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COMMENT

A note about the enumeration of self-avoiding walks

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Abstract. General Möbius inversion is used to obtain an explicit formula for the number of self-avoiding walks between two points of the three-dimensional integer lattice. The consequent probabilities and expected values are of interest in physical chemistry, particularly the formation of polymer chains using excluded volume interaction.

1. Introduction

One of the celebrated problems of applied probability is the asymptotic behaviour of the number of self-avoiding walks (SAW) on lattices such as the three-dimensional integer lattice. These walks are interesting, particularly for modelling the formation of polymers using excluded volume interaction (thus molecules in the polymer chain may not occupy the same site of the lattice). The background and conjectures for the asymptotic number of SAW are well known and useful summaries of this may be found in Torrie and Whittington (1975) and Freed (1981). Considerable attention has also been given to the enumeration of the number of SAW with a small number of steps; generally this is done through computer generation of SAW, such as Martin *et al* (1967) and Wall and Seitz (1979) but more explicit techniques have been used, in particular the recursions of Chay (1971).

This comment demonstrates how Möbius inversion as described by Rota (1964) gives an explicit expression for the number of SAW with n steps between two points of any lattice in terms of the numbers of (non-self-avoiding) paths of the lattice. The intention behind the development of this formula was to use it to investigate the asymptotic questions, but this proves difficult as discussed in the remarks of § 3. However, the result still seems worth reporting for its own interest as a non-trivial application of Möbius inversion and for its application to the enumeration of short SAW. Since (2.2) is an explicit formula it always presents the possibility of providing a means to answering the asymptotic questions. Theorem 2.1 covers SAW on the three-dimensional integer lattice, but it is clear that the technique transfers quite generally to any lattice and furthermore to SAW restricted in some way, such as through absorption at a barrier (see Hammersley *et al* 1982). In this case the paths appearing on the right-hand side of (2.2) need not be self-avoiding but must satisfy the other restrictions imposed.

2. SAW on the integer lattice

The walks considered here may be regarded as mappings $\omega\colon [n]=\{0,1,2,\ldots,n\}\to S=\mathbb{Z}^3$ with the requirement that each step moves the walk to a neighbouring site of the

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lattice so that for $0 \leqslant i < n$, $|\omega(i) - \omega(i+1)| = 1$ where for $x, y \in S$, $|x-y| = |x_1 - y_1| + |x_2 - y_2| + |x_3 - y_3|$. Thus as the basic sets of walks starting at $0 \in S$ take

$$\mathscr{W}_n = \{\omega\colon \omega(0) = 0, |\omega(i) - \omega(i+1)| = 1, 0 \leqslant i < n\}$$

then the SAW of n steps starting at 0 are given by

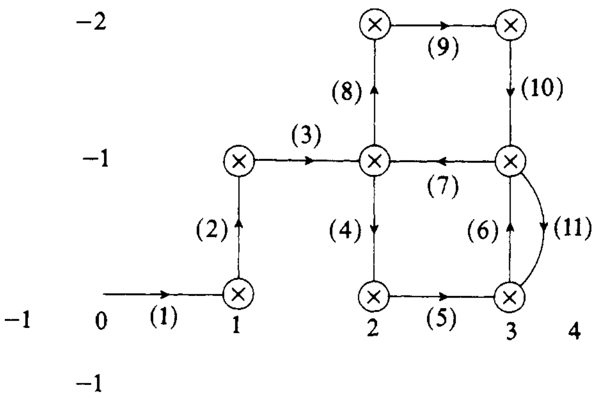
$$\mathscr{S}_n = \{\omega \in \mathscr{W}_n\colon \omega(i) \neq \omega(j), 0 \leqslant i \neq j \leqslant n\}.$$

In the first instance it is easier to use

$$\mathscr{W}_n^a = \{\omega \in \mathscr{W}_n\colon \omega(n) = a\} \qquad \mathscr{S}_n^a = \mathscr{S}_n \cap \mathscr{W}_n^a \qquad a \in S$$

walks ending at a. Then Möbius inversion gives $s_n(a) = |\mathscr{S}_n^a|$ in terms of $\{w_m(b)\colon b \in S, 1 \leqslant m \leqslant n\}$ where $w_m(b) = |\mathscr{W}_m^b|$.

In order to state theorem 2.1, we define a further set C_n of mappings $\xi : C = C(\xi) \subset [n] \to S$ which satisfies the property that $\xi \subset \omega$ for some $\omega \in \mathscr{W}_n$ (alternatively, $\xi \in C_n$ if it can be extended to a walk in $\mathscr{W}_n$). Let $i_\xi = |\mathrm{Im}(\xi)| = |\{\xi(c)\colon c \in C \subset [n]\}|$ the cardinality of the image, and hence define the vector $([\xi]_1, [\xi]_2, \ldots)$ where $[\xi]_j =$ number of $s \in \mathrm{Im}(\xi)$ for which $j = |\xi^{-1}(s)|$, so that necessarily $[\xi]_j = 0, j > i_\xi$. Then by definition $\Sigma_j j[\xi]_j = c_\xi = |C(\xi)|$ and $\Sigma_j [\xi]_j = i_\xi$. The mapping $C(\xi)$ picks a subset of the n steps of the walk $\omega(W_n)$ as the pre-image and maps this to the sites of the lattice visited at those steps. Thus c_ξ denotes the number of steps selected in the pre-image and i_ξ the number of sites visited on those steps. To illustrate this we consider the corresponding definitions on $\mathbb{Z}^2$ and take $n = 11$ with the following walk ω (the order in which sites are visited are given in parentheses):



(2.1)

Then, for example, we take ξ defined by ω and $C(\xi) = \{2, 3, 5, 7, 8, 9, 10, 11\}$ (thus $c_\xi = |C(\xi)| = 8$). At the steps in $C(\xi)$ the walk visits the circled sites and these give $\mathrm{Im}(\xi) = \{(1,1), (2,1), (3,0), (2,2), (3,2), (3,1)\}$; two of these sites are visited twice on steps included in $C(\xi)$. Thus $i_\xi = 6$ and $[\xi]_1 = 4$, $[\xi]_2 = 2$, $[\xi]_j = 0$, $j \geqslant 3$ (four sites visited once in $C(\xi)$, two sites visited twice, none visited more than twice).

The basic enumeration result for SAW is contained in the following theorem: the summation in (2.2) extends over a subset C_n^* of C_n corresponding to choices of ξ in which each site in $\mathrm{Im}(\xi)$ is visited at least twice at steps in $C(\xi)$ (C_n^* is more explicitly defined below).

Theorem 2.1. For $a \in S$ such that there exists $\omega \in \mathscr{S}_n$ satisfying $\omega(n) = a$, the following holds:

$$s_n(a) = \sum_{\xi \in C_n^*} (-1)^{c_\xi - i_\xi + 1} \left(\prod_{j>1} (j-1)^{[\xi]_j} \right) \left(\prod_{k=0}^{c_\xi} w_{\Delta c_k}\big((\Delta\xi)_k\big) \right) \tag{2.2}$$

where for $0 \leqslant k \leqslant i_\xi$, $c_0 = 0$, $c_{c_\xi+1} = n$, $\Delta c_k = c_{k+1} - c_k$ where $C(\xi) = \{c_1 < c_2 < \ldots < c_{c_\xi}\}$ and $(\Delta\xi)_k = \xi(c_{k+1}) - \xi(c_k)$, defining $\xi(c_0) = 0 \in S$, $\xi(c_{c_\xi+1}) = \xi(n) = a$.

Furthermore, for $b = (b_1, b_2, b_3)$,

$$w_m(b) = \Sigma_{(m)}\, m!\left(\prod_{j=1}^{3} [\tfrac{1}{2}(m_j + b_j)]! \prod_{j=1}^{3} [\tfrac{1}{2}(m_j - b_j)]!\right)^{-1}$$

where the summation is over $\{(m_1, m_2, m_3)\colon m_1, m_2, m_3 \geqslant 0, m_1 + m_2 + m_3 = m\}$ and if $m_j + b_j$ or $m_j - b_j$ are not even, then the term in the summation equals 0. Alternatively

$$w_m(b) = (2^{m-3}/\pi^3) \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} \exp[-\mathrm{i}(b_1\theta_1 + b_2\theta_2 + b_3\theta_3)]$$
$$\times [\exp(\mathrm{i}\theta_1) + \exp(\mathrm{i}\theta_2) + \exp(\mathrm{i}\theta_3)]^m \, \mathrm{d}\theta_1 \, \mathrm{d}\theta_2 \, \mathrm{d}\theta_3.$$

Proof. General Möbius inversion as in (2.3) for a suitably defined partially ordered set (poset) gives (2.2); standard inclusion–exclusion (as in p 345 of Rota (1964)) also gives (2.2) but this requires a certain amount of manipulation whereas general Möbius inversion works directly once $\mu(\cdot,\cdot)$ is evaluated. First define the appropriate poset $C_n^* \subset C_n$ by

$$C_n^* = \{\xi \in C_n\colon [\xi]_1 = 0\}.$$

Thus C_n^* consists of mappings $\xi\colon C \to S$, $C \subset [n]$ (including $C = \varnothing$, the empty set) where all points in $\mathrm{Im}(\xi)$ are repeated, i.e. for each $c \in C(\xi) \neq \varnothing$, there exists $c' \in C$, $c' \neq c$, such that $\xi(c) = \xi(c')$. Define a partial ordering $<$ on C_n^* by $\xi_1 < \xi_2$ when $C(\xi_1) \subseteq C(\xi_2)$ and for each $c \in C(\xi_1)$, $\xi_1(c) = \xi_2(c)$ (thus $<$ is standard inclusion of functions). In the two-dimensional example given earlier one may take $C(\xi^*) = \{3, 5, 6, 7, 10, 11\}$ when each of the sites $(2, 1)$, $(3, 1)$ and $(3, 0)$ is visited twice; then $\xi_1 < \xi^*$ when $C(\xi_1) = \{3, 7\}$ or $\xi_2 < \xi^*$ when $C(\xi_2) = \{5, 6, 10, 11\}$ but obviously $\xi_1 \not< \xi_2$ or vice versa. Then for any $f\colon C_n^* \to \mathbb{R}$, Möbius inversion as described by Rota (1964) using the Möbius function $\mu(\cdot,\cdot)$ on $(C_n^*, <)$ gives

$$f(0) = \sum_{\xi} \mu(0, \xi) \sum_{\pi > \xi} f(\pi) \tag{2.3}$$

where $0 \in C_n^*$ is defined by $C(\xi) = \varnothing$. It remains to choose $f(\cdot)$ and determine $\mu(0, \cdot)$.

Define the repeated states $R(\omega)$ of path $\omega \in \mathscr{W}_n^a$ as $\xi = R(\omega) \in C_n^*$ given by $C(\xi) = \{i \in [n]$: there exists $j \neq i$, $j \in [n]$, such that $\omega(i) = \omega(j)\}$ and $\xi(c) = \omega(c)$, $c \in C(\xi)$ (possibly $\xi = 0$). Then (2.3) will be applied to

$$f(\xi) = |\{\omega \in \mathscr{W}_n^a\colon R(\omega) = \xi\}| \qquad \xi \in C_n^*$$

which counts the number of walks (of n steps, starting at 0 and ending at a) with visits specified by $\xi \in C_n^*$. Thus for ω to be counted, for each $c \in C(\xi)$, $\omega(c) = \xi(c)$ must be satisfied while if $c \notin C(\xi)$ then $\omega(c)$ must be visited exactly once. Dropping the last restriction on the sites visited at $c \notin C(\xi)$ leads to the following mapping defined for $\xi \in C_n^*$:

$$F(\xi) = \sum_{\pi > \xi} f(\pi) = |\{\omega\colon \omega(c) = \xi(c), c \in C(\xi)\}|$$

and

$$s_n(a) = f(0).$$

Now show that for $\xi \in C_n^*$, giving the vector $([\xi]_1 = 0, [\xi]_2, \ldots)$,

$$\mu(0, \xi) = (-1)^{c_\xi - i_\xi + 1} \prod_{j>1} (j-1)^{[\xi]_j}. \tag{2.4}$$

To calculate $\mu(0, \xi)$ in general it suffices to take $i_\xi = |\mathrm{Im}(\xi)| = 1$ so that $[\xi]_j = 1, [\xi]_k = 0$, $k \neq j$ and apply proposition 5 of § 3 of Rota (1964). Effectively one writes $\xi: C(\xi) \to \mathrm{Im}(\xi) = \{r_1, \ldots, r_{i_\xi}\}$ as the union of mappings $\xi_1, \ldots, \xi_{i_\xi}, \xi_j \subset \xi$, where ξ_j has domain $\xi^{-1}(r_j) \subset C(\xi)$ (and image r_j) in which case $\mu(0, \xi) = \mu(0, \xi_1) \times \ldots \times \mu(0, \xi_{i_\xi})$. Now under the special assumption $i_\xi = 1$, $\mu(0, \xi)$ is just the Möbius function for subsets of $C(\xi)$ when all singleton subsets are deleted. By definition

$$\mu(0, \xi) = -\sum_{0<\pi<\xi} \mu(0, \pi)$$

and so using induction together with the relationships $\mu(0, 0) = 1$ and

$$1 + \sum_{r=2}^{j} \binom{j}{r}(r-1)(-1)^{r+1} = 0$$

gives (2.4).

Then (2.2) follows from (2.3) since for $C(\xi) = \{c_1 < \ldots < c_{c_\xi}\}$,

$$F(\xi) = |\{\text{paths through } (c_j, \xi(c_j)), j = 0, \ldots, c_\xi + 1\}| = \prod_{k=0}^{c_\xi} w_{\Delta c_k}((\Delta\xi)_k).$$

The formulae for $w_{m(b)}$ given in the statement are standard expressions for the number of paths in a three-dimensional random walk.

Other quantities of interest in dealing with SAW may be obtained either from (2.2) or using slight modifications of the right-hand side. Thus, for instance,

$$s_n = |\mathcal{S}_n| = \sum_{\xi \in C_n^*} (-1)^{c_\xi - i_\xi + 1} \left(\prod_{j>1} (j-1)^{[\xi]_j} \right) \left(\prod_{k=0}^{c_\xi - 1} w_{\Delta c_k}((\Delta\xi)_k) \right) 6^{n - c_{c_\xi}}$$

(since $w_m = |\mathcal{W}_m| = 6^m$).

In order to obtain some appreciation of the calculations involved in (2.2), let us examine the first three terms on the right-hand side in more detail.

(a) $c_\xi = 2 (i_\xi = 1)$:

$$\sum_{\xi: c_\xi = 2} \prod_{k=0}^{c_\xi} w_{\Delta c_k}((\Delta\xi)_k) = \sum_{\substack{r_1, r_2, r_3 > 0, \\ r_1 + r_2 + r_3 = n, \\ r_2 \text{ even}}} w_{r_2}(0) \sum_{e \in K(r_1, r_3)} w_{r_1}(e) w_{r_3}(a - e)$$

where the points reachable from 0 in r_1 steps and from a in r_3 steps may be described by

$$K(r, s) = \{e: |e|^0 < r, |a - e|^0 < s\}$$

with $|a| = |a_1| + |a_2| + |a_3|$ and $|a|^0 < t$ if $|a| \leqslant t$ and $t - |a|$ is even.

(b) $c_\xi = 3 (i_\xi = 1)$:

$$\sum_{\xi: c_\xi = 3} \prod_{k=0}^{c_\xi} w_{\Delta c_k}((\Delta\xi)_k) = \sum_{\substack{r_1, r_2, r_3, r_4 > 0, \\ r_1 + r_2 + r_3 + r_4 = n, \\ r_2, r_3 \text{ even}}} w_{r_2}(0) w_{r_3}(0) \sum_{e \in K(r_1, r_4)} w_{r_1}(e) w_{r_4}(a - e).$$

(c) $c_\xi = 4(i_\xi = 1 \text{ or } 2)$:

$$\sum_{\xi: c_\xi = 4, i_\xi = 1} \prod_{k=0}^{c_\xi} w_{\Delta c_k}((\Delta\xi)_k) = \sum_{\substack{r_1, r_2, r_3, r_4, r_5 > 0, \\ r_1 + r_2 + r_3 + r_4 + r_5 = n, \\ r_2, r_3, r_4 \text{ even}}} w_{r_2}(0) w_{r_3}(0) w_{r_4}(0) \sum_{e \in K(r_1, r_5)} w_{r_1}(e) w_{r_5}(a - e)$$

$$\sum_{\xi: c_\xi = 4, i_\xi = 2} \prod_{k=0}^{c_\xi} w_{\Delta c_k}((\Delta\xi)_k) = \Sigma_{(1)} + \Sigma_{(2)}$$

where

$$\Sigma_{(1)} = \sum_{\substack{r_1, r_2, r_3, r_4, r_5 > 0, \\ r_1 + r_2 + \ldots + r_5 = n, \\ r_2, r_4 \text{ even}}} w_{r_2}(0) w_{r_4}(0) \sum_{e_1, e_2 \in K(r_1, r_3, r_5)} w_{r_1}(e_1) w_{r_3}(e_2 - e_1) w_{r_5}(a - e_2)$$

and

$$\Sigma_{(2)} = \sum_{\substack{r_1, r_2, r_3, r_4, r_5 > 0, \\ r_1 + r_2 + r_3 + r_4 + r_5 = n}} \sum_{e_1, e_2 \in K(r_1, r_2, r_3, r_4, r_5)} w_{r_1}(e_1) w_{r_2}(e_2 - e_1) w_{r_3}(e_1 - e_2) w_{r_4}(e_2 - e_1) w_{r_5}(a - e_2)$$

with

$$K(r, s, t) = \{(e_1, e_2): |e_1|^0 < r, |e_2 - e_1|^0 < s, |a - e_2|^0 < t\}$$

and

$$K(r_1, r_2, r_3, r_4, r_5) = \{(e_1, e_2): |e_1|^0 < r_1, |a - e_2|^0 < r_5, |e_2 - e_1|^0 < r_2, r_3, r_4\}.$$

These special cases illustrate the way in which the formula in (2.2) may be developed into an algorithm for computation. Although it compares favourably with techniques for enumeration mentioned in the introduction as far as obtaining results for small n, it is the author's belief that the real use of theorem 2.1 may be rather in application to the important unsolved asymptotic questions about S_n. This is now briefly discussed.

3. Remarks

The enumeration result reported here as theorem 2.1 represents the starting point for a, by now, long-running attempt at deriving detailed asymptotic results about $s_n(a)$ from (2.2). This investigation also includes closely related problems about Hamilton circuits in graphs. Little tangible success has come from this approach, mainly it would seem because a sufficiently neat analytic expression for $\Sigma_{\xi \in C_n^*}$ seems out of reach. It remains therefore an interesting open question whether formulae such as (2.2), obtained using Möbius inversion, may provide a useful technique for asymptotic analysis of $s_n(a)$ or not. The analogy for hoping that such an approach might deliver results is with the sieving techniques of analytic number theory which as their very basic starting point use Möbius inversion for the integers (ordered by divisibility) (see, for example, ch 1 and the opening pages of ch 2 of Halberstam and Richert (1974)).

References

Chay T R 1971 *J. Chem. Phys.* **54** 1852–65
Freed K F 1981 *Ann. Prob.* **9** 537–51
Halberstam H and Richert H E 1974 *Sieve Methods* (London: Academic)
Hammersley J M, Torrie G M and Whittington S G 1982 *J. Phys. A: Math. Gen.* **15** 539–71
Martin J L, Sykes M F and Hioe F T 1967 *J. Chem. Phys.* **46** 3478–81
Rota G C 1964 *Z. Wahrscheinlichkeitstheorie* **2** 340–68
Torrie G M and Whittington S G 1975 *J. Phys. A: Math. Gen.* **8** 1178–84
Wall F T and Seitz W A 1979 *J. Chem. Phys.* **70** 1860–3