Exact Algorithm for d-Dimensional Walks on Finite and Infinite Lattices with Traps

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An *exact* algorithm is formulated to calculate the expected walk length $\langle n \rangle$ for a walker (atom, molecule) undergoing random displacements on a finite or infinite (periodic) d-dimensional lattice with traps (reactive sites). The method is illustrated for the case of a single deep trap surrounded by shallow traps and the calculated value of $\langle n \rangle$ agrees to within 0.3% of the Monte Carlo result for all lattices considered. The theory introduced is capable of generalization to many new classes of problems in lattice statistics.

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To investigate the interplay between spatial extent and dimensionality in influencing reaction-diffusion processes, we have undertaken recently a program of Monte Carlo calculation of random walks on lattices with traps.[1-3] In the course of analyzing recent data generated in these studies, we have found that a quite general algorithm can be written down to predict the number $\langle n \rangle$ of steps required before trapping (i.e., the expected walk length) on finite and infinite (i.e., periodic) lattices subject to a variety of boundary conditions. Moreover, the method developed seems capable of much further generalization so that although we consider specifically the case of a deep trap (trapping probability, $T = 1$) surrounded by $N - 1$ sites which may be partially absorbing (trapping probability, $0 \leq s < 1$), a great variety of other situations seems accessible to analysis. The method is based on a classification of the symmetry of the sites surrounding the deep trap and a coding of the fate of the random walker as it encounters a site of given symmetry. We illustrate the method using two simple examples and cite a number of additional, representative results to show the generality of the method.

Consider a 5×5 periodic lattice with a deep trap ($T = 1$) at the center and $N - 1 = 24$ surrounding sites, each characterized by a trapping probability s. From the symmetry of the unit cell, it is seen that there are five "types" of lattice sites (apart from the central trap); for definiteness, we code these sites as follows:

5	4	3	4	5
4	2	1	2	4
3	1	T	1	3
4	2	1	2	4
5	4	3	4	5

Suppose now that the walker is situated at one of the sites labeled 1 and let us denote by $\langle n \rangle_1$ the expected walk length for a walk originating from this site. Considering the simplest case first, we suppose that the trapping probability s at this site is zero. Now, there is one chance in four that the walker will move one step to a site labeled 3. Assuming this has been realized, we note that the walker, after having landed on this new site, has no memory of ever having been on the original site 1. The walker will continue his walk just as if he had started from the site 3, except that his walk length must be incremented by the one previously taken step. So, taking into account all four sites surrounding the site labeled 1, together with the attendant probability $p = \frac{1}{4}$ of a neighboring site being reached in a random displacement from the site 1, we conclude that the following relation must hold:

$$\langle n \rangle_1 = \tfrac{1}{4}(\langle n \rangle_T + 1) + \tfrac{1}{4}(\langle n \rangle_2 + 1) + \tfrac{1}{4}(\langle n \rangle_2 + 1) + \tfrac{1}{4}(\langle n \rangle_3 + 1).$$

Since the expected walk length from a deep trap ($T = 1$), $\langle n \rangle_T$, is zero this expression simplifies to

$$\langle n \rangle_1 = \tfrac{1}{4}[1 + 2(\langle n \rangle_2 + 1) + (\langle n \rangle_3 + 1)].$$

A more general situation arises if one assumes that the labeled site 1 is characterized by a nonvanishing probability of trapping (i.e., $0 \leq s < 1$). Then, the factor on the right-hand side of the last result must be weighted by the further probability $(1 - s)$. To account for the possibility that the walker is trapped at the site 1 to begin with, we include the (normalization) factor $s\{1\}$. Overall, then, the de-

sired generalization is

$$\langle n\rangle_1 = s\{1\} + \tfrac{1}{4}(1-s)[1 + 2(\langle n\rangle_2 + 1) + (\langle n\rangle_3 + 1)], \tag{1}$$

an expression from which one recovers the correct limiting behavior when one sets $s = 0$ and $s = 1$. Analogous expressions for $\langle n\rangle_2, \ldots, \langle n\rangle_5$ can be written down by inspection:

$$\langle n\rangle_2 = s\{1\} + \tfrac{1}{4}(1-s)[2(\langle n\rangle_1 + 1) + 2(\langle n\rangle_4 + 1)], \tag{2}$$

$$\langle n\rangle_3 = s\{1\} + \tfrac{1}{4}(1-s)[(\langle n\rangle_1 + 1) + (\langle n\rangle_3 + 1) + 2(\langle n\rangle_4 + 1)], \tag{3}$$

$$\langle n\rangle_4 = s\{1\} + \tfrac{1}{4}(1-s)[(\langle n\rangle_2 + 1) + (\langle n\rangle_3 + 1) + (\langle n\rangle_4 + 1) + (\langle n\rangle_5 + 1)], \tag{4}$$

$$\langle n\rangle_5 = s\{1\} + \tfrac{1}{4}(1-s)[2(\langle n\rangle_4 + 1) + 2(\langle n\rangle_5 + 1)]. \tag{5}$$

As is evident, the above system (1)–(5) represents five equations in five unknowns which can be solved via Cramer's rule to determine the quantities $\langle n\rangle_1, \ldots, \langle n\rangle_5$. Designating $q = \frac{1}{4}(1-s)$, the system is reduced to

$$\begin{bmatrix} 1 & -2q & -q & 0 & 0 \\ -2q & 1 & 0 & -2q & 0 \\ -q & 0 & 1-q & -2q & 0 \\ 0 & -q & -q & 1-q & -q \\ 0 & 0 & 0 & -2q & 1-2q \end{bmatrix} \begin{bmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \\ n_5 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

in which form standard routines may be applied. Once the $\langle n\rangle_1, \ldots, \langle n\rangle_5$ are known, the overall, expected walk length $\langle n\rangle$ can be computed from

$$\langle n\rangle = \frac{4\langle n\rangle_1 + 4\langle n\rangle_2 + 4\langle n\rangle_3 + 8\langle n\rangle_4 + 4\langle n\rangle_5}{24}. \tag{6}$$

The above procedure generalizes at once to d-dimensional lattices, and to boundary conditions other than periodic boundary conditions [we report later results for confining (nontransmitting) and reflecting boundary conditions]. Thus, for the case of a $5\times 5\times 5$ periodic lattice with a centrally located deep trap and $N - 1 = 124$ surrounding sites each characterized by an absorption probability $0 \leq s < 1$, inspection of a three-dimensional model (we used Tinkertoys(R)) shows that only nine distinct sites need be considered:

9 8 6 8 9	8 7 5 7 8	6 5 4 5 6	8 7 5 7 8	9 8 6 8 9
8 7 5 7 8	7 3 2 3 7	5 2 1 2 5	7 3 2 3 7	8 7 5 7 8
6 5 4 5 6	5 2 1 2 5	4 1 T 1 4	5 2 1 2 5	6 5 4 5 6
8 7 5 7 8	7 3 2 3 7	5 2 1 2 5	7 3 2 3 7	8 7 5 7 8
9 8 6 8 9	8 7 5 7 8	6 5 4 5 6	8 7 5 7 8	9 8 6 8 9

The corresponding determinantal equation is then

$$\begin{bmatrix} 1 & -4q & 0 & -q & 0 & 0 & 0 & 0 & 0 \\ -2q & 1 & -2q & 0 & -2q & 0 & 0 & 0 & 0 \\ 0 & -3q & 1 & 0 & 0 & 0 & -3q & 0 & 0 \\ -q & 0 & 0 & 1-q & -4q & 0 & 0 & 0 & 0 \\ 0 & -q & 0 & -q & 1-q & -q & -2q & 0 & 0 \\ 0 & 0 & 0 & 0 & -2q & 1-2q & 0 & -2q & 0 \\ 0 & 0 & -q & 0 & -2q & 0 & 1-q & -2q & 0 \\ 0 & 0 & 0 & 0 & 0 & -q & -2q & 1-2q & -q \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3q & 1-3q \end{bmatrix} \begin{bmatrix} \langle n\rangle_1 \\ \langle n\rangle_2 \\ \langle n\rangle_3 \\ \langle n\rangle_4 \\ \langle n\rangle_5 \\ \langle n\rangle_6 \\ \langle n\rangle_7 \\ \langle n\rangle_8 \\ \langle n\rangle_9 \end{bmatrix} = \underline{1}$$

TABLE I. A comparison of results generated via Monte Carlo simulation vs those generated via the algorithm for d-dimensional periodic lattices with a centrally located deep trap ($T = 1$).

Lattice	s	$\langle n\rangle_{MC}$	$\langle n\rangle_{ALG}$	% ERROR
8 x 1	0.	11.96[a]	12.00	+ 0.33
	0.1	5.501	5.491	- 0.18
20 x 1	0.	70.00[b]	70.00	0.0
	0.1	8.223	8.233	+ 0.12
4 x 4	0.	18.26[c]	18.31	+ 0.27
	0.1	6.656	6.650	- 0.09
	0.3	2.938	2.933	- 0.17
	0.5	1.887	1.885	- 0.11
5 x 5	0.	31.61[d]	31.67	+ 0.19
	0.01	24.18	24.15	- 0.12
	0.1	7.701	7.711	+ 0.13
	0.3	3.082	3.080	- 0.06
	0.5	1.925	1.928	+ 0.16
	0.75	1.318	1.316	- 0.16
5 x 5 x 5	0.	157.5	157.3	- 0.13
	0.01	61.23	61.25	+ 0.03
	0.1	9.420	9.435	+ 0.16

[a]The exact result (Refs. 4–6) for a linear chain, $\langle n\rangle = N(N+1)/6$, leads to $\langle n\rangle = 12.00$ in this case.

[b]The exact result (Refs. 4–6) for a linear chain leads to $\langle n\rangle = 70.00$ in this case; this is the number entered in the table.

[c]The asymptotic estimate (Refs. 4–6) for a square lattice, $\langle n\rangle = [\pi^{-1}N\ln N + 0.195056N - 0.1170 - 0.051N^{-1} + O(N^{-2})]N/(N-1)$, leads to $\langle n\rangle = 18.26$ in this case.

[d]The asymptotic estimate (Refs. 4–6) for a square lattice leads to $\langle n\rangle = 31.63$ in this case.

where here $q = \frac{1}{6}(1 - s)$ and $\underline{1}$ is the unit vector.

We present in Table I a comparison of the results obtained using the exact algorithm described here versus those generated in our full-scale Monte Carlo simulations, for dimension one (the 8×1 and 20×1 lattices), dimension two (the 4×4 and 5×5 lattices), and dimension three (the $5\times 5\times 5$ lattice). Here the lattices were assumed to be *periodic*, with the deep trap ($T = 1$) centrally located and the probability of trapping at all other sites set equal to s. However, the algorithm applies equally well to boundary conditions other than periodic ones; in particular, we may also consider lattices of finite spatial extent. We list in Table II results obtained for a 8×1 lattice subjected to confining boundary conditions (implemented by the restriction that if the walker attempts to step on the boundary it must return to the lattice site from which it started) and a 5×5 lattice subjected to reflecting boundary conditions [implemented by the restriction that if the walker attempts to step on the boundary it is displaced to one (interior) lattice point further removed from the boundary than the lattice site from whence it started]. In all cases, the differences between the Monte Carlo results and the results generated via application of the algorithm were essentially negligible. What makes this especially remarkable is that, whereas the Monte Carlo calculations are very expensive, implementation of the algorithm requires hardly any time at all. For example, to obtain $\langle n\rangle$ for the three-dimensional, $5\times 5\times 5$ lattice with a central, deep trap ($T = 1$) and absorption probability at the other sites set at $s = 0.1$, the Monte Carlo simulation required 270 *minutes* of central processing unit time on an IBM 330 (9000 walks initiated from each site were required to produce good histograms); use of the algorithm, i.e., solution of the determinantal equation (6), required 1.74 *seconds*.

TABLE II. A comparison of the results generated via Monte Carlo simulation vs those generated via the algorithm for d-dimensional finite lattices with a centrally located deep trap ($T = 1$).

Lattice	Boundary Conditions	s	$\langle n\rangle_{MC}$	$\langle n\rangle_{ALG}$	% ERROR
8 x 1	confining (non-transmitting)	0.1	5.536	5.521	- 0.27
5 x 5	reflecting	0.	19.09	19.06	- 0.16
		0.01	16.21	16.20	- 0.06
		0.1	6.883	6.880	- 0.04

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