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Nonergodicity of Local, Length-Conserving Monte Carlo Algorithms for the Self-Avoiding Walk

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It is proved that every dynamic Monte Carlo algorithm for the self-avoiding walk based on a finite repertoire of local, N-conserving elementary moves is nonergodic (here N is the number of bonds in the walk). Indeed, for large N, each ergodic class forms an exponentially small fraction of the whole space. This invalidates (at least in principle) the use of the Verdier–Stockmayer algorithm and its generalizations for high-precision Monte Carlo studies of the self-avoiding walk.

KEY WORDS: Self-avoiding walk; polymer; Monte Carlo; algorithm; lattice model; ergodicity; Verdier–Stockmayer.

1. INTRODUCTION

Dynamic Monte Carlo methods have been widely employed in the numerical study of the self-avoiding walk (SAW) and related models of polymer molecules. In this note we prove that a large class of such methods—including most of the commonly employed ones—are, as a matter of principle, *invalid* for the purpose for which they were designed.

More precisely, we consider dynamic Monte Carlo algorithms for the SAW that are based on a finite repertoire of *local, N-conserving* elementary moves (here N is the number of bonds in the walk; a precise definition of this class of algorithms is given in Section 2). Algorithms of this type have been proposed by Delbrück,[1] Verdier and Stockmayer,[2,3] and many others.[4–12] We show here that every algorithm of this type is *nonergodic* for sufficiently large N: some SAWs cannot be transformed into some

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others by any sequence of allowed moves. Indeed, we show that for large N, each ergodic class includes only an *exponentially small fraction* of the SAW configuration space. Precise statements of these results are given in Section 2 (Theorems 1 and 2).

In fact, the nonergodicity of the Verdier–Stockmayer algorithm was noticed already more than 15 years ago by Heilmann[4] and Verdier,[3],[3] although it has perhaps not been widely appreciated since then; one recent discussion is that of Heilmann and Rotne.[11] Our contribution here is to show that this phenomenon is a very general one, which is inherent in a wide class of algorithms; it cannot be evaded merely by tinkering with the bead-movement rules. The *practical* implications of these facts for Monte Carlo studies of the SAW are perhaps somewhat controversial; we discuss them at length in Section 4.

2. DEFINITIONS AND RESULTS

An *N-step self-avoiding walk* (SAW) ω on the d-dimensional simple (hyper)cubic lattice $\mathbb{Z}^d$ is a sequence of *distinct* points $\omega_0, \omega_1, \ldots, \omega_N \in \mathbb{Z}^d$ such that each point is a nearest neighbor of its predecessor, i.e., $|\omega_i - \omega_{i-1}| = 1$ for $1 \leqslant i \leqslant N$. We shall sometimes refer to the points ω_i of the walk as "beads" and to the steps (ω_{i-1}, ω_i) as "bonds."

Let $S^{(N)}$ be the set of all N-step SAWs on $\mathbb{Z}^d$ that begin at the origin ($\omega_0 = 0$) and end anywhere. In what follows, N will be fixed, and $S^{(N)}$ will be our configuration space. [Alternatively, one could define $S^{(N)}$ to be the space of equivalence classes of N-step SAWs modulo translation; our definition of $S^{(N)}$ corresponds to choosing one particular representative from each equivalence class.]

Our theorems apply to all dynamic algorithms for the SAW that are based on a *finite repertoire of local, N-conserving elementary moves*. By a "local" move we mean one that acts on a contiguous group of beads of no more than some finite maximum number. We formalize this concept mathematically as follows:

Let ω, ω' be N-step SAWs and let $k \geqslant 1$ be an integer. We say that ω *and ω' are directly connected by a k-bead move* if ω and ω' are identical except perhaps for some contiguous group of k or fewer beads, i.e., if there exists an index i ($0 \leqslant i \leqslant N-k+1$) such that $\omega_j = \omega'_j$ for $j = 0, 1, \ldots, i-1$, $i+k, \ldots, N$. We say that ω *and ω' are connected by k-bead moves* if there exists a finite sequence $\omega \equiv \omega^{(0)}, \omega^{(1)}, \ldots, \omega^{(m)} \equiv \omega'$ of N-step SAWs such that $\omega^{(l-1)}$ and $\omega^{(l)}$ are directly connected by a k-bead move for each l

[3] Actually, Heilmann[4] and Verdier[3] found *two distinct* causes of nonergodicity: "knots" and "double culs-de-sac," respectively. See the discussion in Section 3.

($1 \leqslant l \leqslant m$). Finally, we say that ω *and* ω' *are connected by k-bead moves and translation* if there exists an N-step SAW $\tilde{\omega}$ and a vector $\tau \in \mathbb{Z}^d$ such that ω and $\tilde{\omega}$ are connected by k-bead moves, and $\omega_j' = \tilde{\omega}_j + \tau$ for all j ($0 \leqslant j \leqslant N$).

The relation of "connection by k-bead moves and translation" is easily seen to be reflexive, symmetric, and transitive—i.e., an equivalence relation—so the space $S^{(N)}$ decomposes into equivalance classes, which we shall call *ergodic classes*. The k-bead algorithm is said to be *ergodic* (for the given N) if there is only one ergodic class (i.e., all of $S^{(N)}$).

A full specification of a dynamic Monte Carlo algorithm would require, of course, a listing not only of the "allowed elementary moves," but also of their probabilities. For our purposes, however, this detailed information is unnecessary. All we need to know is that, for any algorithm based on a "finite repertoire of local, N-conserving moves," the set of allowed elementary moves (i.e., those having nonzero probability) must be a subset of the k-bead moves as defined above, for some finite integer k.

Remarks. 1. Note that there is a slight difference between k-bead moves affecting an "internal k-bead group" (i.e., $1 \leqslant i \leqslant N-k$) and those affecting an "end k-bead group" ($i=0$ or $i=N-k+1$). In the former case, we remove a segment of $k+1$ bonds and replace it by another segment of $k+1$ bonds having the same initial point ω_{i-1} and the same final point ω_{i+k}. In the latter case, say for $i=0$, we remove a segment of k bonds and replace it by another segment of k bonds having the same final point $\omega_{i+k} = \omega_k$, but *not* necessarily the same initial point ω_0; the case $i = N-k+1$ is analogous, with "initial" and "final" interchanged.

2. Our concept of "k-bead move" is a slight generalization of Meirovitch's[12] concept of "transition to a new allowed local conformation (ALC)." The only difference is that he restricts himself to the case $k=3$, and imposes an additional condition of "contour noncrossability."

Theorem 1 ($d=2$). Let k be any positive integer. Then, for all sufficiently large N ($N \geqslant 16k+63$ will do), there exists an N-step SAW that is not connected to any other N-step SAW by k-bead moves. In particular, the k-bead algorithm is nonergodic.

Proof. Fix $a \geqslant k$, and let ω be the $(6a+17)$-step SAW

$$\mathrm{N}^a\mathrm{E}\mathrm{S}^{a+1}\mathrm{W}^2\mathrm{N}^{a+2}\mathrm{E}^5\mathrm{S}^{a+2}\mathrm{W}^2\mathrm{N}^{a+1}\mathrm{E}\mathrm{S}^a$$

where we have denoted the successive steps of the walk as north (N), south (S), east (E), or west (W). (This walk is drawn for $a=5$ in Fig. 1.) We shall show that ω is not connected to any other $(6a+17)$-step SAW by k-bead moves.

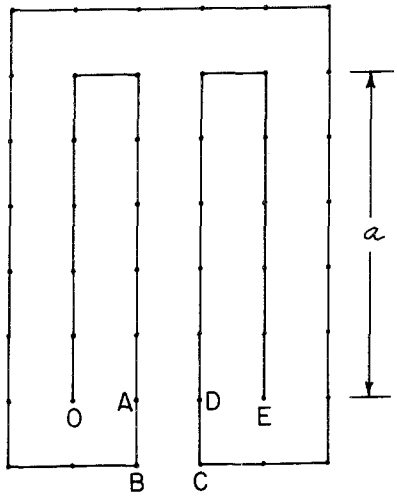


Fig. 1. A frozen configuration, drawn here for $a = 5$.

Suppose that we excise a k-bead segment $\omega_i,\ldots,\omega_{i+k-1}$ (here $0 \leqslant i \leqslant N-k+1$ and $N \equiv 6a+17$). Then we have to replace it with a $(k+1)$-step SAW going from ω_{i-1} to ω_{i+k} (or, if $i=0$, with a k-step SAW going from anywhere to $\omega_{i+k}=\omega_k$; or, if $i=N-k+1$, with a k-step SAW going from $\omega_{i-1}=\omega_{N-k}$ to anywhere) which lies entirely in the set

$$W^* \equiv \mathbb{Z}^2 \setminus \{\omega_0, \omega_1,\ldots, \omega_{i-2}, \omega_{i+k+1},\ldots, \omega_N\}$$

We shall show that there is a *unique* such SAW, namely the original one $\omega_{i-1},\ldots,\omega_{i+k}$ (or $\omega_0,\ldots,\omega_k$ in case $i=0$, or $\omega_{N-k},\ldots,\omega_N$ in case $i=N-k+1$).

Let us call "outside beads" those numbered $2a+2$ through $N-(2a+2)$, inclusive (that is, B through C in Fig. 1), and "inside beads" all the rest. We then distinguish three cases:

1. The beads $i-1,\ldots, i+k$ are all outside beads.
2. The beads $i-1,\ldots, i+k$ are all inside beads.
3. The beads $i-1,\ldots, i+k$ include both outside and inside beads.

Case 1. $2a+3 \leqslant i \leqslant N-(2a+2)-k$. Since the inside beads are immobile, we have

$$W^* \subset W^{**} \equiv \mathbb{Z}^2 \setminus \{\omega_0,\ldots, \omega_{2a+1}, \omega_{N-(2a+1)},\ldots, \omega_N\}$$

Since $k+1 < \frac{1}{2}(\text{perimeter of outside}) = a+7$, it follows that $\omega_{i-1},\ldots,\omega_{i+k}$ is the unique shortest path in W^{**} from ω_{i-1} to ω_{i+k}, hence the unique $(k+1)$-step SAW in W^{**} from ω_{i-1} to ω_{i+k}.

Case 2a. Beads $i-1,..., i+k$ are all contained in the initial segment of inside beads (OA in Fig. 1), but are not an end group ($1 \leqslant i \leqslant 2a+1-k$). It is easily seen that the only $(2a+1)$-step SAW ω' from $O=\omega_0$ to $A=\omega_{2a+1}$ lying entirely in $\mathbb{Z}^2 \setminus \{\omega_0,..., \omega_{2a+1}\}$ is the original one $\omega_0,..., \omega_{2a+1}$. (*Proof*: ω'_1 must be ω_1, and ω'_{2a} must be ω_{2a}, because they are the only available neighbors. Continue with ω'_2 and ω'_{2a-1}, etc.)

Case 2b. Beads $i-1,..., i+k$ are all contained in the final segment of inside beads (DE in Fig. 1), but are not an end group ($N-2a \leqslant i \leqslant N-k$). This case is exactly analogous to case 2a.

Case 2c. $i=0$ (end-group move). Because $a \geqslant k$, the points $\omega_0,..., \omega_k$ all lie in a single vertical line. Thus, the only k-step SAW ω' from *anywhere* to ω_k lying entirely in W^* is the original one $\omega_0,..., \omega_k$. (*Proof*: ω'_{k-1} must be ω_{k-1}, because it is the only available neighbor, etc.)

Case 2d. $i=N-k+1$ (end-group move). This case is exactly analogous to case 2c.

Case 3a. Beads $i-1,..., i+k$ include some from the initial segment of inside beads (OA in Fig. 1) and some outside beads ($2a+2-k \leqslant i \leqslant 2a+2$). Arguing as in case 2a, we conclude that the beads up to and including B are forced to be in their original positions (i.e., $\omega'_j = \omega_j$ for $j=i,..., 2a+2$). But we are then reduced to case 1.

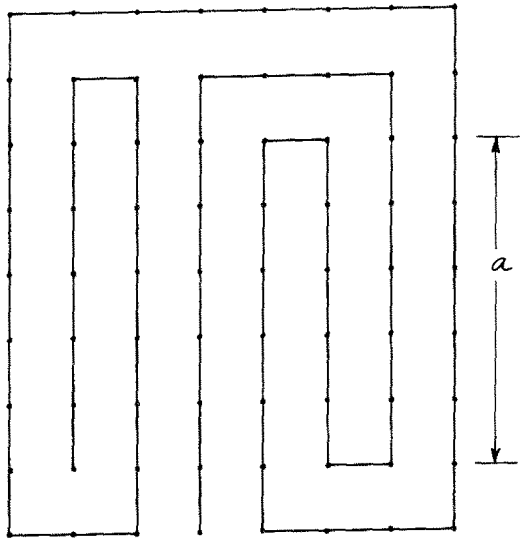
Case 3b. Beads $i-1,..., i+k$ include some from the final segment of inside beads (DE in Fig. 1) and some outside beads $[N-(2a+1)-k \leqslant i \leqslant N-(2a+1)]$. This case is exactly analogous to case 3a.

This proves the theorem for the special case $N \geqslant 6k+17$ with $N \equiv 5 \pmod 6$.

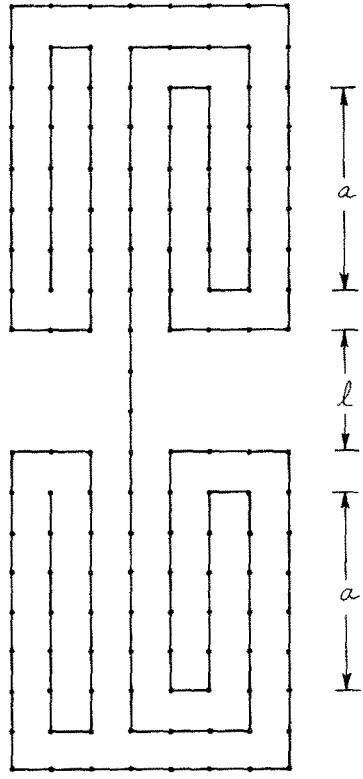
We now sketch the proof of theorem for arbitrary large N, leaving the details to the reader. Fix $a \geqslant k$, and consider the $(8a+31)$-step SAW

$$N^{a+1}ES^{a+2}W^2N^{a+3}E^7S^{a+3}W^3N^{a+1}ES^aEN^{a+1}W^3S^{a+2}$$

(This walk is drawn for $a=5$ in Fig. 2a.) It is straightforward to show, by a slight extension of the foregoing proof, that this SAW is not connected to any other $(8a+31)$-step SAW by k-bead moves. Now, imagine connecting the walk of Fig. 2a to an inverted image of itself, with the connection being a straight rod of length $l \geqslant 1$ (see Fig. 2b). It is then easy to see that this $(16a+62+l)$-step SAW is not connected to any other by k-bead moves. (The top and bottom pieces are "frozen" as in Fig. 2a, and the connecting



(a)



(b)

Fig. 2. More frozen configurations, drawn here for $a = 5$.

rod is "frozen" because it is taut.) This completes the proof of the theorem for arbitrary $N \geqslant 16k + 63$. ∎

Remark. Obviously our lower bound on N is far from optimal. An alternate bound can be obtained by considering the configuration of Fig. 2a with some (but not too many!) of the final beads missing—details are left to the reader. Also, a quick proof of nonergodicity for all $N \geqslant 8k + 31$ can be obtained by appending a "tail" to the configuration of Fig. 2a: although this SAW is not completely "frozen," it is nevertheless not deformable into a straight rod by k-bead moves.

Our next goal is to show that for large N, each ergodic class includes only an exponentially small fraction of the SAW configuration space. Our main tool is a deep theorem of Kesten,[13] which we now proceed to explain. Let $\omega \in S^{(M)}$ and $\omega' \in S^{(N)}$, with $N \geqslant M$; we refer to ω as a *pattern*, and say that ω *occurs at the* rth *step of* ω' $(0 \leqslant r \leqslant N - M)$ if $\omega'_{r+i} = \omega'_r + \omega_i$ for $0 \leqslant i \leqslant M$. There exist patterns that may occur once or twice on SAWs in $\mathbb{Z}^d$ but never more than twice (see Hammersley and Whittington[14] for an example). But three times is always enough:

Lemma. Let ω be a pattern. Then the following are equivalent:

(a) There exists a SAW on which ω occurs at least three times.

(b) There exists an infinite SAW on which ω occurs infinitely many times.

(c) There exists a SAW ω' on which ω occurs, and a cube D such that ω' lies in D and has its endpoints at vertices of D.

The implications (c) $\Rightarrow$ (b) $\Rightarrow$ (a) are obvious, and (b) $\Rightarrow$ (c) is not difficult. The only nontrivial part of this Lemma is (a) $\Rightarrow$ (b), which was proven by Hammersley and Whittington.[14]

Now let

$$c_N \equiv \text{card}(S^{(N)}) \equiv \text{the number of distinct } N\text{-step SAWs} \tag{2.1}$$

and, for each pattern ω,

$$c_N(j, \omega) \equiv \text{card}(\{\omega' \in S^{(N)}\text{: } \omega \text{ occurs on } \omega' \text{ at most } j \text{ times}\}) \tag{2.2}$$

Kesten's theorem then states that any pattern ω that is capable of occurring at least three times on a SAW must in fact occur at least εN times on an N-step SAW, with the exception of "exponentially few" $\omega' \in S^{(N)}$:

Kesten's Theorem (Ref. 13, Theorem 1). Let ω be a pattern satisfying the conditions of the lemma. Then there exist constants ε, C_1, $C_2 > 0$ such that

$$c_N(\varepsilon N, \omega)/c_N \leqslant C_1 e^{-C_2 N} \tag{2.3}$$

for all N. (Kesten's theorem actually states a bit more than this, but this is all we shall need.)

We can now state our second main result:

Theorem 2 ($d=2$). Let k be any positive integer, and let

$$c_N^{(k)} \equiv \max\{\mathrm{card}(\mathscr{C}): \mathscr{C} \text{ is an ergodic class of } S^{(N)} \text{ for the } k\text{-bead algorithm}\} \tag{2.4}$$

Then there exist constants C_3, $C_4 > 0$ (depending on k) such that

$$c_N^{(k)}/c_N \leqslant C_3 e^{-c_4 N} \tag{2.5}$$

for all N.

Proof. Fix $a \geqslant k$, and let P be the SAW

$$N^{a+2}W^3S^{a+1}EN^aES^{a+1}W^3N^{a+3}E^9S^{a+3}W^3N^{a+1}ES^aEN^{a+1}W^3S^{a+2}$$

of total length $L = 10a + 39$. (This walk is drawn for $a=4$ in Fig. 3.) Now let ω be an N-step SAW ($N \geqslant L$). Reasoning as in the proof of Theorem 1 shows that if P occurs in ω at the mth step, and ω is connected to ω' by k-bead moves, then P must occur in ω' at the mth step. (In fact, we must have $\omega_j = \omega'_j$ for $m \leqslant j \leqslant m + L$.) For $0 \leqslant m_1 < m_2 < \cdots < m_t < N$, let

$$E^N(m_1, m_2, \ldots, m_t) \equiv \{\omega \in S^{(N)}: P \text{ occurs in } \omega \text{ at } m_j \text{ for each } j = 1, \ldots, t \text{ and nowhere else in } \omega\} \tag{2.6}$$

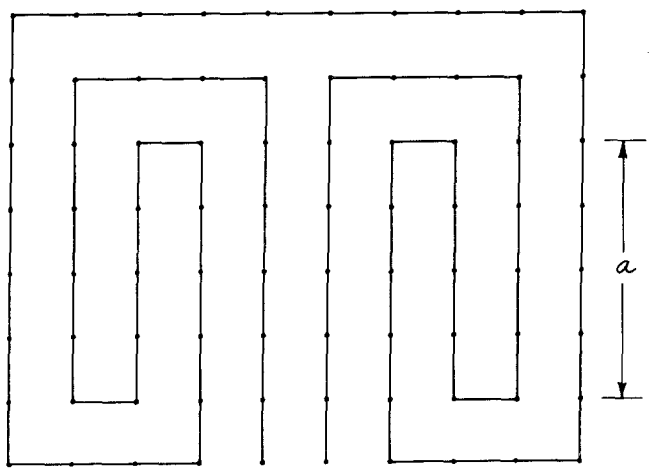


Fig. 3. The pattern P employed in the proof of Theorem 2, drawn here for $a=4$.

For $t=0$, this is the set of ω in which P nowhere occurs. (For $t \geqslant 2$, it is easy to see that successive occurrences of P in ω cannot overlap, so we must have $m_j - m_{j-1} > L$.) From the foregoing it follows that each ergodic class for the k-bead algorithm is contained in some $E^N(m_1, m_2, \ldots, m_t)$. By Kesten's theorem there exist constants ε, C_1, $C_2 > 0$ such that

$$c_N^{-1} \operatorname{card}\left(\bigcup_{t \leqslant \varepsilon N} \bigcup_{m_1 < m_2 < \cdots < m_t} E^N(m_1, m_2, \ldots, m_t) \right)$$
$$\equiv c_N(\varepsilon N, P)/c_N \leqslant C_1 e^{-C_2 N} \tag{2.7}$$

Now define the following map, which "chops off" each occurrence of P and replaces it by a single bond:

$$f: E^N(m_1, m_2, \ldots, m_t) \to S^{[N-t(L-1)]}$$

is given by

$$(f(\omega))_i = \begin{cases} \omega_i & \text{for } 0 \leqslant i \leqslant m_1 \\ \omega_{i+r(L-1)} & \text{for } m_r - (r-1)(L-1) < i \leqslant m_{r+1} - r(L-1) \\ & \text{and } 1 \leqslant r < t \\ \omega_{i+t(L-1)} & \text{for } m_t - (t-1)(L-1) < i \leqslant N - t(L-1) \end{cases} \tag{2.8}$$

Since f is one-to-one, it follows that

$$\operatorname{card}(E^N(m_1, m_2, \ldots, m_t)) \leqslant C_{N-t(L-1)} \tag{2.9}$$

Moreover, it is known[15] that $\mu^M \leqslant c_M \leqslant C_5 \mu^M \exp(C_6 \sqrt{M})$ for suitable constants μ, C_5, and C_6. It follows that if $t > \varepsilon N$, then

$$c_{N-t(L-1)}/c_N \leqslant C_7 e^{-C_8 N} \tag{2.10}$$

for some constants C_7, $C_8 > 0$. The theorem then follows from (2.7) combined with (2.9)–(2.10). ∎

The extension of Theorems 1 and 2 to $d=3$ uses identical arguments to those we have used in proving the $d=2$ case, so we will omit all details except for the construction of a SAW that is not connected to any other SAW by k-bead moves, and plays the role of the pattern P in Theorem 2.

Fix $k \geqslant 4$ (obviously this is no loss of generality). We will construct a SAW ω of length $N \equiv k^3 + 9k^2 + 6k - 23$ that lies in the box

$$B = \{(x, y, z): 0 \leqslant x \leqslant k+6,\ 0 \leqslant y \leqslant k-1,\ -1 \leqslant z \leqslant k\}$$

has both endpoints on the boundary of this box, and is connected to no other N-step SAW by k-bead moves.

The solid lines in Fig. 4a show the middle part of ω; it is contained in the boundary of the box B. The rest of ω fills up the interior of B (as the dashed lines in Fig. 4a begin to indicate), and the middle part wraps it up tightly so that nothing can move. Figure 4b is a top view (xy-plane projection) of ω, for the case $k = 6$. A solid dot signifies a segment of the walk

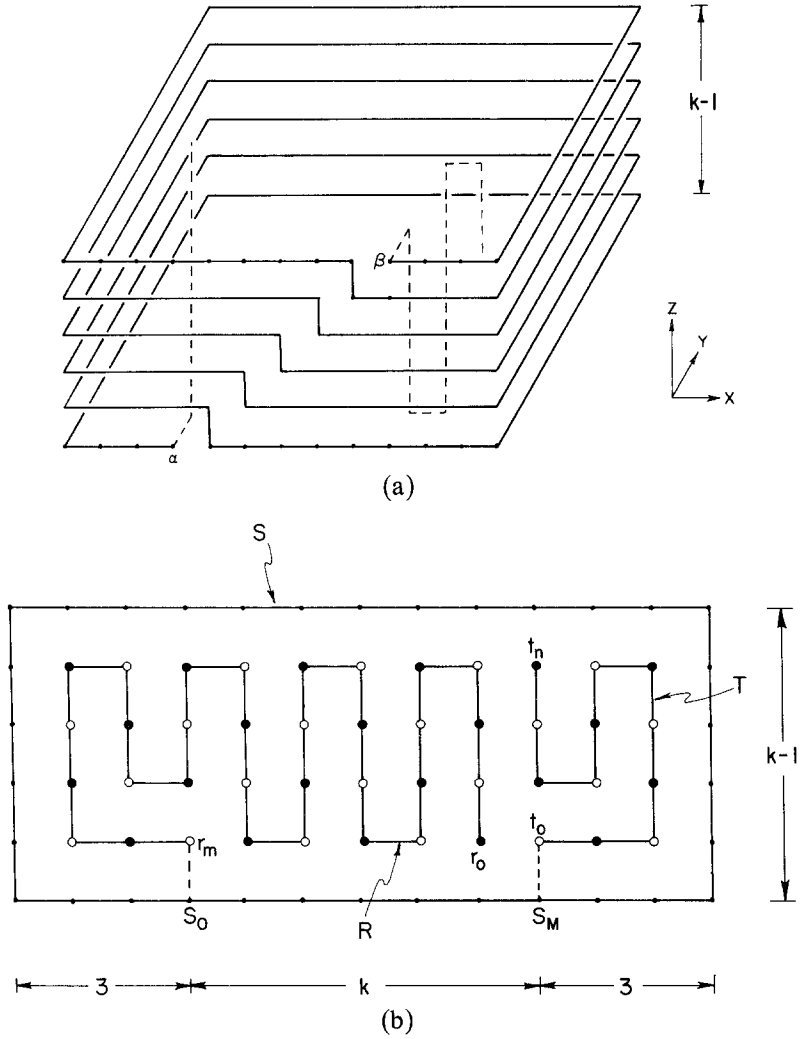


Fig. 4. The walk ω. (a) Perspective view: (—) The middle part of ω (called S); (– –) beginning to indicate the first and last parts. Here $\alpha = (3, 0, 0)$ and $\beta = (k+3, 0, k-1)$. (b) Top view: (●) Segments of the walk going in the $+z$ direction; (○) segments of the walk going in the $-z$ direction.

going in the $+z$ direction; an open dot signifies a segment going in the $-z$ direction. We now describe the construction in detail.

First we construct a shorter SAW, S, of length $M \equiv 4k^2 + 10k - 1$, which will be the "middle" part of ω as shown in Fig. 4a. For $0 \leqslant i \leqslant k-1$, let U^i be the $(4k+9)$-step SAW with starting point $(i+3, 0, i)$ and terminal point $(i+4, 0, i)$ which passes through the points

$$\{(x, y, i) \in B: x = 0 \text{ or } x = k+6 \text{ or } y = 0 \text{ or } y = k-1\}$$

Also, let V^i be the one-step SAW from $(i+4, 0, i)$ to $(i+4, 0, i+1)$. Then S is the walk formed by concatenating U^0, V^0, U^1, V^1,..., U^{k-2}, V^{k-2}, U^{k-1}. Thus, the endpoints of S are $(3, 0, 0)$ and $(k+3, 0, k-1)$.

Next, we construct the template for the rest of ω. First, let

$$C = \{(x, y): 0 < x < k+6 \text{ and } 0 < y < k-1\}$$

Then let $R = (r_0, r_1, ..., r_m)$ and $T = (t_0, t_1, ..., t_n)$ be SAWs in $\mathbb{Z}^2$ such that: $m \geqslant 2$ and $n \geqslant 2$; $r_m = (3, 1)$ and $t_0 = (k+3, 1)$; R and T are disjoint, and the union of their ranges is precisely C. [In particular, it follows that $m + n + 2 = (k+5)(k-2)$.] One possible choice of R and T is shown in Fig. 4b for the case $k = 6$. Essentially, R and T will be the projections onto $\mathbb{Z}^2$ of the "first" and "last" parts of ω, respectively. The general scheme is: ω goes "up" ($+z$ direction) k steps, then takes a "horizontal" (xy-plane) step according to R or T, then goes "down" k steps, then takes another "horizontal" step, and so on.

Notation. For a point $r = (x, y) \in \mathbb{Z}^2$ and an integer z, let (r, z) denote (x, y, z).

We are now ready to define $\omega = (\omega_0, \omega_1, ..., \omega_N)$:

1. For $0 \leqslant j < m$ and $0 \leqslant i \leqslant k+1$, define

$$\omega_{j(k+2)+i} = \begin{cases} (r_j, i-1) & \text{if } m-j \text{ is odd} \\ (r_j, k-i) & \text{if } m-j \text{ is even} \end{cases}$$

2. For $0 \leqslant i \leqslant k$, define $\omega_{m(k+2)+i} = (r_m, k-i)$.
3. Define $\omega_{m(k+2)+k+1} = (3, 0, 0)$.
4. For $0 \leqslant i \leqslant 4k^2 + 10k - 1$, define $\omega_{m(k+2)+k+1+i} = S_i$.

[Let $J = 4k^2 + 10k + m(k+2) + k$. So we are so far up to $\omega_J = (k+3, 0, k-1)$.]

5. For $1 \leqslant i \leqslant k+1$, define $\omega_{J+i} = (k+3, 1, k-i)$.

6. For $1 \leqslant j \leqslant n$ and $0 \leqslant i \leqslant k+1$, define

$$\omega_{J+j(k+2)+i} = \begin{cases} (t_j, i-1) & \text{if } j \text{ is odd} \\ (t_j, k-i) & \text{if } j \text{ is even} \end{cases}$$

This completes the definition of ω. It is now left to the reader to show, as in Theorems 1 and 2, that ω is not connected to any other N-step SAW by k-bead moves.

We expect that Theorems 1 and 2 hold also in lattice dimensions $d \geqslant 4$, but we have not worked out a proof: this is left as an exercise for readers whose capacity for multidimensional geometric visualization surpasses our own.

3. SOME REMARKS (HISTORICAL AND OTHER)

The proofs given in Section 2 are very general, but very crude: the lower bounds on N given there are far from optimal. It is perhaps of interest, therefore, to look at some specific algorithms in the literature.

Figure 5 shows some examples of k-bead moves with $k = 1, 2$, and 3. Moves A–C are a complete listing of the one-bead moves. Moves D–F are a partial listing of the two-bead moves (there are, in addition, numerous two-bead end-group moves, and in $d \geqslant 3$ there are some additional two-bead internal-group moves as well). Move G is a typical three-bead move (there are many others). All of the local, N-conserving algorithms in Refs. 2–11 are based on some subset of moves A–F; the algorithm of Delbrück[1] uses some additional two-bead moves, and the algorithm of Meirovitch[12] uses some additional two-bead and three-bead moves.

The foregoing algorithms are nonergodic already for small values of N:

1. The "double cul-de-sac" configuration shown in Fig. 6a is completely "frozen" under elementary moves A, B, and D–F. It follows that the original Verdier–Stockmayer algorithm[2,3] and most of its generalizations[4,6–11] are nonergodic (in $d = 2$) already for $N = 11$.

2. If move C is allowed, then the configuration of Fig. 6a is no longer frozen, but that of Fig. 6b still is. Thus, any algorithm based on moves A–F is nonergodic (in $d = 2$) for $N = 15$.

3. If two-bead end-group moves are allowed, then the configuration of Fig. 6b is no longer frozen, but that of Fig. 6c still is. Thus, any algorithm based on one-bead and two-bead moves is nonergodic (in $d = 2$) for $N = 19$.

4. When three-bead moves are allowed, it is not sufficient simply to make the "double cul-de-sac" taller. Indeed, *any* double cul-de-sac of the

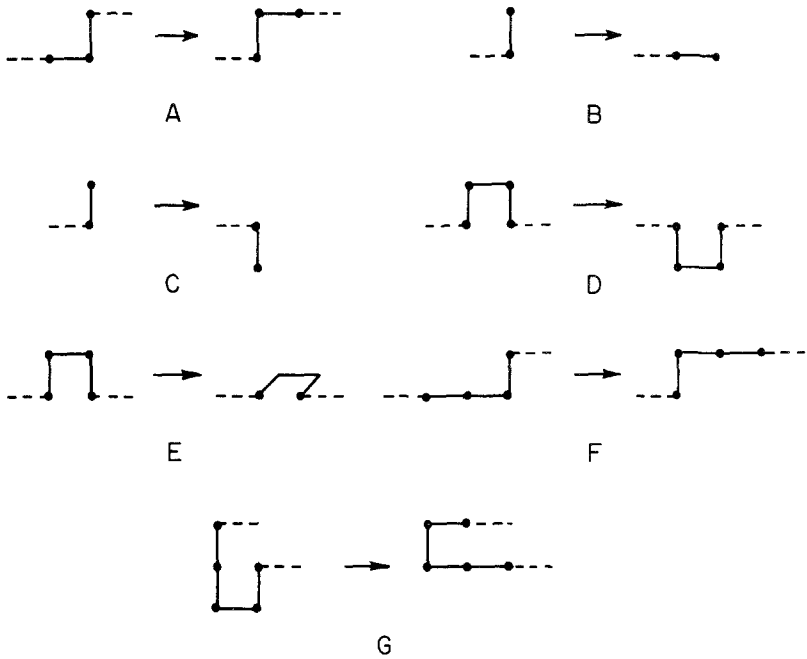


Fig. 5. Some examples of local, N-conserving elementary moves. One-bead moves: (A) 180° kink-jump, (B) 90° end-bond rotation, (C) 180° end-bond rotation. Two-bead moves: (D) 180° crankshaft, (E) 90° crankshaft ($d \geqslant 3$ only), (F) two-bead kink-jump. A three-bead move: (G) three-bead L flip.

kind shown in Fig. 6, no matter how tall, can be unfolded into a straight rod by repeated use of the moves A, B, and G. (The reader might find it amusing to work out the required sequence of moves.) But only one additional trick is needed: by folding the double cul-de-sac once more, as in Fig. 1, a frozen configuration can be obtained for the k-bead algorithm for arbitrary k.

The nonergodicity of the Verdier–Stockmayer algorithm due to double culs-de-sac was noticed already by Verdier[3] in 1969. Indeed, his article shows a three-dimensional analogue of the double cul-de-sac, with $N = 21$.

An entirely different type of nonergodicity arises in dimension $d = 3$ (and only there) because of the possibility of knots, as was first pointed out by Heilmann[4] in 1968. The simplest knotted configuration is shown in Fig. 7: it has $N = 18$, and although it is not completely "frozen," it nevertheless cannot be deformed to a straight rod using moves A–F. We believe that analogous knots can be constructed for the k-bead algorithm for arbitrary k, although we have not worked out the details. (An excellent

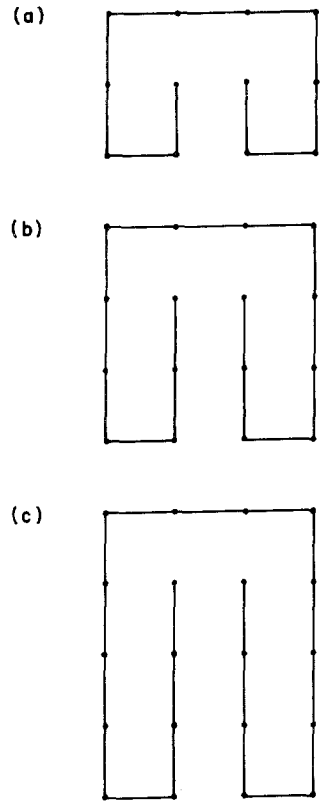


Fig. 6. Some "double cul-de-sac" configurations, frozen in the Verdier–Stockmayer algorithm and its generalizations.

bibliography on knots in polymer physics can be found in an article of Michels and Wiegel.[16])

In this paper we have restricted attention, for simplicity, to SAWs on the simple (hyper)cubic lattice $\mathbb{Z}^d$, but analogous results presumably hold for other regular lattices. Local, N-conserving Monte Carlo algorithms for SAWs on the tetrahedral lattice have been employed by Monnerie and Gény[17] and Kremer *et al.*[18]

An analogue of the Verdier–Stockmayer algorithm has also been devised[19,20] for models of continuum polymer chains. In the "pearl-necklace" model, for example, hard spheres of diameter D are connected by freely jointed rods of length L ($D \leqslant L$). The "kink-jump" algorithm[19,20] then moves a bead ω_i randomly along the circle defined by the fixed neighboring beads ω_{i-1} and ω_{i+1}. Perhaps this algorithm is also nonergodic, at least for D/L sufficiently close to 1; this is an open question.

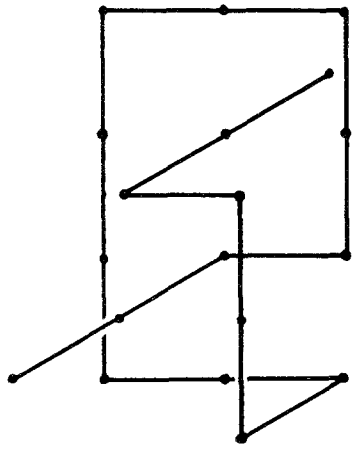


Fig. 7. A "knot" that cannot be deformed to a straight rod using moves A–F.

A very different type of nonergodicity occurs in the "slithering-snake" (reptation) algorithm of Kron[21,22] and Wall and Mandel.[23,24] The elementary moves of this algorithm are "slithering" motions: one step is appended at one end of the walk, and one step is simultaneously deleted from the other end. Such a move is N-conserving, but is *nonlocal* according to our definition. In this algorithm, frozen configurations occur[22,23] when both ends of the walk are trapped in culs-de-sac. The simplest such configuration is shown (for $d=2$) in Fig. 8, and has $N=14$. The superficial resemblance between Figs. 1 and 8 is, however, very misleading: the nonergodicities in the two types of algorithms are of radically different natures. In the local, N-conserving algorithms, nonergodicity is caused by the occurrence of a frozen conformation *anywhere* along the walk (cf. Fig. 3 and the proof of Theorem 2). In the slithering-snake algorithm, by contrast, nonergodicity occurs only if the *ends* of the walk are trapped in culs-de-sac. Indeed, in the slithering-snake algorithm, the ergodic class of the N-step straight rod includes all N-step SAWs that can occur on some

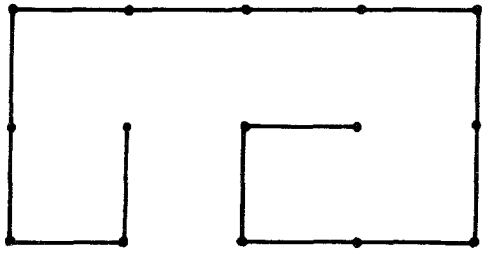


Fig. 8. A "double cul-de-sac" frozen in the slithering-snake (reptation) algorithm.

$2N$-step SAW in the sense defined preceding Theorem 2.[4] In particular, any N-step SAW that can be extended to a $2N$-step SAW belongs to the ergodic class of the straight rod. Let d_N be the number of N-step SAWs that can be extended to a $2N$-step SAW. Clearly $c_{2N} \leqslant d_N^2$, so that $d_N \geqslant c_{2N}^{1/2}$. Hence, the fraction of $S^{(N)}$ that belongs to the ergodic class of the straight rod is $\geqslant d_N/c_N \geqslant c_{2N}^{1/2}/c_N$. This quantity behaves as follows:

1. Nonrigorously, $c_{2N}^{1/2}/c_N \sim N^{-(\gamma-1)/2}$. (This follows from the believed scaling behavior $c_N \sim \mu^N N^{\gamma-1}$.)

2. Rigorously, $c_{2N}^{1/2}/c_N \geqslant C_9 \exp(-C_{10}\sqrt{N})$. (This follows from the rigorous bounds[15] $\mu^N \leqslant c_N \leqslant C_5 \mu^N \exp(C_6\sqrt{N})$ noted earlier.)

Thus, the analogue of Theorem 2 for the slithering-snake algorithm is *false*! (It would be interesting to know, even heuristically, the behavior of d_N/c_N.)

4. PRACTICAL IMPLICATIONS

What are we to make of these failures of ergodicity? Most workers in the field seem to have ignored the question entirely; among those who have considered it, the general belief[3,4,23] seems to be that the "forbidden" configurations are rare, and therefore that their exclusion will cause a negligible error in practice. Heilmann[4] argues, for example, that "the number of configurations with tight knots is a very small fraction, only, of the total number of configurations. Therefore disregarding these configurations totally ... probably introduces only a negligible difference." Similarly, Wall and Mandel,[23] commenting on the slithering-snake algorithm, argue that "the probability of one cul-de-sac is small, especially in three dimensions; accordingly, the probability of two cul-de-sacs [*sic*] for the same molecule will be exceedingly small indeed, being of the order of the square of the probability for one.... The difference [due to nonergodicity] should be very small indeed and can be neglected for most purposes. (This is borne out by numerical calculations.)"

More recently, however, Heilmann and Rotne[11] have sounded a cautionary note: "For moderate values of N it is only a small fraction of the conformations which is separated from the main ergodic class ... But as N increases the probability of having a locked conformation in part of the

[4] *Proof*: Let $\omega \in S^{(N)}$ occur on $\omega' \in S^{(2N)}$; we wish to show that ω can be deformed by the reptation algorithm into a rod. Let R be the smallest rectangular box containing ω', and let ω'_j be a point of ω' that lies on the boundary of R. Now let ω'' be the N-step SAW $(\omega'_j, \omega'_{j+1}, \ldots, \omega'_{j+N})$ if $j \leqslant N$, or $(\omega'_{j-N}, \ldots, \omega'_j)$ if $j > N$. Clearly, ω can be deformed into ω'' (by "slithering" along ω'), and ω'' can be deformed into a rod (by "pulling" at the end that touches the boundary of R).

chain increases (to one in the limit $N \to \infty$) and the fraction of conformations which belong to the main ergodic class (the class with all the open conformations) will decrease (to zero in the limit $N \to \infty$)." This statement is correct, for all local, N-conserving algorithms—indeed, our Theorem 2 makes rigorous a very strong form of this assertion. Unfortunately, we have no quantitative estimate of the constants C_3 and C_4 in Theorem 2 (they could in principle be inferred from our proof together with the proofs of Kesten[13] and Hammersley and Welsh[15]), so we are unable to say quantitatively how serious this nonergodicity is for any given value of N. (Our proof is in any case very crude: the true value of C_4 is clearly much larger than our proof would indicate.) But the examples given in the preceding section do show that this nonergodicity arises already for quite small values of N.

Good numerical evidence on the size of the systematic error due to nonergodicity is, unfortunately, hard to come by. What is required is to compare expectation values in the standard SAW ensemble (all SAWs) to those in a suitably restricted ensemble (e.g., ergodic class of the straight rod). We see four potentially viable methods for doing this:

(a) Exact enumeration versus exact enumeration.

(b) Exact enumeration versus Monte Carlo simulation.

(c) Extrapolated exact enumeration versus Monte Carlo simulation.

(d) Monte Carlo simulation versus Monte Carlo simulation.

We discuss these in turn.

(a) Exact enumeration versus exact enumeration. For small N, one can explicitly enumerate both the ensemble of all SAWs and the ergodic classes of a given Monte Carlo algorithm. For example, for $d=2$ and $N=11$, the ensemble of all SAWs has[25]

$$c_{11} = 120{,}292$$

$$c_{11}\langle \omega_{11}^2 \rangle = 3{,}610{,}884$$

$$\langle \omega_{11}^2 \rangle \approx 30.017657$$

while the ergodic class of the straight rod under moves A, B, D, F has[5]

$$c'_{11} = 120{,}284$$

$$c'_{11}\langle \omega_{11}^2 \rangle' = 3{,}610{,}876$$

$$\langle \omega_{11}^2 \rangle' \approx 30.019587$$

[5] There are eight "frozen" configurations (Fig. 6a in various orientations), each of which has $\omega_{11}^2 = 1$. All other configurations are deformable to a rod.

Thus, for $N=11$, the systematic error in $\langle\omega_N^2\rangle$ is roughly 0.006%. For $d=2$ and $N=13$ the corresponding values are[25]

$$c_{13}=881{,}500$$
$$c_{13}\langle\omega_{13}^2\rangle=33{,}765{,}276$$
$$\langle\omega_{13}^2\rangle\approx 38.304340$$

and[6]

$$c'_{13}=881{,}436$$
$$c'_{13}\langle\omega_{13}^2\rangle'=33{,}765{,}212$$
$$\langle\omega_{13}^2\rangle'\approx 38.307049$$

for a systematic error of 0.007%. For $d=2$ and $N=15$ the values are[25]

$$c_{15}=6{,}416{,}596$$
$$c_{15}\langle\omega_{15}^2\rangle=302{,}977{,}204$$
$$\langle\omega_{15}^2\rangle\approx 47.217747$$

and[7]

$$c'_{15}=6{,}416{,}332$$
$$c'_{15}\langle\omega_{15}^2\rangle'=302{,}976{,}940$$
$$\langle\omega_{15}^2\rangle'\approx 47.219648$$

for a systematic error of 0.004%. Thus, right at the threshold of nonergodicity the effect is very small, since it is caused by very few configurations; this is hardly surprising. Presumably the effect gets larger at larger N. Unfortunately, the exact enumeration of ergodic classes is a rather difficult task: it is equivalent to finding the connected components of a graph with c_N vertices and (for the local, N-conserving algorithms) $O(N)$ edges per vertex. This is at least a factor of N more computationally complex than the enumeration of SAWs.

(b) Exact enumeration versus Monte Carlo simulation. The quantity $\langle\omega_N^2\rangle$ in the standard SAW ensemble has been computed for $N\leqslant 27$ on the square lattice and for $N\leqslant 20$ on the simple cubic lattice.[26] It would be

[6] There are 64 configurations not deformable to a rod (only 16 of which are "frozen"), each of which has $\omega_{13}^2=1$.

[7] There are (if we have counted correctly) 264 configurations not deformable to a rod (only 40 of which are "frozen"), each of which has $\omega_{15}^2=1$.

possible in principle, therefore, to do high-precision Monte Carlo simulations in the region of nonergodicity ($N \geqslant 11$ for Verdier–Stockmayer in $d=2$, and $N \geqslant 18$ in $d=3$), which could be compared against exact enumeration. However, we are not aware of *any* existing computations in this region.[8,9] In any case, the sought-for systematic error would most likely be hidden under a much larger statistical error, for any reasonable CPU time on a currently available supercomputer. Indeed, the autocorrelation time τ for the local, N-conserving Monte Carlo algorithms grows rapidly with N, roughly like $N^{2+2\nu}$ ($\sim N^{\approx 3.2}$ in $d=3$)[32]; and roughly τ/ε^2 iterations are needed for relative accuracy ε. This is an enormous computational demand. Quite honestly, we do not think this problem is worth the effort.

(c) Extrapolated exact enumeration versus Monte Carlo simulation. Monte Carlo measurements of $\langle \omega_N^2 \rangle'$ can, of course, be compared to *extrapolations* from exact-enumeration data. The Monte Carlo data in Refs. 2, 12, 27, 28, and 30 do appear to agree with such extrapolations to within statistical error, typically ~ 0.2–1%. This statistical error is quite large, for the reasons noted previously. Moreover, there is a logical difficulty here: Suppose we were to perform an *infinitely* long Monte Carlo run, thereby obtaining measurements of $\langle \omega_N^2 \rangle'$ with *zero* statistical error; and suppose that these data were to agree with extrapolated exact enumeration to within the subjective error estimates for that extrapolation. This would confirm that the systematic error of the Monte Carlo algorithm is smaller than or equal to the estimated extrapolation error, at the given value of N; but it would provide *no logical justification whatsoever* for using the Monte Carlo algorithm to *test* the extrapolations, or to make measurements of *higher* accuracy, or to work at *higher* values of N. In other words, it would provide no logical justification for using Monte Carlo to do anything that has not already been done by extrapolated exact enumeration. And in that case, what's the point of Monte Carlo?

(d) Monte Carlo simulation versus Monte Carlo simulation. There do exist Monte Carlo algorithms for the SAW that are both ergodic and

[8] Virtually all existing work of which we are aware (see, e.g., Refs. 2, 4, 11, 27–30) has been performed in $d=3$ at $N \leqslant 16$ (where the Verdier–Stockmayer algorithm is still ergodic) or at $N \geqslant 31$ (beyond the reach of exact enumeration). Gurler *et al.*[31] have one run at $N=23$, and Romiszowski and Stockmayer[30] have one run at $N=24$. Meirovitch[12] has a run at $N=20$, but we do not know whether his algorithm is ergodic there.

[9] For the slithering-snake algorithm, Mandel[24] presents Monte Carlo data at $N=20$ that agree with exact enumeration to within statistical error, roughly 0.2%. He also presents data at values of N from 40 to 600 which agree well with *extrapolated* exact enumeration (see below for discussion). The earlier data of Wall and Mandel[23] at $N=10$ are, however, irrelevant for present purposes, since the slithering-snake algorithm is ergodic at $N=10$.

efficient (see below). So one could in principle use an algorithm of this type to make high-precision measurements in the standard SAW ensemble, and then compare them to measurements made using a nonergodic algorithm. But this test procedure suffers from the same two difficulties as in case (c). And what's the point of using a Monte Carlo algorithm that is nonergodic and inefficient, when there exist alternative algorithms that are both ergodic and efficient?

In our opinion the seriousness of the nonergodicity problem depends on the type of information one is seeking. If one is seeking moderately accurate numerical data for modest values of N, then perhaps the exclusion of some configurations will cause only a small error. But the most interesting questions about the SAW concern the critical behavior, i.e., the behavior as $N \to \infty$, and here the problem is extremely serious: the exclusion of certain configurations means that one is really studying a *different model* with *different long-range excluded-volume interactions* from those of the standard SAW; thus, it is quite possible that this model lies in a *different universality class* and has *different critical exponents.* (This is admittedly a speculation for which we have no hard evidence.) Moreover—and this is a general objection to any Monte Carlo algorithm with an uncontrollable systematic error—to pin one's hopes on the expected "smallness" of the error is to give up one of the main advantages of the Monte Carlo method, namely that one knows exactly what model one is studying and that one has complete control over all errors except statistical fluctuations. Finally, there is no excuse for using nonergodic (and inefficient!) algorithms, when there exist alternative algorithms that are both ergodic and efficient.[10]

[10] There is one exception to this statement. Heretofore we have assumed tacitly that the goal is to compute *static* quantities (i.e., equilibrium expectation values) in the standard SAW. From this point of view the Monte Carlo algorithm is merely a *computational method*; the choice between competing algorithms is to be made solely on grounds of efficiency. Polymer physicists are, however, also interested in the *dynamics* of polymer molecules. In this case it is important to use a Monte Carlo algorithm that at least roughly mimics the true physical dynamics (perhaps in some approximation). For example, the local, N-conserving algorithms are intended to simulate the dynamics of a single polymer chain in a good solvent in the "free-draining" limit, i.e., neglecting hydrodynamic interactions. (This limit does not correspond to any physically realizable situation, for in fact the hydrodynamic interactions always dominate the dynamics.) For such problems it is perhaps reasonable to use a nonergodic algorithm, since appropriate alternative algorithms are not available (at present), and the systematic error due to nonergodicity is probably small compared to the modest accuracy desired. However, even in this case it is worth exploring the possibility of devising ergodic algorithms that adequately represent the desired dynamics. For example, one possibility might be the continuum "kink-jump" algorithm.

We conclude that dynamic Monte Carlo algorithms based on a finite repertoire of local, N-conserving elementary moves are not suitable for high-precision studies of the standard (equal-weight) SAW distribution.

What options remain, then, for Monte Carlo studies of the SAW? We see three main classes of viable algorithms:

1. *Static or quasistatic algorithms.* For these algorithms the question of ergodicity does not arise. At least three algorithms in this class appear to be reasonably efficient: dimerization,[33-36] enrichment,[37,38] and the Redner–Reynolds algorithm.[39] For enrichment and Redner–Reynolds, the CPU time required to generate one "effectively independent" sample appears[38] to be of order N^2.

2. *Nonlocal, N-conserving dynamic algorithms.* A very interesting algorithm in this class was invented by Lal[40] and subsequently rediscovered by MacDonald *et al.*[41]; a comprehensive study is currently in preparation.[42] The elementary moves of this algorithm are "pivot" moves: one "half" of the walk is rotated (or reflected) around a pivot point chosen randomly along the walk. This algorithm is *nonlocal* according to our definition, since the number of beads that may participate in a single move is unbounded. It can be proven[42] that this algorithm is ergodic. This algorithm also appears to be extraordinarily efficient: modulo some subtleties (discussed in detail in Ref. 42), the CPU time per "effectively independent" sample is of order N.

3. *Non-N-conserving dynamic algorithms.* We know of three algorithms in this class:

(a) Kron *et al.*[22] proposed a generalization of the "slithering-snake" algorithm that cures its nonergodicity. The CPU time per "effectively independent" sample is of order $\langle N \rangle^2$.

(b) Berretti and Sokal[43] proposed a closely related algorithm, which may be dubbed the "slithering tortoise." It generates SAWs in a "grand canonical" ensemble with one endpoint fixed and the other endpoint free. This algorithm is easily proven[43] to be ergodic. The CPU time per "effectively independent" sample is of order $\langle N \rangle^2$.

(c) Berg and Foerster[44] and Aragão de Carvalho *et al.*[45,46] (BFACF) proposed an algorithm that generates SAWs in a "grand canonical" ensemble with both endpoints fixed, e.g., one endpoint at the origin and the other at x ($\neq 0$). The ergodicity situation for this algorithm is rather complicated:

(i) In dimension $d=2$, it can be proven[47] that the BFACF algorithm is ergodic, for all choices of x.

(ii) In dimension $d=3$, it can be proven[47,48] that the BFACF algorithm is *nonergodic* (due to knots) if $|x|_\infty \equiv \max(|x_1|, |x_2|, |x_3|) = 1$.

(iii) In dimension $d=3$ with $|x|_\infty \geqslant 2$, or in dimension $d \geqslant 4$, we do not know whether the BFACF algorithm is ergodic (but we suspect that it is). This is an important open question, as the main application of this algorithm will be in dimensions 3 and 4.

The dynamical behavior of this algorithm, and thus its computational complexity per "effectively independent" sample, are not well understood at present; see Refs. 32 and 49.

There is thus no lack of efficient, ergodic Monte Carlo algorithms for the self-avoiding walk. We urge that they be used!

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