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The Number of Distinct Sites Visited in a Random Walk on a Lattice*

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Abstract

A general formalism is developed from which the average number of distinct sites visited in n steps by a random walker on a lattice can be calculated. The asymptotic value of this number for large n is shown to be $\sqrt{\frac{8n}{\pi}}$ for a one dimensional lattice and cn for lattices of three or more dimensions. The constant c is evaluated exactly, with the help of Watson's integrals, for the simple cubic, body centered cubic, and face centered cubic lattices. An analogy is drawn with an electrical network in which unit resistors replace all near neighbor bonds in a lattice, and the resistance of such a network on each of the three cubic lattices is evaluated.

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DISCLAIMER

1. INTRODUCTION

Despite the attention devoted to random walks on a lattice,[1,2] the simple question of the number of distinct sites visited by a walker in n steps has not, to our knowledge, been treated before in a systematic way.[3] The problem has practical importance in the theory of annealing of point defects in crystals. A defect, such as an interstitial or a vacancy, diffuses by a random walk on a lattice, and the rate at which defects are annihilated at point sinks is proportional to the average rate at which defects are arriving at fresh sites on the lattice, that is, at sites which have not been visited previously. The physical side of this problem will be treated at some length in a forthcoming book by Damask and Dienes.[4]

In this note we show how to determine the average number of distinct sites visited by a walker in n steps, examine the limiting behavior of this number in one and three dimensions for large n, and present numerical results for cubic lattices. The larger question of the distribution of number of distinct sites visited in n steps is not treated.

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[1] S. Chandrasekhar, Rev. Mod. Phys. 15, 1 (1943).

[2] E. Montroll, J. Soc. Ind. and Appl. Math. 4, 241 (1956).

[3] J. R. Beeler, Jr., and J. A. Delaney (unpublished) have studied random walks by Monte Carlo methods on a computing machine and have deduced results on the asymptotic number of distinct sites visited.

[4] A. C. Damask and G. J. Dienes, Point Defects in Metals, to be published.

2. GENERAL FORMALISM

Consider a random walk on a Bravais lattice of any number of dimensions. Let the coordination number of the lattice be z. The walker is allowed to step only to nearest neighbor sites, and to step to each of these with probability 1/z. If a site is considered to be marked with a "footprint" as soon as the walker visits it, a cloud of footprints develops in the lattice as the walk progresses. On the average this cloud will have the symmetry of the lattice, and, if viewed from the current position of the walker at any stage, will also, on the average, possess the lattice symmetry. Our strategy is to calculate the average density of this cloud of footprints, for the rate at which fresh sites are being visited is just the probability that a site adjoining the walker does not bear a footprint.

Thus, define the probability $p_n(\underset{\sim}{r})$ that, after n steps, the site at $\underset{\sim}{r}$ from the present position of the walker has been visited at least once. These probabilities obey the following relations:

$$p_{n+1}(\underset{\sim}{r}) = \frac{1}{z}\sum_{\underset{\sim}{b}} p_n(\underset{\sim}{r} + \underset{\sim}{b}), \qquad r \neq 0, \quad n = 0,1,2,\ldots, \tag{1}$$

$$p_n(0) = 1, \qquad n = 0,1,2,\ldots, \tag{2}$$

$$p_0(\underset{\sim}{r}) = 0, \qquad \underset{\sim}{r} \neq 0, \tag{3}$$

where $\underset{\sim}{b}$ denotes a nearest neighbor displacement and $\sum_{\underset{\sim}{b}}$ means summation over the set of z nearest neighbor displacements.

Equations (2) and (3) are obvious. To prove Eq. (1) observe that in the step n + 1 the walker might be displaced by a vector $\underset{\sim}{b}$, in which case the site previously at $\underset{\sim}{r} + \underset{\sim}{b}$ relative to the walker becomes the site at $\underset{\sim}{r}$. Since $\underset{\sim}{r} \neq 0$ the walker has not moved on to this site, and so the probability that the site has been visited has not changed. Allowing the probability 1/z for the particular displacement $\underset{\sim}{b}$, and summing over the possible displacements, one arrives at Eq. 1.

Equations (1) and (2) and the initial conditions (3) determine the entire set $p_n(\underset{\sim}{r})$.

Let S_n be the average number of distinct sites visited in n steps. The increase, in step n + 1, in average number of distinct sites visited is just the probability that any nearest neighbor site $\underset{\sim}{b}$ has not yet been visited by step n, namely $1-p_n(\underset{\sim}{b})$ (note that symmetry makes $p_n(\underset{\sim}{b})$ the same for all nearest neighbor sites). Thus

$$S_{n+1} - S_n = 1-p_n(\underset{\sim}{b}), \quad n = 0,1,2,\ldots \; ; \; S_0 = 1. \tag{4}$$

Equations (1) and (4) determine the set S_n.

Directly from the definitions of S_n and $p_n(\underset{\sim}{r})$ one can also write the relation

$$S_n = \sum_{\underset{\sim}{r}} p_n(\underset{\sim}{r}), \tag{5}$$

where the summation is over all lattice vectors. The consistency of Eqs. (4) and (5) is easy to prove, with the aid of Eqs. (1) and (2).

Without seeking explicit solutions of Eqs. (1) - (4) certain general conclusions can be drawn. For n large $p_n(\underset{\sim}{r})$ becomes indepent of n. Let this limiting value be called $p_\infty(\underset{\sim}{r})$. From Eq. (1) $p_\infty(\underset{\sim}{r})$ is determined by

$$p_\infty(\underset{\sim}{r}) = \frac{1}{z}\sum_{b} p_\infty(\underset{\sim}{r} + \underset{\sim}{b}), \qquad \underset{\sim}{r} \neq 0 , \tag{6}$$

$$p_\infty(0) = 1.$$

These equations can be understood more easily by the following analogy: If an electrical network is constructed[5] with nodes at the lattice points and unit resistors replacing all near neighbor bonds, and if the nodes at infinity are grounded and the node at the origin is held at unit potential, $p_\infty(\underset{\sim}{r})$ will be the potential of the node at $\underset{\sim}{r}$. From this consideration one can demonstrate that, for networks of 3 or more dimensions, $0 < p_\infty(\underset{\sim}{b}) < 1$.

Equations (4) lead in three or more dimensions to a limiting form, for large n,

$$S_n = a + [1-p_\infty(\underset{\sim}{b})]\, n, \tag{7}$$

where a is a constant.

For 1 or 2 dimensional lattices, the electrical network analogy shows that $p_\infty(\underset{\sim}{b}) = 1$, and here S_n must increase less rapidly than linearly with n.

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[5] Electrical networks have also been employed in random walk problems by K. Compaan and Y. Havens, Trans. Faraday Soc. 52, 786 (1956).

3. LIMITING VALUES IN 1 DIMENSION

For 1 dimension the limiting growth is found by passing from Eq. (1) to a differential equation for $p_n(r)$, valid in the limit of large n:

$$2\frac{\partial p_n(x)}{\partial n} = \frac{\partial^2 p_n(x)}{\partial x^2}, \qquad p_n(0) = 1. \tag{8}$$

The solution of (8) is

$$p_n(x) = 1\text{-Erf}\left(\frac{x}{\sqrt{2n}}\right).$$

In the same limit $\frac{d S_n}{dn} = 1-p_n(1) = \text{Erf}\left(\frac{1}{\sqrt{2n}}\right) \underset{n \to \infty}{\longrightarrow} \sqrt{\frac{2}{\pi n}}$. (9)

Equation (9) has the solution

$$S_n = a + 2\sqrt{\frac{2n}{\pi}}, \quad (n \to \infty), \tag{10}$$

showing a square root growth of S_n with n. The meaning of this is evident from the consideration that the r.m.s. excursion of the walker is proportional to $\sqrt{n}$, and, in one dimension, sites inside this distance will almost always have been visited, sites outside it will not.

4. LIMITING VALUES IN THREE DIMENSIONS

Consider a 3 dimensional cubic Bravais lattice and let half the cubic cell edge be the unit of length. Let the Cartesian components of a near neighbor vector $\underset{\sim}{b}$ be donoted b_1, b_2, b_3, and of a lattice vector $\underset{\sim}{r}$ be denoted r_1, r_2, r_3; all of these components will be integers. The general solution of the Eqs. (6) for $p_\infty(\underset{\sim}{r})$ can now be written down:

$$p_\infty(\underset{\sim}{r}) = \frac{1}{F} \int_0^\pi\int_0^\pi\int_0^\pi \frac{\cos(ur_1)\,\cos(vr_2)\,\cos(wr_3)}{1 - z^{-1} \sum_{\underset{\sim}{b}} \cos(ub_1)\,\cos(vb_2)\,\cos(wb_3)}\,du\,dv\,dw, \quad (11)$$

where

$$F = \int_0^\pi\int_0^\pi\int_0^\pi \frac{du\,dv\,dw}{1 - z^{-1} \sum_{\underset{\sim}{b}} \cos(ub_1)\,\cos(vb_2)\,\cos(wb_3)} \,. \quad (12)$$

To demonstrate that (11) is a solution of (6), write the latter in the form

$$\Omega\, p_\infty(\underset{\sim}{r}) = 0 \,, \qquad \underset{\sim}{r} \neq 0$$

where Ω is an operator defined by

$$\Omega\, f(\underset{\sim}{r}) \equiv f(\underset{\sim}{r}) - z^{-1} \sum_{\underset{\sim}{b}} f(\underset{\sim}{r} + \underset{\sim}{b}) \,.$$

Observe that, by virtue of the cubic symmetry, $\cos(ur_1)\,\cos(vr_2)\,\cos(wr_3)$ is an eigenfunction of Ω with eigenvalue

$$1 - z^{-1} \sum_{\underset{\sim}{b}} \cos(ub_1)\,\cos(vb_2)\,\cos(wb_3) \,.$$

Then, applying Ω to the expression (11)

for $p_\infty(r)$, one finds

$$\Omega\, p_\infty(\underset{\sim}{r}) = \frac{1}{F}\int_0^\pi\int_0^\pi\int_0^\pi \cos(ur_1)\cos(vr_2)\cos(wr_3)\,du\,dv\,dw$$

$$= \frac{1}{F}\prod_{j=1}^{3}\frac{\sin\pi r_j}{r_j} = 0\,,\quad (\underset{\sim}{r} \neq 0).$$

Finally, from the definition of F, it is evident that $p_\infty(0) = 1$, which completes the demonstration.

For the three lattices simple cubic (s.c.), body centered cubic (b.c.c.), and face centered cubic (f.c.c.), $p_\infty(\underset{\sim}{b})$ may readily be evaluated. One uses the relation $z^{-1}\sum_{\underset{\sim}{b'}} p_\infty(\underset{\sim}{b'}) = p_\infty(\underset{\sim}{b})$ to rewrite (11) as

$$p_\infty(\underset{\sim}{b}) = \frac{1}{F}\int_0^\pi\int_0^\pi\int_0^\pi \frac{z^{-1}\sum_{\underset{\sim}{b'}}\cos(ub_1')\cos(vb_2')\cos(wb_3')}{1 - z^{-1}\sum_{\underset{\sim}{b'}}\cos(ub_1')\cos(vb_2')\cos(wb_3')}\,du\,dv\,dw$$

$$= \frac{1}{F}\int_0^\pi\int_0^\pi\int_0^\pi \left[\frac{1}{1 - z^{-1}\sum_{\underset{\sim}{b'}}\cos(ub_1')\cos(vb_2')\cos(wb_3')} - 1\right]du\,dv\,dw$$

$$= \frac{1}{F}\left[F - \pi^3\right].$$

Finally, for s.c. lattices $F = 3\pi^3 I_3$, for b.c.c. $F = \pi^3 I_1$, and for f.c.c. $F = 3\pi^3 I_2$, where I_1, I_2, and I_3 are integrals which have been evaluated by Watson.[6]

The asymptotic rate of change of S_n with n, as seen from Eq. (7), is $1-p_\infty(\underset{\sim}{b})$. Values of this quantity, as determined here, and also as found by Beeler and Delaney in their Monte Carlo treatments of diffusion are given in Table I.

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[6] G.N. Watson, Quarterly J. of Math. 10, 266 (1939).

Finally, one notes that, from the electrical network analogy cited above, the resistance from a node to infinity in a lattice in which unit resistors have replaced all near neighbor bonds can be written

$$\frac{1}{z[1-p_\infty(b)]}$$

This resistance is 0.25273, 0.17415, and 0.11206 ohms for the s.c., b.c.c. and f.c.c. lattices, respectively.

5. ACKNOWLEDGEMENTS

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Table I. $\lim_{n\to\infty} \frac{dS_n}{dn}$, where S_n is average number of distinct sites visited in n steps.

Lattice	Present Calculations	Beeler and Delaney
s.c.	0.659 462 670	0.667
b.c.c.	0.717 770 010	0.72
f.c.c.	0.743 681 763	-----