}, \tag{2.106}$$

which satisfies $0<\rho<1$ and maximises the left-hand side of (2.105), as an easy calculation shows. This gives

$$\theta^+(q,p)+(\tfrac{1}{2}q-2p)\log(1+e^{-\psi})-p\psi\leq\theta^+(q). \tag{2.107}$$

2.15.

Suppose we are given q with $0<q<1$. We can find a sequence $\{p_i(q)\}_{i=1,2,\ldots}$ such that

$$\lim_{i\to\infty}\theta^+(q,p_i(q))=\theta^+(q), \tag{2.108}$$

in view of (2.47). Since $\theta^+(q,p)=-\infty$ if (p,q) does not belong to Δ^+, we can suppose without loss of generality that $(p_i(q),q)$ belongs strictly to the interior of Δ^+ for all i: that is to say

$$0<p_i(q)<\min(\tfrac{1}{2}q,\tfrac{1}{2}-\tfrac{1}{2}q)\qquad(i=1,2,\ldots). \tag{2.109}$$

So the sequence $\{p_i(q)\}$ is bounded and has at least one limit point $p(q)$ satisfying

$$0\leq p(q)\leq\min(\tfrac{1}{2}q,\tfrac{1}{2}-\tfrac{1}{2}q). \tag{2.110}$$

By replacing $\{p_i(q)\}$ by a suitable subsequence of itself, we may suppose without loss of generality that

$$\lim_{i\to\infty}p_i(q)=p(q). \tag{2.111}$$

Note that we do *not*, of course, claim that $\theta^+(q,p(q))=\theta^+(q)$ since we have not established that $\theta^+(q,p)$ actually attains its supremum $\theta^+(q)$.

2.16.

We shall next prove that

$$p(q)\geq\frac{q\log(1+e^{-\psi(q)})}{2\psi(q)+4\log(1+e^{-\psi(q)})}=\phi(q), \tag{2.112}$$

where $\phi(q)$ is defined by (2.112). We note in the first place that $(p,1)\in\Delta^+$ if and only if $p=0$ by virtue of (2.40). Also $\theta^+(1,p)=-\infty$ if $(p,1)\notin\Delta^+$. Hence

$$\theta^+(1)=\theta^+(1,0)=\kappa', \tag{2.113}$$

by (2.103). Suppose $0<\delta<q$. Then, by the concavity of $\theta^+(q)$

$$\theta^+(q)=\theta^+\left[\left(\frac{1-q}{1-\delta}\right)\delta+\left(\frac{q-\delta}{1-\delta}\right)1\right]\geq\left(\frac{1-q}{1-\delta}\right)\theta^+(\delta)+\left(\frac{q-\delta}{1-\delta}\right)\theta^+(1). \tag{2.114}$$

Let $\delta \to 0+$ in (2.114), and use (2.65) and (2.113) to obtain

$$\theta^+(q) \geq (1-q)\kappa + q\kappa' > q\kappa'. \tag{2.115}$$

Hence, from (2.104), $\psi(q) > 0$, and thence (2.112) yields

$$\phi(q) < \tfrac{1}{4}q. \tag{2.116}$$

Now suppose, for the sake of a contradiction, that (2.112) is false; so that

$$0 \leq p(q) < \phi(q) < \tfrac{1}{4}q. \tag{2.117}$$

It follows from (2.117) that we may without loss of generality suppose that

$$0 < p_i(q) < \tfrac{1}{4}q \qquad (i = 1, 2, \ldots) \tag{2.118}$$

by choosing a similar subsequence of the original $p_i(q)$ if necessary. Now (2.110) and (2.118) show that all the $p_i(q)$ satisfy (2.84), and therefore we may substitute $p = p_i(q)$ in (2.107). We then let $i \to \infty$ and use (2.108) and (2.111) to obtain

$$\theta^+(q) + (\tfrac{1}{2}q - 2p(q)) \log(1 + e^{-\psi}) - p(q)\psi \leq \theta^+(q), \tag{2.119}$$

and hence

$$p(q) \geq \phi(q), \tag{2.120}$$

which contradicts (2.117). So (2.117) is false, and we have proved (2.112).

2.17.

Now we shall prove that

$$\theta(q, p) \geq \theta^+(q, p) + p \log 2 \tag{2.121}$$

whenever (p, q) lies strictly in the interior of Δ^+. By the continuity of $\theta(q, p)$ and $\theta^+(q, p)$ in the interior of Δ^+, which is contained in the interior of Δ, it is enough to prove (2.121) for rational p, q. So let n be a positive integer in I_{pq}, and consider any $w \in \mathscr{B}^+_{n,nq,np}$. If we reflect some of the np excursions of w in the hyperplane $x = 0$, we shall obtain a new SAW $w_1 \in \mathscr{B}_{n,nq,np}$. The total number of different ways in which we can reflect these excursions is 2^{np}, including the possibilities that all or none of the excursions are reflected. These 2^{np} SAWS are all different members of $\mathscr{B}_{n,nq,np}$. Moreover, if we started with two different SAWS w and w', the 2^{np} SAWS obtained from w would all be different from the 2^{np} SAWS obtained from w'. Hence

$$b_{n,nq,np} \geq 2^{np} b^+_{n,nq,np}. \tag{2.122}$$

Take logarithms of (2.122), divide by n, and let $n \to \infty$ through members of I_{pq}, and we obtain (2.121).

2.18.

From (2.121) we have *a fortiori*

$$\theta(q) \geq \theta^+(q, p) + p \log 2. \tag{2.123}$$

In (2.123) we can substitute $p = p_i(q)$ using the sequence (2.109) defined in § 2.15. Let $i \to \infty$, use (2.108) and (2.111) to obtain

$$\theta(q) \geq \theta^+(q) + p(q) \log 2. \tag{2.124}$$

Then (2.112) yields

$$\theta(q) \geqslant \theta^{+}(q) + \phi(q) \log 2. \tag{2.125}$$

Hence, by (2.82),

$$\omega_0^{+} - \omega_0 \geqslant \liminf_{q \to 0+} q^{-1} \phi(q) \log 2. \tag{2.126}$$

However (2.65) and (2.104) show that

$$\lim_{q \to 0+} \psi(q) = 2\kappa. \tag{2.127}$$

On the other hand $q^{-1}\phi(q)$ is a continuous function of ψ according to (2.112). Hence

$$\liminf_{q \to 0+} q^{-1}\phi(q) = \lim_{q \to 0+} q^{-1}\phi(q) = \frac{\log(1+\mathrm{e}^{-2\kappa})}{4\kappa + 4\log(1+\mathrm{e}^{-2\kappa})} \tag{2.128}$$

and (1.9) follows from (2.126) and (2.128).

2.19.

Next we turn to the proof of (1.7). We fix $\omega > \omega_0$, and write (2.52) in the form

$$A(\omega) = \sup_{0<q\leqslant 1} \{\theta(q) + q\omega\}, \qquad A^{+}(\omega) = \sup_{0<q\leqslant 1} \{\theta^{+}(q) + q\omega\}, \tag{2.129}$$

this being possible because $A(\omega) \geqslant A^{+}(\omega) \geqslant \kappa$, while $\theta(q)$ and $\theta^{+}(q)$ are both $-\infty$ for $q \leqslant 0$ or $q > 1$. We can then find a sequence $\{q_i(\omega)\}$ such that

$$0 < q_i(\omega) < 1 \tag{2.130}$$

and

$$A^{+}(\omega) = \lim_{i \to \infty} \{\theta^{+}[q_i(\omega)] + q_i(\omega)\omega\}. \tag{2.131}$$

Moreover, by considering a suitable subsequence of the bounded sequence (2.130), we can suppose without loss of generality that

$$\lim_{i \to \infty} q_i(\omega) = q(\omega). \tag{2.132}$$

There are then three cases to consider:

$$0 < q(\omega) < 1, \tag{2.133}$$

$$q(\omega) = 0, \tag{2.134}$$

$$q(\omega) = 1. \tag{2.135}$$

2.20.

First consider the case (2.133). We have seen that $\phi(q)$ is a continuous function of q in $0 < q < 1$, so that (2.125), (2.129), (2.131) and (2.132) yield

$$\begin{aligned} A(\omega) &\geqslant \limsup_{i \to \infty} \{\theta(q_i) + q_i\omega\} \geqslant \limsup_{i \to \infty} \{\theta^{+}(q_i) + q_i\omega + \phi(q_i) \log 2\} \\ &\geqslant A^{+}(\omega) + \phi[q(\omega)] \log 2. \end{aligned} \tag{2.136}$$

But (2.104) and (2.112) show that $\phi[q(\omega)]>0$ when (2.133) holds. This proves (1.7) in this case.

2.21.

Next we consider the case (2.134). From (2.131) and (2.134) we obtain

$$A^+(\omega)=\kappa, \tag{2.137}$$

by virtue of (2.130) and (2.65). However, $A(\omega)>\kappa$ when $\omega>\omega_0$, so (1.7) is true in this case.

2.22.

The case (2.135) is more difficult, and to deal with it we first prove that

$$\limsup_{q\to 1-} \theta(q)=\kappa'. \tag{2.138}$$

Let s'_n be the number of n-SAWs that are completely confined to the hyperplane $x=0$. Then we know that

$$\lim_{n\to\infty} n^{-1}\log s'_n=\kappa'. \tag{2.139}$$

Consider any arbitrary $\lambda>\kappa'$. Then, by (2.139), there exists a number γ_λ, depending on λ, such that

$$s'_n\leqslant\gamma_\lambda\, \mathrm{e}^{\lambda n}, \qquad \gamma_\lambda\geqslant 1, \tag{2.140}$$

for all positive integers n.

Let (p, q) be any rational point in the interior of Δ, let n be a positive integer belonging to I_{pq}, and consider a SAW $w\in\mathscr{B}_{n,nq,np}$. There are $np+1$ incursions in w, and each of these incursions is a SAW wholly confined to the hyperplane $x=0$. Suppose the ith incursion has ν_i+1 points on it. Then

$$\sum_{i=1}^{np+1}(\nu_i+1)=nq+1, \tag{2.141}$$

the total number of visits on w. Hence

$$\sum_i \nu_i=n(q-p). \tag{2.142}$$

The first incursion of w starts at the origin $z=\mathbf{0}$; the remaining incursions may start at any one of the remaining n points of w. Hence the starting points of the incursions can be chosen in at most $\binom{n}{np}$ different ways. By (2.140) and (2.142), the steps of the incursions can be formed in at most

$$\binom{n}{np}s'_{\nu_1}s'_{\nu_2}\ldots s'_{\nu_{np+1}}\leqslant\binom{n}{np}\gamma_\lambda^{np+1}\,\mathrm{e}^{\lambda n(q-p)} \tag{2.143}$$

different ways. There are also $n-nq$ steps on w, which do not belong to incursions, and can be chosen in at most $(2D)^{n(1-q)}$ ways. Hence

$$b_{n,nq,np}\leqslant\binom{n}{np}\gamma_\lambda^{np+1}(2D)^{n(1-q)}\,\mathrm{e}^{\lambda n(q-p)}. \tag{2.144}$$

Take logarithms, divide by n, and let $n \to \infty$ through members of I_{pq}, and we find from (2.90)

$$\theta(q, p) \leqslant -p \log p - (1-p) \log(1-p) + p \log \gamma_\lambda + (1-q) \log(2D) + \lambda(q-p). \tag{2.145}$$

Suppose $\frac{1}{3} < q < 1$. Then, by (2.39) $0 < p < \frac{1}{2}(1-q) < \frac{1}{3}$ because (p, q) lies in the interior of Δ; so (2.145) yields

$$\theta(q, p) \leqslant -\tfrac{1}{2}(1-q) \log \tfrac{1}{2}(1-q) - \tfrac{1}{2}(1+q) \log \tfrac{1}{2}(1+q) + \tfrac{1}{2}(1-q) \log \gamma_\lambda + (1-q)\log(2D) + \lambda q, \tag{2.146}$$

because $-p \log p - (1-p) \log(1-p)$ is an increasing function of p for $0 < p < \frac{1}{3}$. The right-hand side of (2.146) is independent of p; so we may write $\theta(q)$ instead of $\theta(q, p)$ on the left-hand side of (2.146). By the continuity of $\theta(q)$ in $0 < q < 1$, we have thus proved that

$$\theta(q) \leqslant -\tfrac{1}{2}(1-q) \log \tfrac{1}{2}(1-q) - \tfrac{1}{2}(1+q) \log \tfrac{1}{2}(1+q) + \tfrac{1}{2}(1-q) \log \gamma_\lambda + (1-q)\log(2D) + \lambda q \tag{2.147}$$

for all real q satisfying $\frac{1}{3} < q < 1$. Letting $q \to 1-$, we deduce

$$\limsup_{q \to 1-} \theta(q) \leqslant \lambda. \tag{2.148}$$

However, λ is any arbitrary number greater than κ'. So

$$\limsup_{q \to 1-} \theta(q) \leqslant \kappa'. \tag{2.149}$$

Since $\theta(q)$ and $\theta^+(q)$ are concave functions, bounded above by κ and satisfying (2.64) and (2.65), they are non-increasing functions of q for $q > 0$. Also $\theta(q) \geqslant \theta^+(q) \geqslant \theta^+(1) = \kappa'$ by (2.113). Hence (2.149) implies

$$\lim_{q \to 1-} \theta(q) = \lim_{q \to 1-} \theta^+(q) = \kappa'. \tag{2.150}$$

2.23.

Next consider a rational q such that $\frac{1}{2} < q < 1$. Put

$$p = \tfrac{1}{2}(1-q) \tag{2.151}$$

and let n be a positive integer belonging to I_{pq}. Let w be a SAW belonging to $\mathscr{B}^+_{n,nq,np}$, which is possible because of (2.37). The total number of non-visits on w is $n+1-(nq+1) = 2np$, and these occur on np excursions. Each excursion must have at least two non-visits; and therefore every excursion on w has exactly two non-visits. Hence, if we remove all the excursions on w (replacing each of these three-step excursions by a single step connecting the first and last points of that excursion), we shall obtain an nq-SAW w_1 lying wholly in the hyperplane $x = 0$. Conversely, given any nq-SAW lying wholly in the hyperplane, we can reconstruct a member of $\mathscr{B}^+_{n,nq,np}$ by replacing np of its steps by three-step excursions. Different nq-SAWS w_1 and different positions of these excursions will all lead to different members of $\mathscr{B}^+_{n,nq,np}$. Hence

$$b^+_{n,nq,np} = h^+ s'_{nq}, \tag{2.152}$$

where h^+ is the number of ways that np steps can be selected from nq steps to provide these excursions. The last step of w_1 is not available for replacement, because w would not then satisfy (2.1) and (2.2); nor may two successive steps on w_1 be replaced, because w would not then be self-avoiding. Hence h^+ is the number of ways of selecting np integers $\nu_1, \ldots, \nu_{np}$ from the set $\{1, 2, \ldots, nq-1\}$ such that

$$1 \leq \nu_1 < \nu_2 < \ldots < \nu_{np} \leq nq-1 \qquad \text{and } \nu_{i+1} > \nu_i + 1. \tag{2.153}$$

Such a selection can be placed in (1, 1) correspondence with a set of np distinct integers selected from $\{1, 2, \ldots, nq-np\}$, namely

$$1 \leq \nu_1 < \nu_2 - 1 < \nu_3 - 2 < \ldots < \nu_{np} - np + 1 \leq nq - np. \tag{2.154}$$

Hence

$$h^+ = \binom{nq-np}{np} = \binom{\frac{1}{2}n(3q-1)}{\frac{1}{2}n(1-q)}. \tag{2.155}$$

From (2.152) and (2.155) we obtain

$$n^{-1} \log b^+_{n,nq,np} = n^{-1} \log\binom{\frac{1}{2}n(3q-1)}{\frac{1}{2}n(1-q)} + n^{-1} \log s'_{nq}; \tag{2.156}$$

and thence, on letting $n \to \infty$ through members of I_{pq}, we have

$$\begin{aligned}\theta^+(q, \tfrac{1}{2} - \tfrac{1}{2}q) = q\kappa' - \tfrac{1}{2}(1-q) \log(1-q) - \tfrac{1}{2}(4q-2) \log(4q-2) \\ + \tfrac{1}{2}(3q-1) \log(3q-1).\end{aligned} \tag{2.157}$$

Since the left-hand side of (2.157) is a continuous function of q for $\frac{1}{2} < q < 1$, equation (2.157) holds for all real q in $\frac{1}{2} \leq q \leq 1$. The sum of the third and fourth terms in (2.157) is concave for $\frac{1}{2} \leq q \leq 1$, and so they are not less than $\frac{1}{2}(1-q) \log \frac{1}{2}$. Hence

$$\theta^+(q) \geq \theta^+(q, \tfrac{1}{2} - \tfrac{1}{2}q) \geq q\kappa' - \tfrac{1}{2}(1-q) \log(1-q) - \tfrac{1}{2}(1-q) \log 2$$

and

$$\frac{\theta^+(q) - \kappa'}{1-q} \geq -\tfrac{1}{2} \log(1-q) - \kappa' - \tfrac{1}{2} \log 2 \qquad (\tfrac{1}{2} \leq q < 1). \tag{2.158}$$

2.24.

Now, for the sake of a contradiction, suppose that (2.135) holds. Letting $i \to \infty$ in (2.131), we have from (2.52), (2.130), (2.135) and (2.150)

$$\sup_q \{\theta^+(q) + q\omega\} = A^+(\omega) = \kappa' + \omega, \tag{2.159}$$

and hence

$$\theta^+(q) + q\omega \leq \kappa' + \omega \qquad (\tfrac{1}{2} \leq q < 1) \tag{2.160}$$

which gives

$$(\theta^+(\omega) - \kappa')/(1-q) \leq \omega \qquad (\tfrac{1}{2} \leq q < 1). \tag{2.161}$$

Putting $q = 1 - \frac{1}{4} \exp[-2(\omega + \kappa')]$ in (2.158) and (2.161), we obtain the contradiction that $\omega + \frac{1}{2} \log 2 \leq \omega$. This shows that (2.135) is false; and the proof of (1.7) is complete.

2.25.

Finally, we shall prove (1.12) and (1.13). We shall require an equation for $\theta(q, \frac{1}{2}-\frac{1}{2}q)$ like (2.157). We consider a rational q such that $\frac{1}{3}<q\leqslant 1$ and we define p by (2.151). Then $(p, q)\in\Delta$ by (2.39), and we can find $w\in\mathscr{B}_{n,nq,np}$ when n is a positive integer belonging to I_{pq}. As in § 2.23, we see that each of the excursions on w are three-step excursions, so that we can delete them to obtain an nq-SAW w_1 lying wholly in the hyperplane $x=0$. Corresponding to (2.152) we obtain

$$b_{n,nq,np}=hs'_{nq}, \tag{2.162}$$

where h is the number of ways that np steps can be selected from nq steps of w_1 to provide these excursions. However, these excursions can now lie on either side of the hyperplane $x=0$. As before, the last step of w_1 is not available for selection. So we have to select np integers $\nu_1, \ldots, \nu_{np}$ from the set $\{1, 2, \ldots, nq-1\}$ and we have to attach to each of them symbols $\eta_1, \ldots, \eta_{np}$ (each equal to 0 or 1) to indicate which side of the hyperplane $x=0$ the excursion is to occupy. So in place of (2.153) we have

$$1\leqslant\nu_1(\eta_1)<\nu_2(\eta_2)<\ldots<\nu_{np}(\eta_{np})\leqslant nq-1. \tag{2.163}$$

If $\eta_i=\eta_{i+1}$, then two successive excursions lie on the same side of $x=0$, so we must have $\nu_{i+1}(\eta_{i+1})>\nu_i(\eta_i)+1$. But if $\eta_i\neq\eta_{i+1}$, we only require $\nu_{i+1}(\eta_{i+1})\geqslant\nu_i(\eta_i)+1$. Define $\rho_i=1$ or 0 according as $\eta_{i+1}\neq\eta_i$ or $\eta_{i+1}=\eta_i$, and write

$$\sum_{i=1}^{np-1}\rho_i=t. \tag{2.164}$$

Then the selection (2.163) can be placed in (1, 1) correspondence with the selection of np distinct integers from the set $\{1, 2, \ldots, nq-np+t\}$, namely

$$\begin{aligned}1\leqslant\nu_1(\eta_1)&<\nu_2(\eta_2)-1+\rho_1<\nu_3(\eta_3)-2+\rho_1+\rho_2\\&<\ldots<\nu_{np}(\eta_{np})-np+1+t\leqslant nq-np+t\end{aligned} \tag{2.165}$$

together with any admissible selection of the η_i. Suppose temporarily that t is fixed. Then the number of selections of integers in (2.165) is $\binom{nq-np+t}{np}$. Moreover, the values of $\eta_1, \eta_2, \ldots, \eta_{np}$ determine and are uniquely determined by the values of η_1, ρ_1, $\rho_2, \ldots, \rho_{np-1}$. Now η_1 can be chosen in two ways. Also $\rho_1, \rho_2, \ldots, \rho_{np-1}$ are determined by specifying which ones, of the available $np-1$ ρ's, are equal to 1. Hence the specification of the η's can be made in $2\binom{np-1}{t}$ ways. So for fixed t, we can select the excursions in

$$h(t)=2\binom{np-1}{t}\binom{nq-np+t}{np} \tag{2.166}$$

different ways. Since t can take any of the values $t=0, 1, \ldots, np-1$, we obtain

$$h=\sum_{t=0}^{np-1}h(t). \tag{2.167}$$

Now

$$\frac{h(t)}{h(t-1)}=\left(\frac{nq-np}{t}+1\right)\left(\frac{np-t}{nq-2np+t}\right) \tag{2.168}$$

is a strictly decreasing function of t. Hence the largest term in the sum (2.167) is $h([\tau])$, where

$$\left(\frac{nq-np}{\tau}+1\right)\left(\frac{np-\tau}{nq-2np+\tau}\right)=1. \tag{2.169}$$

Therefore

$$h([\tau])\leqslant h\leqslant nph([\tau]), \tag{2.170}$$

and thence

$$\lim_{n\to\infty} n^{-1}\log h=\lim_{n\to\infty} n^{-1}\log h([\tau]). \tag{2.171}$$

If we put

$$\tau=\tfrac{1}{2}nr, \tag{2.172}$$

we find from (2.151) and (2.169) that

$$(3q-1+r)(1-q-r)=r(4q-2+r), \tag{2.173}$$

and hence

$$r=1-2q+\{\tfrac{1}{2}q^2+\tfrac{1}{2}(1-2q)^2\}^{1/2}. \tag{2.174}$$

Here we have to choose the positive square root in solving the quadratic equation (2.173), because we require $0\leqslant[\tau]\leqslant np$, given that $\tfrac{1}{2}<q\leqslant 1$. From (2.166) and (2.171) and Stirling's formula, we deduce that

$$\begin{aligned}\lim_{n\to\infty} n^{-1}\log h&=\lim_{n\to\infty} n^{-1}\log\left[2\binom{\tfrac{1}{2}n(1-q)-1}{[\tfrac{1}{2}nr]}\binom{\tfrac{1}{2}n(3q-1)+[\tfrac{1}{2}nr]}{\tfrac{1}{2}n(1-q)}\right]\\&=\tfrac{1}{2}(3q-1+r)\log(3q-1+r)-\tfrac{1}{2}(4q-2+r)\log(4q-2+r)\\&\quad-\tfrac{1}{2}(1-q-r)\log(1-q-r)-\tfrac{1}{2}r\log r.\end{aligned} \tag{2.175}$$

So, letting $n\to\infty$ through members of I_{pq} in (2.162), we obtain

$$\begin{aligned}\theta(q,\tfrac{1}{2}-\tfrac{1}{2}q)&=q\kappa'+\tfrac{1}{2}(3q-1+r)\log\left(\frac{3q-1+r}{q}\right)-\tfrac{1}{2}(4q-2+r)\log\left(\frac{4q-2+r}{q}\right)\\&\quad-\tfrac{1}{2}(1-q-r)\log\left(\frac{1-q-r}{q}\right)-\tfrac{1}{2}r\log\frac{r}{q}.\end{aligned} \tag{2.176}$$

Here we have been able to insert denominators q throughout because the sum of the coefficients of the logarithms is zero. This result, established for rational q, persists for all real $\tfrac{1}{3}<q\leqslant 1$ by continuity. Writing

$$Q=2-1/q, \qquad -1<Q\leqslant 1, \tag{2.177}$$

we obtain

$$(\kappa-\theta(q,\tfrac{1}{2}-\tfrac{1}{2}q))/q=F(Q), \tag{2.178}$$

where

$$\begin{aligned}F(Q)&=2\kappa-\kappa'-\kappa Q-\tfrac{1}{2}(1+Q)\log\{1+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}\}+\tfrac{1}{2}(1-Q)\log\{1-(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}\}\\&\quad+\log\{Q+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}\}.\end{aligned} \tag{2.179}$$

Differentiating F with respect to Q, we find (after some manipulation in which extraneous terms cancel out) that

$$F'(Q)=-\kappa-\tfrac{1}{2}\log\{1+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}\}-\tfrac{1}{2}\log\{1-(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}\}$$
$$+\log\{Q+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}\}. \tag{2.180}$$

We now choose Q to minimise $F(Q)$. Thus

$$F'(Q)=0; \tag{2.181}$$

and so

$$e^{2\kappa}=\frac{\{Q+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}\}^2}{\{1+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}\}\{1-(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}\}}=\frac{Q+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}{-Q+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}. \tag{2.182}$$

Also, from (2.179), (2.180) and (2.181), we have

$$F(Q)=2\kappa-\kappa'-\log\frac{1+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}{1-(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}=2\kappa-\kappa'-\lambda, \tag{2.183}$$

where

$$e^{2\lambda}=\frac{1+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}{1-(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}. \tag{2.184}$$

Now, by (2.182) and (2.184),

$$\begin{aligned}2\cosh^2\kappa&=1+\cosh 2\kappa\\&=\frac{1}{2}\left(\frac{Q+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}{-Q+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}+\frac{-Q+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}{Q+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}\right)+1\\&=\frac{2Q^2+2}{1-Q^2}=\frac{1}{2}\left(\frac{1+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}{1-(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}+\frac{1-(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}{1+(\tfrac{1}{2}+\tfrac{1}{2}Q^2)^{1/2}}\right)-1\\&=-1+\cosh 2\lambda=2\sinh^2\lambda.\end{aligned} \tag{2.185}$$

Since $\lambda>0$ by (2.184), we deduce that $\cosh\kappa=\sinh\lambda$. Hence

$$\inf_{\frac{1}{3}<q\leq 1}\frac{\kappa-\theta(q,\tfrac{1}{2}-\tfrac{1}{2}q)}{q}=2\kappa-\kappa'-\sinh^{-1}\cosh\kappa. \tag{2.186}$$

But $\kappa-\theta(q)$ is a convex function of q tending to zero as $q\to 0+$. Hence, from (2.80),

$$\begin{aligned}\omega_0=\lim_{q\to 0+}\frac{\kappa-\theta(q)}{q}=\inf_{q>0}\frac{\kappa-\theta(q)}{q}\leq\inf_{q>0}\frac{\kappa-\theta(q,\tfrac{1}{2}-\tfrac{1}{2}q)}{q}\\ \leq 2\kappa-\kappa'-\sinh^{-1}\cosh\kappa.\end{aligned} \tag{2.187}$$

This proves (1.13).

2.26.

To obtain (1.12), we make the substitution (2.177) in (2.157), after inserting denominators q into arguments of the logarithms (for the same reasons as in (2.176)).

Table 1. Values of $\frac{1}{2}a_{nv}$ for $D=2$.

n \ v	0	1	2	3	4	5
1	1	1				
2	3	2	1			
3	7	8	2	1		
4	19	18	10	2	1	
5	49	50	28	12	2	1
6	131	130	78	34	14	2
7	339	354	222	112	40	16
8	899	926	608	318	140	46
9	2 345	2 490	1 668	956	426	174
10	6 199	6 554	4 530	2 646	1 288	538
11	16 225	17 514	12 296	7 564	3 820	1 712
12	42 811	46 202	33 166	20 740	11 014	5 112
13	112 285	122 990	89 456	57 842	31 702	15 464
14	296 051	324 782	240 164	157 426	89 248	44 794
15	777 411	862 646	645 046	433 092	251 648	131 204
16	2 049 025	2 278 822	1 726 282	1 172 422	698 100	372 728
17	5 384 855	6 044 126	4 622 384	3 197 050	1 941 914	1 067 440
18	14 190 509	15 968 174	12 342 712	8 620 470	5 334 640	2 991 004
19	37 313 977	42 310 562	32 974 042	23 365 294	14 697 726	8 432 054
20	98 324 565	111 781 490	87 898 024	62 810 306	40 101 716	23 389 414
21	258 654 441	295 971 310	234 413 500	169 501 498	109 710 704	65 193 582

n \ v	6	7	8	9	10	11	12
6	1						
7	2	1					
8	18	2	1				
9	52	20	2	1			
10	212	58	22	2	1		
11	670	254	64	24	2	1	
12	2 204	818	300	70	26	2	1
13	6 778	2 794	982	350	76	28	2
14	20 808	8 784	3 484	1 162	404	82	30
15	62 154	27 674	11 198	4 282	1 358	462	88
16	183 716	83 962	36 136	14 052	5 196	1 570	524
17	537 070	254 024	111 860	46 468	17 386	6 234	1 798
18	1 549 930	750 596	344 288	146 634	58 916	21 240	7 404
19	4 454 472	2 213 558	1 035 902	459 944	189 468	73 752	25 654
20	12 645 968	6 414 988	3 093 404	1 405 932	605 528	241 590	91 264
21	35 860 450	18 577 856	9 117 080	4 266 308	1 881 504	786 646	304 336

n \ v	13	14	15	16	17	18	19	20	21
13	1								
14	2	1							
15	32	2	1						
16	94	34	2	1					
17	590	100	36	2	1				
18	2 042	660	106	38	2	1			
19	8 714	2 302	734	112	40	2	1		
20	30 668	10 172	2 578	812	118	42	2	1	
21	111 756	36 322	11 786	2 870	894	124	44	2	1

Table 2. Values of a^{+}_{nv} for $D = 2$.

n \ v	0	1	2	3	4	5
1	1	2				
2	3	2	2			
3	7	8	2	2		
4	19	16	10	2	2	
5	49	42	24	12	2	2
6	131	106	56	28	14	2
7	339	282	148	78	32	16
8	899	718	384	194	92	36
9	2 345	1 898	988	544	250	110
10	6 199	4 906	2 572	1 376	674	298
11	16 225	12 946	6 692	3 690	1 830	844
12	42 811	33 674	17 512	9 510	4 838	2 244
13	112 285	88 734	45 708	25 362	12 922	6 256
14	296 051	231 718	119 772	65 802	34 140	16 504
15	777 411	610 330	313 440	174 602	90 798	45 126
16	2 049 025	1 597 518	822 352	454 974	239 360	119 050
17	5 384 855	4 207 198	2 155 512	1 204 316	634 754	321 898
18	14 190 509	11 029 230	5 660 424	3 146 908	1 672 128	848 710
19	37 313 977	29 045 886	14 853 388	8 317 976	4 426 452	2 278 494
20	98 324 565	76 227 402	39 031 572	21 775 920	11 657 950	6 005 826
21	258 654 441	200 754 406	102 505 956	57 508 486	30 824 676	16 050 558

n \ v	6	7	8	9	10	11	12
6	2						
7	2	2					
8	18	2	2				
9	40	20	2	2			
10	130	44	22	2	2		
11	356	152	48	24	2	2	
12	1 018	420	176	52	26	2	2
13	2 780	1 224	490	202	56	28	2
14	7 700	3 376	1 458	566	230	60	30
15	20 996	9 518	4 074	1 722	648	260	64
16	56 974	25 958	11 618	4 874	2 018	736	292
17	154 488	71 944	32 066	14 078	5 784	2 348	830
18	415 198	194 460	89 306	39 242	16 926	6 812	2 714
19	1 119 464	533 286	244 702	110 416	47 678	20 202	7 966
20	2 991 024	1 432 790	671 502	304 440	135 454	57 514	23 948
21	8 027 274	3 897 632	1 830 076	843 758	376 714	165 034	68 912

n \ v	13	14	15	16	17	18	19	20	21
13	2								
14	2	2							
15	32	2	2						
16	68	34	2	2					
17	326	72	36	2	2				
18	930	362	76	38	2	2			
19	3 118	1 036	400	80	40	2	2		
20	9 254	3 562	1 148	440	84	42	2	2	
21	28 208	10 684	4 048	1 266	482	88	44	2	2

Table 3. Values of $\frac{1}{2}a_{nv}$ for $D=3$.

n \ v	0	1	2	3	4
1	1	2			
2	5	4	6		
3	21	24	12	18	
4	93	100	84	36	50
5	409	444	384	288	100
6	1 853	1 956	1 724	1 356	900
7	8 333	8 900	7 828	6 472	4 456
8	37 965	40 164	35 880	30 020	21 992
9	172 265	183 772	164 608	141 400	106 788
10	787 557	836 804	758 212	656 340	512 144
11	3 593 465	3 839 812	3 492 176	3 072 848	2 441 200
12	16 477 845	17 574 860	16 116 732	14 276 664	11 565 004
13	75 481 105	80 840 124	74 392 240	66 650 852	54 695 876
14	346 960 613	371 306 084	343 825 152	309 769 972	257 656 616

n \ v	5	6	7	8	9
5	142				
6	284	390			
7	2 840	780	1 086		
8	14 252	8 580	2 172	2 958	
9	73 692	44 304	26 064	5 916	8 134
10	367 116	235 968	135 572	76 908	16 268
11	1 817 456	1 219 980	750 276	407 864	227 752
12	8 805 552	6 161 280	3 965 100	2 320 168	1 213 908
13	42 636 584	30 659 012	20 584 596	12 638 388	7 143 436
14	204 022 244	150 626 248	104 170 920	66 832 632	39 662 020

n \ v	10	11	12	13	14
10	22 050				
11	44 100	60 146			
12	661 500	120 292	162 466		
13	3 574 688	1 924 672	324 932	440 750	
14	21 590 520	10 440 252	5 523 844	881 500	1 187 222

We obtain

$$\frac{\kappa-\theta^+(q,\frac{1}{2}-\frac{1}{2}q)}{q}=2\kappa-\kappa'-\kappa Q+\tfrac{1}{2}(1-Q)\log(1-Q)+Q\log 2Q$$
$$-\tfrac{1}{2}(1+Q)\log(1+Q) \qquad (0\leqslant Q\leqslant 1). \tag{2.188}$$

The right-hand side of (2.188) attains its minimum when

$$Q/(1-Q^2)^{1/2}=\tfrac{1}{2}\,e^{\kappa}, \tag{2.189}$$

and this minimum is

$$\inf_{\frac{1}{2}\leq q\leq 1} \frac{\kappa-\theta^{+}(q,\frac{1}{2}-\frac{1}{2}q)}{q} = 2\kappa-\kappa'-\tfrac{1}{2}\log\frac{1+Q}{1-Q}$$
$$= 2\kappa-\kappa'-\log\left\{\frac{Q}{(1-Q^2)^{1/2}}+\left(1+\frac{Q^2}{1-Q^2}\right)^{1/2}\right\}$$
$$= 2\kappa-\kappa'-\sinh^{-1}(\tfrac{1}{2}e^{\kappa}); \qquad (2.190)$$

whereupon (1.12) follows from (2.81), as in (2.187).

3. Exact enumeration results

We have obtained exact values of a_{nv} and a_{nv}^{+} for the square lattice for $n\leq 21$ and exact values of a_{nv} for the simple cubic lattice for $n\leq 14$, using a modified version of a counting programme which has been described elsewhere (Torrie and Whittington 1975). The results are given in tables 1–3. (The corresponding results for a_{nv}^{+} for the simple cubic lattice can be extracted from data in Middlemiss *et al* (1977).) Note in particular that our tables 1 and 3 quote values for $\frac{1}{2}a_{nv}$, whereas table 2 quotes values of a_{nv}^{+} (*without* the factor $\frac{1}{2}$).

For fixed ω we calculate $A_n(\omega)$ (equation (1.1)) and form the sequence of ratio estimates

$$\mu_n(\omega) = \left(\frac{A_n(\omega)}{A_{n-2}(\omega)}\right)^{1/2} \qquad (3.1)$$

up to the largest value of n for which exact data are available. As $n\to\infty$ we expect $\mu_n(\omega)$ to converge to $\exp[A(\omega)]$ and we carry out the extrapolation against n^{-1} using an appropriate Neville table. We form the sequence of extrapolants

$$\mu_n^{(k)}(\omega) = (2k)^{-1}(n\mu_n^{(k-1)}(\omega)-(n-2k)\mu_{n-2}^{(k-1)}(\omega)) \qquad (3.2)$$

with $\mu_n^{(0)}(\omega)=\mu_n(\omega)$.

Our estimates for $A(\omega)$ and $A^{+}(\omega)$ for the square lattice are shown in figure 1, and our estimates of $A(\omega)$ for the simple cubic lattice in figure 2. The value of κ is known

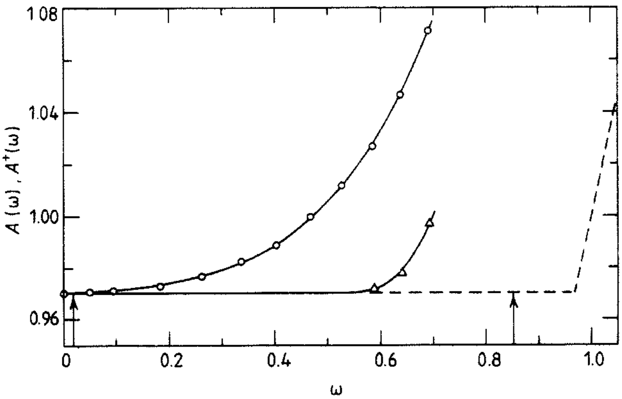


Figure 1. $A(\omega)$ and $A^{+}(\omega)$ for the square lattice. The broken line is the lower bound (1.5) and the arrows are the lower and upper bounds (1.9) and (1.12) for ω_0^{+}.

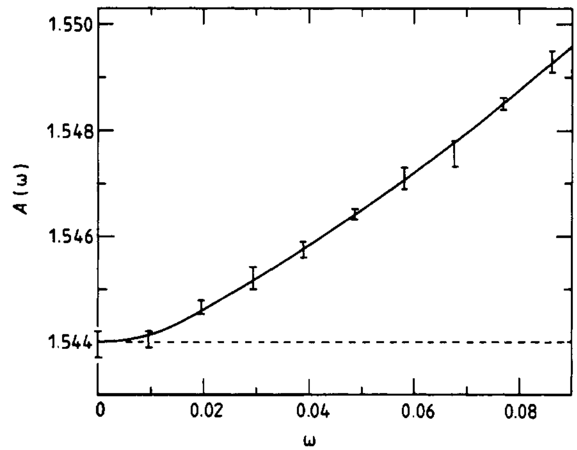


Figure 2. $A(\omega)$ for the simple cubic lattice.

rather accurately from series analysis work: $e^{\kappa} \simeq 2.6385$ for $D = 2$, and $e^{\kappa} = 4.6835$ for $D = 3$ (Sykes *et al* 1972).

Since we know that $\omega_0 \geq 0$ from § 2 and $\bar{\omega}_0 = 0$ it is tempting to conjecture that $\omega_0 = 0$. From figures 1 and 2 we see that this is reasonably consistent with the data. To obtain further evidence for this we look for a value of ω at which we can be reasonably sure that $A(\omega) > \kappa$. In table 4 we give the Neville table, successive entries of which are calculated from (3.2), for $\exp(\omega) = 1.03$ for the cubic lattice. Inspection of this table indicates that $\exp[A(\omega)]$ is about 4.689 and, in view of the behaviour of the linear extrapolants, it is most unlikely to be less than 4.687 which, in turn, is greater than $\exp(\kappa)$. This indicates that $0 \leq \omega_0 < 0.03$ for $D = 3$.

Table 4. Neville table for estimating $\exp[A(\omega)]$ for the simple cubic lattice with $\exp(\omega) = 1.03$.

n	μ_n	$\mu_n^{(1)}$	$\mu_n^{(2)}$	$\mu_n^{(3)}$
6	4.858 273	4.657 900		
7	4.826 089	4.674 273	4.701 442	
8	4.812 690	4.675 941	4.693 983	
9	4.795 818	4.689 871	4.709 369	4.713 332
10	4.787 115	4.684 816	4.698 129	4.700 892
11	4.776 570	4.689 954	4.690 099	4.674 042
12	4.770 418	4.686 934	4.691 168	4.684 207
13	4.763 206	4.689 705	4.689 145	4.688 032
14	4.758 626	4.687 873	4.690 221	4.688 959

The corresponding Neville table for the square lattice when $\exp(\omega) = 1.04$ is given in table 5. Again, it is clear from these results that $A(\omega) > \kappa$ for this value of ω so that $\omega_0 < 0.04$ for the square lattice.

The results for $A_n^+(\omega)$ for the square lattice are rather more difficult to analyse but, proceeding on the above lines, it is fairly clear that $A^+(0.6) > \kappa$ while $A^+(0.5)$ is indistinguishable from κ. Hence we can be quite confident that $\omega_0^+ < 0.6$ though it is

Table 5. Neville table for estimating $\exp[A(\omega)]$ for the square lattice with $\exp(\omega)=1.04$.

n	μ_n	$\mu_n^{(1)}$	$\mu_n^{(2)}$	$\mu_n^{(3)}$
12	2.721 804	2.637 051	2.635 998	2.638 319
13	2.713 911	2.641 753	2.640 051	2.630 337
14	2.709 818	2.637 903	2.640 035	2.645 417
15	2.704 197	2.641 055	2.639 137	2.637 765
16	2.700 930	2.638 712	2.641 138	2.642 977
17	2.696 691	2.640 393	2.638 240	2.636 597
18	2.694 055	2.639 054	2.640 253	2.638 482
19	2.690 734	2.640 102	2.639 013	2.640 689
20	2.688 563	2.639 142	2.639 493	2.637 721
21	2.685 893	2.639 905	2.639 066	2.639 197

more difficult to form a reliable estimate of a lower bound on ω_0^+. Within the accuracy of the ratio analysis which we have carried out, we suggest that ω_0^+ is probably greater than 0.5. In figure 1 we show the ω dependence of $A^+(\omega)$ for the square lattice. The arrows indicate the bounds on ω_0^+ calculated from (1.9) (with $\omega_0=0$) and (1.12), using numerical estimates of κ and κ' (Sykes *et al* 1972).

4. Discussion

This paper has been concerned with two models of polymer adsorption in which excluded volume effects are incorporated by modelling the conformation of the isolated polymer molecule by the conformation of a self-avoiding walk on a lattice. In each case the walk interacts with a lattice plane via a short-range potential. In the first model the walks are free to cross the lattice plane, representing the surface, while in the second they are constrained to lie in or on one side of this lattice plane. We show rigorously that the limiting free energies per step, $A(\omega)$ and $A^+(\omega)$, exist for all values of the interaction parameter ω. In addition there exist critical values of ω, ω_0 and ω_0^+, which are the largest values of ω for which $A(\omega)=\kappa$ and $A^+(\omega)=\kappa$, respectively. We have shown that $\omega_0^+>\omega_0\geqslant 0$ and that $A(\omega)>A^+(\omega)$ for $\omega>\omega_0$.

For walks which are not allowed to penetrate the surface (positive walks), this implies that $\omega_0^+>0$, and, in addition, we have shown that

$$\omega_0^+\leqslant 2\kappa-\kappa'-\sinh^{-1}(\tfrac{1}{2}e^{\kappa})<\kappa-\kappa'. \tag{4.1}$$

The bounds on ω_0^+ (shown as arrows in figure 1), though numerically weak, do rule out the possibilities $\omega_0^+=0$ (which corresponds to an infinite temperature transition) and $\omega_0^+=\kappa-\kappa'$ (the value predicted by a mean field argument).

We have also reported exact enumeration data on the number of walks which visit the surface plane a given number of times. Our analysis of these data suggests that ω_0 is probably zero for both two- and three-dimensional lattices. We have also estimated that $0.5<\omega_0^+<0.6$ for the square lattice.

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References

Barber M N, Guttmann A J, Middlemiss K M, Torrie G M and Whittington S G 1978 *J. Phys. A: Math. Gen.* **11** 1833
Clayfield E J and Lumb E C 1966 *J. Coll. Interface Sci.* **22** 285
Gaunt D S and Guttmann A J 1974 *Phase Transitions and Critical Phenomena* vol 3, ed C Domb and M S Green (London: Academic)
Hammersley J M 1957 *Proc. Camb. Phil. Soc.* **53** 642
—— 1961 *Proc. Camb. Phil. Soc.* **57** 516
—— 1962 *Proc. Camb. Phil. Soc.* **58** 235
—— 1982 *J. Appl. Prob.* **19**A 327
Hammersley J M and Welsh D J A 1962 *Oxford Q. J. Math.* (2) **13** 108
Hardy G H, Littlewood J E and Pólya G 1934 *Inequalities* ch 3 (Cambridge: CUP)
Lax M 1974a *J. Chem. Phys.* **61** 4133
—— 1974b *Macromolecules* **7** 660
Ma L, Middlemiss K M, Torrie G M and Whittington S G 1978 *J. Chem. Soc. Faraday Trans. II* **74** 721
McCrackin F L 1967 *J. Chem. Phys.* **47** 1980
Middlemiss K M, Torrie G M and Whittington S G 1977 *J. Chem. Phys.* **66** 3227
Silberberg A 1967 *J. Chem. Phys.* **46** 1105
Sykes M F, Watts M G and Roberts P D 1972 *J. Phys. A: Gen. Phys.* **5** 653
Torrie G M and Whittington S G 1975 *J. Phys. A: Math. Gen.* **8** 1178
Whittington S G 1975 *J. Chem. Phys.* **63** 779