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Random Walks on Lattices. II

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Formulas are obtained for the mean first passage times (as well as their dispersion) in random walks from the origin to an arbitrary lattice point on a periodic space lattice with periodic boundary conditions. Generally this time is proportional to the number of lattice points.

The number of distinct points visited after n steps on a k-dimensional lattice (with $k \geq 3$) when n is large is $a_1 n + a_2 n^{\frac{1}{2}} + a_3 + a_4 n^{-\frac{1}{2}} + \cdots$. The constants $a_1 - a_4$ have been obtained for walks on a simple cubic lattice when $k = 3$ and a_1 and a_2 are given for simple and face-centered cubic lattices. Formulas have also been obtained for the number of points visited r times in n steps as well as the average number of times a given point has been visited.

The probability $F(c)$ that a walker on a one-dimensional lattice returns to his starting point before being trapped on a lattice of trap concentration c is $F(c) = 1 + [c/(1 - c)] \log c$.

Most of the results in this paper have been derived by the method of Green's functions.

A NUMBER of problems in solid-state physics are directly or indirectly related to various aspects of random walks on periodic space lattices. The theory of such random walks on infinite lattices was first discussed by Polya[1] who was especially concerned with the effect of dimensionality on the probability that a walker starting at a given point eventually returns to that point. Some other types of problems which are of special interest involve the average time required by a walker to go from a given lattice point to another preassigned point for the first time and with the average number of distinct points occupied in a walk of a given number of steps. Results on these topics as well as the effect of a small number of lattice defects on random walks have been discussed in the first paper of this series.[2]

That paper is concerned mainly with random walks which involve jumps to nearest-neighbor lattice points only. Many of the results are generalized here to be applicable to walks which involve steps to more distant neighbors. We also discuss the average number of points occupied k times in an n-step walk as well as the number of times a given point has been occupied in such a walk. The average number of points occupied in an n-step walk was first estimated by Dvoretsky and Erdös,[3] further analysis having been made by Vineyard[4] and one of the authors.[2] Repeated occupancy was first considered by Erdös and Taylor.[5]

Green's function techniques and Tauberian theorems are the main mathematical tools used in this paper. Although emphasis is placed on walks in which steps are taken at regular time intervals, the generalization to those in which the steps are taken at random times is developed in Sec. V.

We also discuss the effect of traps of a given con-

[1] G. Polya, Math. Ann. **84**, 149 (1921).
[2] E. W. Montroll, Proc. Symp. Appl. Math. Am. Math. Soc. **16**, 193 (1964).
[3] A. Dvoretzky and E. Erdos, Proc. 2nd Berkeley Sympos. Math. Stat. and Prob., (University of California Press, Berkeley, 1951), p. 33.
[4] G. H. Vineyard, J. Math. Phys. **4**, 1191 (1963).
[5] P. Erdos and S. J. Taylor, Acta Math. Acad. Sci. Hung. **11**, 137 (1960).

centration on the probability of a walker on a one-dimensional lattice returning to his starting point before being trapped.

Since the first draft of this article was completed, a book by Spitzer[6] has appeared which contains a discussion of some of the topics included here.

I. LATTICE GREEN'S FUNCTIONS AND RANDOM-WALK GENERATING FUNCTIONS

We begin by studying discrete random walks on lattices with periodic boundary conditions (i.e., toroidal lattices), and in particular will assume that there exists an integer N such that the lattice points $\mathbf{s} = (s_1, s_2, \cdots, s_k)$ satisfy

$$(s_1 + j_1N, s_2 + j_2N, \cdots, s_k + j_kN) = (s_1, s_2, \cdots, s_k)$$

when the j's are integers.

There are N^k distinct lattice points on our k-dimensional lattice. Let $P_n(\mathbf{s})$ be the probability that the random walker is at a point $\mathbf{s}$ after the nth step. In view of the periodic boundary conditions,

$$P_n(s_1 + j_1N, s_2 + j_2N, \cdots, s_k + j_kN) = P_n(\mathbf{s}), \quad \text{(I.1)}$$

when the j's are integers. The $\{P_n(\mathbf{s})\}$ satisfy the recursion formula

$$P_{n+1}(\mathbf{s}) = \sum_{\mathbf{s}'} p(\mathbf{s} - \mathbf{s}')P_n(\mathbf{s}'), \qquad \text{(I.2)}$$

if $p(\mathbf{s})$ represents the probability that any step results in a vector displacement $\mathbf{s}$ by a walker. We find the Fourier expansion of $p(\mathbf{s})$

$$\lambda(2\pi\mathbf{r}/N) = \sum_{\mathbf{s}} p(\mathbf{s}) \exp(2\pi i\mathbf{r}\cdot\mathbf{s}/N), \qquad \text{(I.3)}$$

which we call the structure function of the walk, to be of considerable importance. In particular

$$\sum_{\mathbf{s}} p(\mathbf{s}) = 1 \quad \text{and} \quad \lambda(0) = 1 \qquad \text{(I.4)}$$

when walkers are conserved; i.e., when walkers are neither created nor destroyed in the walk. The reader can easily verify that

$$\lambda(\boldsymbol{\vartheta}) = \begin{cases} (c_1 + c_2 + \cdots + c_k)/k \\ \quad \text{for } k\text{-D simple cubic lattice} \\ (c_1c_2 + c_2c_3 + c_3c_1)/3 \\ \quad \text{for 3-D face-centered cubic lattice} \\ c_1c_2c_3, \\ \quad \text{for 3-D body-centered cubic lattice,} \end{cases} \qquad \text{(I.5)}$$

where

$$c_j = \cos\vartheta_j \quad \text{and} \quad \vartheta_j = 2\pi r_j/N. \qquad \text{(I.5a)}$$

Properties of random walks can be described effectively through the random-walk generating function

$$P(\mathbf{s}, z) = \sum_0^\infty z^n P_n(\mathbf{s}). \qquad \text{(I.6)}$$

We restrict ourselves now to the initial condition

$$P_0(\mathbf{s}) = \delta_{\mathbf{s},0} \qquad \text{(I.7)}$$

which corresponds to walks which start from the origin, $\mathbf{s} = 0$. By multiplying (2) by z^n, summing over all n, and applying (7), one finds that $P(\mathbf{s}, z)$ satisfies the Green's function equation

$$P(\mathbf{s}, z) - z \sum_{\mathbf{s}'} p(\mathbf{s} - \mathbf{s}')P(\mathbf{s}', z) = \delta_{\mathbf{s},0}. \qquad \text{(I.8)}$$

This equation can be solved for our generating function $P(\mathbf{s}, z)$ by considering the function

$$u(z, 2\pi\mathbf{r}/N) = \sum_{\mathbf{s}} P(\mathbf{s}, z) \exp(2\pi i\mathbf{r}\cdot\mathbf{s}/N). \qquad \text{(I.9)}$$

If we multiply (8) by $\exp(2\pi i\mathbf{s}\cdot\mathbf{r}/N)$, sum over $\mathbf{s}$ and employ (9) and (3) we find

$$u(z, 2\pi\mathbf{r}/N) = \{1 - z\lambda(2\pi\mathbf{r}/N)\}^{-1}. \qquad \text{(I.10)}$$

Since $P(\mathbf{s}, z)$ is the Fourier inverse of $u(z, 2\pi\mathbf{r}/N)$, we find

$$P(\mathbf{s}, z) = N^{-k} \sum_{\mathbf{r}} \frac{\exp(-2\pi i\mathbf{r}\cdot\mathbf{s}/N)}{1 - z\lambda(2\pi\mathbf{r}/N)}. \qquad \text{(I.11)}$$

In the case of an infinite lattice, $N \to \infty$ and

$$P(\mathbf{s}, z) = \frac{1}{(2\pi)^k} \int_{-\pi}^{\pi} \cdots \int \frac{\exp(-i\mathbf{s}\cdot\boldsymbol{\vartheta})\, d^k\boldsymbol{\vartheta}}{1 - z\lambda(\boldsymbol{\vartheta})}. \qquad \text{(I.12)}$$

From this it is clear that

$$P_n(\mathbf{s}) = \frac{1}{(2\pi)^s} \int_{-\pi}^{\pi} \cdots \int [\lambda(\boldsymbol{\vartheta})]^n e^{-i\mathbf{s}\cdot\boldsymbol{\vartheta}}\, d^k\boldsymbol{\vartheta}. \qquad \text{(I.13)}$$

Also since we assume walkers to be conserved

$$\sum_{\mathbf{s}} P_n(\mathbf{s}) = 1, \qquad \text{(I.14a)}$$

and

$$\sum_{\mathbf{s}} P(\mathbf{s}, z) = (1 - z)^{-1}. \qquad \text{(I.14b)}$$

In all the analysis above we assume $|z| \leq 1$.

We will find it expedient to separate out the singular and nonsingular parts of $P(\mathbf{s}, z)$ by writing

$$P(\mathbf{s}, z) = (1 - z)N^{-k} + \varphi(\mathbf{s}, z), \qquad \text{(I.15)}$$

where

$$\varphi(\mathbf{s}, z) = N^{-k} {\sum_{\mathbf{r}}}' \frac{\exp(2\pi i\mathbf{r}\cdot\mathbf{s}/N)}{1 - z\lambda(2\pi\mathbf{r}/N)}, \qquad \text{(I.16)}$$

[6] F. Spitzer, *Principles of Random Walks* (D. Van Nostrand, Inc., Princeton, New Jersey, 1964).

in which the prime indicates that the term with $r_1 = r_2 = \cdots = r_k = 0$ is to be omitted. In general, when the limit $N \to \infty$ is taken, the sum can be replaced by an integral. Although the resulting integral may be a singular function of z the singularity is weaker than $(1 - z)^{-1}$ as we show later.

We will also be interested in the properties of the first passage time, and for this purpose we define $F_n(\mathbf{s})$ to be the probability that a random walker reaches the point $\mathbf{s}$ for the *first time* at step n. The generating function of the $F_n(\mathbf{s})$ will be denoted by $F(\mathbf{s}, z)$:

$$F(\mathbf{s}, z) = \sum_{n=1}^{\infty} F_n(\mathbf{s}) z^n. \tag{I.17}$$

It is possible to relate the $F_n(\mathbf{s})$ to the $P_n(\mathbf{s})$ since, if the random walker is at step n he must first have reached there at some step j and then returned to s in $n - j$ steps. Taking account of the initial condition of Eq. (I.3), we find

$$P_n(\mathbf{s}) = \delta_{n,0}\delta_{s,0} + \sum_{j=1}^{n} F_j(\mathbf{s}) P_{n-j}(0)$$

The generating functions therefore satisfy

$$F(\mathbf{s}, z) = [P(\mathbf{s}, z) - \delta_{\mathbf{s},0}]/P(0, z). \tag{I.18}$$

The probability that the walker reaches point s at some time is just $F(s, 1)$. For $N < \infty$ the probability of reaching any point on the lattice is one, independent of the dimension. When $N = \infty$ the probability of a return to the origin is $1 - [F(0, 1)]^{-1}$ In one and two dimensions $F(0, 1) = \infty$ and the walker returns to the origin with probability one. In higher dimensions the return to the origin occurs with probability less than one. The same results are true for the first passage to any point $\mathbf{s}$.

Another function that will be useful later is $F_n^{(r)}(\mathbf{s})$, the probability that the random walker reaches $\mathbf{s}$ for the rth time at step n. This function satisfies the recurrence formula

$$F_n^{(r)}(\mathbf{s}) = \sum_{j=1}^{n} F_{n-j}^{(r-1)}(\mathbf{s}) F_j(0), \tag{I.19}$$

and its generating function $F^{(r)}(\mathbf{s}, z)$ is therefore given by

$$F^{(r)}(\mathbf{s}, z) = [F(0, z)]^{r-1} F(\mathbf{s}, z) = \sum_{n=1}^{\infty} F_n^{(r)}(\mathbf{s}) z^n. \tag{I.20}$$

II. STATISTICS OF FIRST-PASSAGE TIME

The first results to be given will be those related to first-passage times. Let $\langle n^j(\mathbf{s})\rangle$ be the jth moment of the first-passage time to reach point $\mathbf{s}$. In terms of $F(\mathbf{s}, z)$, $\langle n^j(\mathbf{s})\rangle$ can be written

$$\langle n^j(\mathbf{s})\rangle = (z\, \partial/\partial z)^j F(\mathbf{s}, z)]_{z=1}. \tag{II.1}$$

In particular, if we substitute the representation of Eq. (II.15) for $P(\mathbf{s}, z)$ into (II.18) we find, for the first two moments

$$\langle n(\mathbf{s})\rangle = \begin{cases} N^k[\varphi(0, 1) - \varphi(\mathbf{s}, 1)], & \mathbf{s} \neq 0, \quad \text{(II.2a)} \\ N^k, & \mathbf{s} = 0, \quad \text{(II.2b)} \end{cases}$$

$$\langle n^2(\mathbf{s})\rangle = [2N^k\varphi(0, 1) + 1]\,\langle n(\mathbf{s})\rangle + 2N^k\left[\frac{\partial\varphi(0, z)}{\partial z} - \frac{\partial\varphi(\mathbf{s}, z)}{\partial z}\right]_{z=1} \quad \text{if} \quad \mathbf{s} \neq 0, \tag{II.3a}$$

$$\langle n^2(0)\rangle = 2N^{2k}\varphi(0, 1) + N^k. \tag{II.3b}$$

Notice that *the expected number of steps required to return to the origin is* N^k, the total number of lattice points, independently of the structure of the lattice. The second moment of the expected number of steps required to return to the origin for the first time does depend on lattice structure as is indicated by the function $\varphi(0, 1)$. Moments of the number of steps to reach other points on the lattice for the first time all depend on the structure.

So far we have given formal results valid for any k-dimensional periodic lattice. In the next few paragraphs we shall illustrate the general theory by evaluating some of the relevant functions for particular lattices. In our evaluation we will need some analytic properties of the functions $\lambda(\boldsymbol{\vartheta})$ and $\varphi(\mathbf{r}, z)$ which appear in many of the formulas derived above. We shall be interested only in symmetric random walks, hence the expansion of $\lambda(\boldsymbol{\vartheta})$ in a neighborhood of the origin is

$$\lambda(\boldsymbol{\vartheta}) = 1 - \frac{1}{2}\sum_{1}^{k} \sigma_i^2\vartheta_i^2 + O(\vartheta^4), \tag{II.4}$$

where

$$\sigma_i^2 = \sum_m m_i^2 p(m). \tag{II.5}$$

We will make use of $\varphi(\mathbf{s}, z)$ for an infinite lattice in the limit $z = 1^-$. The expression for $\varphi(\mathbf{s}, z)$ when $N = \infty$ is

$$\varphi(\mathbf{s}, z) = \frac{1}{(2\pi)^k} \times \int_{-\pi}^{\pi} \cdots \int \frac{\exp(i\boldsymbol{\vartheta}\cdot\mathbf{s})\, d^k\boldsymbol{\vartheta}}{1 - z\lambda(\boldsymbol{\vartheta})} = P(\mathbf{s}, z). \tag{II.6}$$

The function $\varphi(\mathbf{s}, 1)$ is singular in one and two dimensions. We can see this by considering the contribution to $\varphi(\mathbf{s}, 1)$ from a neighborhood of the origin $\boldsymbol{\vartheta} = 0$,

$$\int \cdots \int \frac{d^k\boldsymbol{\vartheta}}{\sigma_1^2\vartheta_1^2 + \cdots + \sigma_k^2\vartheta_k^2}. \tag{II.7}$$

If the integrand is transformed to polar coordinates, there arise contributions of the form

$$\int \cdots \int \frac{r^{k-1}}{r^2}\, dr, \tag{II.8}$$

which diverges in one and two dimensions, but remains finite in higher dimensions. We will be interested in the behavior of $\varphi(\mathbf{s}, z)$ for $\mathbf{s} = 0$ and $\mathbf{s} = (s_1^2 + \cdots + s_k^2)^{\frac{1}{2}}$ large but not large enough to violate the condition $\mathbf{s} \ll N^k$. It will be demonstrated that the properties of $\langle n(\mathbf{s})\rangle/N^k$ can be obtained fairly simply for large distances from the origin.

Let us begin by decomposing the integral defining $\varphi(s, z)$ into two parts:

$$\begin{aligned}\varphi(\mathbf{s}, z) &= \frac{1}{(2\pi)^k}\int_{-\pi}^{\pi}\!\!\cdots\!\int \frac{\exp(i\boldsymbol{\vartheta}\cdot\mathbf{s})\, d^k\boldsymbol{\vartheta}}{1 - z + \frac{1}{2}z(\sigma_1^2\vartheta_1^2 + \cdots + \sigma_k^2\vartheta_k^2)} \\ &\quad + \frac{1}{(2\pi)^k}\int_{-\pi}^{\pi}\!\!\cdots\!\int e^{i\boldsymbol{\vartheta}\cdot\mathbf{s}}\left\{\frac{1}{1 - z\lambda(\boldsymbol{\vartheta})} - \frac{1}{1 - z + \frac{1}{2}z(\sigma_1^2\vartheta_1^2 + \cdots + \sigma_k^2\vartheta_k^2)}\right\} d^k\boldsymbol{\vartheta} \\ &= \varphi_1(\mathbf{s}, z) + \varphi_2(\mathbf{s}, z).\end{aligned} \tag{II.9}$$

The singularity in one and two dimensions at $z = 1$ comes from the function $\varphi_1(\mathbf{s}, z)$ since the integral for $\varphi_2(\mathbf{s}, 1)$ has the form

$$\int \cdots \int r^{k-1}\, dr$$

at the origin of θ space. In higher dimensions both $\varphi_1(\mathbf{s}, z)$ and $\varphi_2(\mathbf{s}, z)$ approach zero as $\mathbf{s} \to \infty$, but

$$\lim_{\mathbf{s}\to\infty} [\varphi_2(\mathbf{s}, 1)/\varphi_1(\mathbf{s}, 1)] = 0. \tag{II.10}$$

This limit can be established by examining the behavior of the integrands in the neighborhood of $\boldsymbol{\vartheta} = 0$, which gives the principal contribution in the range of large $\mathbf{s}$. A detailed justification is given in Appendix A. We therefore see that the significant analytic properties of $\varphi(\mathbf{s}, z)$ are contained in $\varphi_1(\mathbf{s}, z)$ for large $\mathbf{s}$.

We shall recast the form of this function as a Laplace transform and begin by using the identity

$$u^{-1} = \int_0^\infty e^{-ut}\, dt$$

to rewrite it as

$$\varphi_1(\mathbf{s}, z) = \int_0^\infty e^{-(1-z)t}\, dt \times \prod_{j=1}^{k}\left\{\frac{1}{2\pi}\int_{-\pi}^{\pi} \exp(i\vartheta_j s_j - \tfrac{1}{2}zt\sigma_j^2\vartheta_j^2)\, d\vartheta_j\right\}, \tag{II.11}$$

where the interchange of orders of integration can be justified in detail. Thus $\varphi_1(\mathbf{s}, z)$ can be expressed as a Laplace transform

$$\varphi_1(\mathbf{s}, z) = \int_0^\infty e^{-(1-z)t} F(z, t)\, dt, \tag{II.12}$$

where $F(z, t)$ is the product of integrals in Eq. (II.11). Since each of the integral factors of $F(z, t)$ is analytic in z at $z = 1$, we may expand $F(z, t)$ in a Taylor series around $z = 1$,

$$F(z, t) = F(1, t) + (z - 1)[\partial F/\partial z]_{z=1} + \cdots. \tag{II.13}$$

Since we are interested in the behavior of $\varphi_1(\mathbf{s}, z)$ at $z = 1$ we can invoke an Abelian theorem for Laplace transforms[7] which states in the present context that the behavior of $\varphi(\mathbf{s}, z)$ at $z = 1$ is determined by the behavior of $F(z, t)$ at $t = \infty$.

To determine this behavior we note that as $t \to \infty$ the integrand of each of the integrals in $\varphi_1(\mathbf{s}, z)$ is peaked sharply at the origin with negligible contribution coming from values of ϑ_j greater than $2/\sigma_j t^{\frac{1}{2}} z^{\frac{1}{2}}$. Hence the ranges of integration on the ϑ integrals $(-\pi, \pi)$ can, as $t \to \infty$ be replaced by $(-\infty, \infty)$ so that

$$F(z, t) \sim \prod_{j=1}^{k} (2\sigma_j^2\pi t z)^{-\frac{1}{2}} \exp(-s_j^2/2zt\sigma_j^2)$$

and

$$F(1, t) \sim [\sigma_1 \cdots \sigma_k (2\pi t)^{k/2}]^{-1} \exp(-\lambda^2/2t), \tag{II.14a}$$

where

$$\lambda^2 = \sum_{j=1}^{k} (s_j/\sigma_j)^2. \tag{II.14b}$$

In one dimension we find

$$\begin{aligned}\varphi_1(s, z) &\sim \frac{1}{\sigma(2\pi)^{\frac{1}{2}}}\int_0^\infty e^{-(1-z)t - (s^2/2t\sigma^2)}\, t^{-\frac{1}{2}}\, dt \\ &= \frac{2^{\frac{1}{2}} s^{\frac{1}{2}}}{\pi^{\frac{1}{2}}\sigma^{\frac{1}{2}}(1 - z)^{\frac{1}{4}}} K_{\frac{1}{2}}\!\left(\frac{s}{\sigma}[2(1 - z)]^{\frac{1}{2}}\right) \\ &= \frac{\exp\{-(s/\sigma)[2(1 - z)]^{\frac{1}{2}}\}}{\sigma[2(1 - z)]^{\frac{1}{2}}},\end{aligned} \tag{II.15}$$

where $K_{1/2}(x)$ is a Bessel function of the third kind of imaginary argument. The two-dimensional form $\varphi_1(\mathbf{s}, z)$ for $\lambda \neq 0$ is

$$\begin{aligned}\varphi_1(\mathbf{s}, z) &\sim \frac{1}{2\pi\sigma_1\sigma_2}\int_0^\infty t^{-1} \exp\{-(1 - z)t - \lambda^2/2t\}\, dt \\ &= \frac{1}{\pi\sigma_1\sigma_2} K_0(\lambda[2(1 - z)]^{\frac{1}{2}}).\end{aligned} \tag{II.16}$$

[7] D. V. Widder, *The Laplace Transform* (Princeton University Press, Princeton, New Jersey, 1941).

When $\lambda = 0$ we may use an Abelian theorem for Laplace transforms[7] to show that it follows from the asymptotic form $F(1, t) \sim (2\pi\sigma_1\sigma_2 t)^{-1}$ that

$$\varphi_1(0, z) \sim -(1/2\pi\sigma_1\sigma_2) \log (1 - z) \quad \text{(II.17)}$$

for $z \to 1^-$. In three dimensions and higher $\varphi_1(0, 1)$ is defined by a convergent integral and must be calculated numerically. For large λ^2 an asymptotic expression for $\varphi_1(\mathbf{s}, 1)$ is

$$\varphi_1(s, 1) \sim \frac{1}{(2\pi)^{k/2}\sigma_1 \cdots \sigma_k} \int_0^\infty e^{-\lambda^2/2t} t^{-k/2}\, dt$$
$$= \lambda^{2-k}\Gamma(\tfrac{1}{2}k - 1)/2\sigma_1 \cdots \sigma_k \pi^{k/2}. \quad \text{(II.18a)}$$

The 3-D expression for $P(\mathbf{s}, z)$ as $z \to 1$ is

$$P(\mathbf{s},z) \sim (2\pi\lambda\sigma_1\sigma_2\sigma_3)^{-1} \exp\{-\lambda[2(1-z)]^{\frac{1}{2}}\}. \quad \text{(II.18b)}$$

Let us now consider some results for specific lattices. The simplest case is that of a one-dimensional lattice with jumps to nearest neighbors with probability $\frac{1}{2}$. For this case we can calculate an explicit expression for[2] $P(s, z)$:

$$P(s, z) = \frac{1}{N} \sum_{r=0}^{N-1} \frac{\exp(2\pi i r s/N)}{1 - z \cos(2\pi r/N)}$$
$$= \frac{(1 - z^2)^{-\frac{1}{2}}(U^s + U^{N-s})}{(1 - U^N)}, \quad \text{(II.19a)}$$

where

$$U = z^{-1}\{1 - (1 - z^2)^{\frac{1}{2}}\}. \quad \text{(II.19b)}$$

It is known that the mean recurrence time for return to the origin is infinite for an infinite lattice, even though the return probability[8] is 1. Likewise the expected time to reach any point is infinite although the probability of reaching any point is 1. This difficulty is avoided in the case of a finite lattice. Here, in contrast to the Polya case, return to the origin or to any lattice point occurs with probability one in any number of dimensions. We shall calculate the expected time to reach any point for the first time for nearest-neighbor jumps, and then present the generalization for different one-dimensional random walks, in the limit of large N. For the lattice with jumps to nearest neighbors only, we find[2] by an exact calculation starting from Eqs. (II.2a) and (II.19)

$$\langle n(s) \rangle = s(N - s). \quad \text{(II.20)}$$

To treat the case of the general one-dimensional walk for which $N \gg \mathbf{s}$, we use Eqs. (II.2a) and (II.15) to find

$$\lim_{N\to\infty} \langle n(s) \rangle / N = \varphi(0, 1) - \varphi(s, 1)$$
$$\sim \lim_{z\to 1} [\varphi_1(0, z) - \varphi_1(s, z)] = s/\sigma^2. \quad \text{(II.21)}$$

In the two-dimensional case, since

$$K_0\{\lambda[2(1 - z)]^{\frac{1}{2}}\} \sim -\tfrac{1}{2} \log (1 - z) - \log \lambda + O(1)$$

for large λ, we have the expression

$$\lim_{N\to\infty} \langle n(\mathbf{s}) \rangle / N^2 \sim \frac{\log \lambda}{\pi\sigma_1\sigma_2}. \quad \text{(II.22)}$$

For the symmetric random walk on a simple square lattice with jumps to nearest neighbors, $\sigma_1 = \sigma_2 = 2^{-\frac{1}{2}}$ and the mean passage time is

$$\lim_{N\to\infty} \frac{\langle n(\mathbf{s}) \rangle}{N^2} = \frac{2 \log s}{\pi}. \quad \text{(II.23)}$$

The three-dimensional first-passage time is given by

$$\lim_{N\to\infty} \frac{\langle n(\mathbf{s}) \rangle}{N^3}$$
$$= \varphi(0, 1) - \frac{1}{2\pi\sigma_1\sigma_2\sigma_3\lambda} + \cdots, \quad \mathbf{s} \neq 0. \quad \text{(II.24)}$$

It is interesting to note that, in one and two dimensions, the first term in the asymptotic expansion for the mean first-passage time depends only on λ and the σ_i and not on any further detailed description of the lattice. Furthermore, $\langle n(\mathbf{s}) \rangle / N^k$ is an increasing function of λ for large λ in one and two dimensions. In three and higher dimensions the mean first-passage time depends in a detailed way on the lattice [through $\varphi(0, 1)$] and to a first approximation is a constant, independent of λ.

Calculation of the variances of the first passage times is considerably more difficult because, at the very least, the expression for the variance contains $\varphi(0, 1)$. For the one-dimensional random walk with jump probabilities of $\frac{1}{2}$ to either nearest neighbor, the detailed expansion of $P(s, z)$ around $z = 1$ is from Eq. (II.19)

$$P(s, z) = 1 - s(N - s)(1 - z) + \tfrac{1}{6}s(N - s)$$
$$\times (N^2 + sN - s^2 - 5)(1 - z)^2 + \cdots. \quad \text{(II.25)}$$

From this expression we derive

$$\sigma^2(s) = \langle n^2(s) \rangle - \langle n(s) \rangle^2$$
$$= \tfrac{1}{3}s(N - s)[N^2 - 2s(N - s) - 2], \quad s \neq 0. \quad \text{(II.26)}$$

For $s = 0$ we have

$$F(0, z) = 1 - [P(0, z)]^{-1} = 1 - N(1 - z)$$
$$+ \tfrac{1}{6}N(N^2 - 1)(1 - z)^2 - \cdots, \quad \text{(II.27)}$$

[8] W. Feller, *An Introduction to Probability Theory and its Applications* (John Wiley & Sons, Inc., New York, 1951).

from which it follows that[2]

$$\sigma^2(0) = \tfrac{1}{3}N(N-1)(N-2). \qquad \text{(II.28)}$$

It is possible to derive an asymptotic value for $\sigma^2(0)$ for any 1-D transition probabilities by noticing that in the limit $N=\infty$, the principal contributions in

$$\varphi(0,1) = \frac{1}{N}\sum_{j=1}^{N-1}\left\{1-\lambda\left(\frac{2\pi j}{N}\right)\right\}^{-1}$$
$$= \frac{2}{N}\sum_{j=1}^{[\frac{1}{2}(N-1)]}\left\{1-\lambda\left(\frac{2\pi j}{N}\right)\right\}^{-1}$$
$$+\frac{1}{2N}[1+(-1)^N]\left\{1-\lambda\left(\frac{2\pi[\frac{1}{2}(N-1)]+2\pi}{N}\right)\right\}^{-1}$$

come from small j. We therefore expand $\lambda(2\pi j/N)$ according to Eq. (II.4) and find

$$\varphi(0,1) \sim \frac{N}{\pi^2\sigma_1^2}\sum_{j=1}^{[\frac{1}{2}(N-1)]} j^{-2}. \qquad \text{(II.29)}$$

In the limit of large N the series can be replaced by its sum to infinity $\frac{1}{6}\pi^2$, and the asymptotic expression for the variance becomes

$$\sigma^2(0) \sim N^3/3\sigma_1^2 \qquad \text{(II.30)}$$

in agreement with the special result given in Eq. (II.28). It is also possible to derive an expression for $\sigma^2(s)$ for $s \ll N$ by this technique. A calculation similar to the preceding serves to show that

$$\frac{\partial\varphi(0,1)}{\partial z} - \frac{\partial\varphi(s,1)}{\partial z} = \frac{Ns^2}{6\sigma_1^4}; \qquad \text{(II.31)}$$

hence the principal contribution to $\sigma^2(s)$ comes from the first term in the expression for $\langle n^2(s)\rangle$. Using the expression for $\varphi(0,1)$ given in Eq. (II.29) we find

$$\sigma^2(s) = (sN^3)/(3\sigma_1^4). \qquad \text{(II.32)}$$

It is shown in Appendix B that the asymptotic form for $\varphi(0,1)$ in the 2-D case as $N\to\infty$ is

$$\varphi(0,1) \sim (\pi\sigma_1\sigma_2)^{-1}\log N. \qquad \text{(II.33)}$$

Hence in 2D the variance in the return time to the origin is

$$\sigma^2(0) \sim (2/\pi\sigma_1\sigma_2)N^4\log N. \qquad \text{(II.34)}$$

The sum defining $\varphi(0,1)$ converges in three dimensions and greater. As $N\to\infty$, $\varphi(0,1)$ has the integral form (II.6). These integrals have been calculated by Watson[9] for cubic lattices. From the numerical values one obtains the following estimates of $\sigma^2(0)$ for the cubic lattices:

s.c. $\sigma^2(0)/N^6$

$$\sim \frac{2}{(2\pi)^3}\iiint_{-\pi}^{\pi}\frac{d^3\vartheta}{1-\frac{1}{3}(c_1+c_2+c_3)} - 1 = 2.032,$$

f.c. $\sigma^2(0)/N^6$

$$\sim \frac{2}{(2\pi)^3}\iiint_{-\pi}^{\pi}\frac{d^3\vartheta}{1-\frac{1}{3}(c_1c_2+c_2c_3+c_3c_1)} - 1 = 1.690,$$

b.c. $\sigma^2(0)/N^6$

$$\sim \frac{2}{(2\pi)^3}\iiint_{-\pi}^{\pi}\frac{d^3\vartheta}{1-c_1c_2c_3} - 1 = 1.786.$$

It is of incidental interest that the expression for the variance

$$\sigma^2(0) = N^{2k}[2\varphi(0,1)-1]+N^k \qquad \text{(II.35)}$$

shows that, for $k\geq 3$,

$$\varphi(0,1)\geq \tfrac{1}{2}, \qquad \text{(II.36)}$$

a result which seems otherwise difficult to prove.

III. NUMBER OF POINTS VISITED r TIMES IN AN n-STEP WALK

We now turn to the statistics of the number of distinct lattice points visited during an n-step walk. We will be concerned mainly with the large n case, although some results will also be given for any integer n.

Let S_n be the average number of lattice points visited in an n-step walk. Then

$$S_n = 1+\sum_{\mathbf{s}}{}'\{F_1(\mathbf{s})+F_2(\mathbf{s})+\cdots+F_n(\mathbf{s})\}, \qquad \text{(III.1)}$$

where the primed summation proceeds over all lattice points except the origin. The integer 1 represents the fact that the walker was originally at the origin. As before $F_j(\mathbf{s})$ is the probability that the walker arrives at $\mathbf{s}$ for the first time after the jth step. Hence the summand of (III.1) represents the probability that the point $\mathbf{s}$ has been occupied at least once in the first n steps.

It is convenient to define a quantity Δ_k by

$$\Delta_k = S_k - S_{k-1}, \qquad k=1,2,\cdots. \qquad \text{(III.2)}$$

Since $S_0=1$ and $S_1=2$ we find $\Delta_1=1$. Then

$$\Delta_n = \sum_{\mathbf{s}}{}' F_n(\mathbf{s}) = -F_n(0)+\sum_{\mathbf{s}} F_n(\mathbf{s}). \qquad \text{(III.3)}$$

[9] G. N. Watson, Quar. J. Math. Oxford, Ser. 10, 266 (1939).

Hence the generating function for Δ_k is

$$\Delta(z) = \sum_{1}^{\infty} z^n \Delta_n$$
$$= -\sum_{1}^{\infty} z^n F_n(0) + \sum_{\mathbf{s}} \sum_{n=1}^{\infty} z^n F_n(\mathbf{s}), \qquad \text{(III.4)}$$

so that

$$\Delta(z) = -F(0, z) + \sum_{\mathbf{s}} F(\mathbf{s}, z). \qquad \text{(III.5)}$$

However from Eq. (I.18)

$$F(\mathbf{s}, z) = \frac{P(\mathbf{s}, z) - \delta_{\mathbf{s},0}}{P(0, z)} \qquad \text{(III.6)}$$

and

$$\Delta(z) = -1 + \sum_{\mathbf{s}} \frac{P(\mathbf{s}, z)}{P(0, z)}. \qquad \text{(III.7)}$$

Then Eq. (I.14b) implies

$$\Delta(z) = -1 + \{(1 - z)P(0, z)\}^{-1}. \qquad \text{(III.8)}$$

The generating function $S(z)$ can be obtained immediately from this expression since

$$S_0 = 1,$$
$$S_1 = 1 + \Delta_1,$$
$$\cdots$$
$$S_n = 1 + \Delta_1 + \Delta_2 + \cdots + \Delta_n \quad \text{etc.}, \qquad \text{(III.9)}$$

we find

$$S(z) = \frac{1}{1 - z} + \frac{z\Delta_1}{1 - z} + \frac{z^2\Delta_2}{1 - z} + \cdots$$
$$= \frac{1}{1 - z} + \frac{\Delta(z)}{1 - z}.$$

Hence from (III.8)

$$S(z) = \{(1 - z)^2 P(0, z)\}^{-1}. \qquad \text{(III.10)}$$

The asymptotic properties of S_n as $n \to \infty$ can be inferred from the analytic behavior of $\Delta(z)$ as $z \to 1$ by employing the following Tauberian theorem[10]:

Let $A(y) = \sum a_n \exp(-ny)$ be convergent for all $y > 0$ and let $a_n > 0$ for all n. If as $y \to 0$

$$A(y) \sim \varphi(y^{-1}), \qquad \text{(III.11a)}$$

where (i) $\varphi(x) = x^\sigma L(x)$ is a positive increasing function of x for x greater than some x_0, and which increases monotonically to infinity for x sufficiently large; (ii) σ is ≥ 0; and (iii) $L(cx) \sim L(x)$ as $x \to \infty$; then as $n \to \infty$

$$a_1 + a_2 + \cdots + a_n \sim \varphi(n)/\Gamma(\sigma + 1). \qquad \text{(III.11b)}$$

In our problem we interpret $a_1 + \cdots + a_n$ as $\Delta_1 + \cdots + \Delta_n$ and $A(y)$ as $\Delta(e^{-y})$.

[10] G. H. Hardy, *Divergent Series* (Oxford University Press, New York, 1949).

As $z \to 1$ the asymptotic behavior of $P(0, z)$ in one, two, and three dimensions is as follows[2]:

$$\text{1D} \quad P(0, z) = (1 - z^2)^{-\frac{1}{2}}, \qquad \text{(III.12a)}$$
$$\text{2D} \quad P(0, z) \sim -\pi^{-1} \log(1 - z), \qquad \text{(III.12b)}$$
$$\text{3D} \quad P(0, z) \sim P(0, 1) + a(1 - z)^{\frac{1}{2}} + \cdots, \qquad \text{(III.12c)}$$

where a is a constant which depends on the lattice. Then, if we let $z = \exp(-y)$ and let $y \to 0$,

$$\text{1D} \quad \Delta(z) \sim (2/y)^{\frac{1}{2}}, \qquad \text{(III.13a)}$$
$$\text{2D} \quad \Delta(z) \sim (\pi/y)[1/\log(1/y)], \qquad \text{(III.13b)}$$
$$\text{3D} \quad \Delta(z) \sim [yP(0, 1)]^{-1}. \qquad \text{(III.13c)}$$

The Tauberian theorem given above applies directly to our problem[2] if we choose

$$\text{1D} \quad \sigma = \tfrac{1}{2}, \quad L(x) = 2^{\frac{1}{2}}, \qquad \text{(III.14a)}$$
$$\text{2D} \quad \sigma = 1, \quad L(x) = \pi/\log x, \qquad \text{(III.14b)}$$
$$\text{3D} \quad \sigma = 1, \quad L(x) = 1/P(0, 1). \qquad \text{(III.14c)}$$

We therefore find for the number of distinct lattice points visited after n steps

$$\text{1D} \quad S_n \sim (8n/\pi)^{\frac{1}{2}}, \qquad \text{(III.15a)}$$
$$\text{2D} \quad S_n \sim \pi n/\log n, \qquad \text{(III.15b)}$$
$$\text{3D} \quad S_n \sim n/P(0, 1). \qquad \text{(III.15c)}$$

These results have been derived by Erdos and Dvoretsky[3] and by Vineyard[4] by somewhat different methods. The values of $P(0, 1)$ are 1.5164 for a simple cubic lattice, 1.3445 for a face-centered and 1.3932 for a body-centered cubic lattice.[2,4]

It is interesting to note that the 2-D S_n/π has the same asymptotic behavior as the number of primes less than n. Perhaps one can find some deep connection between random walks on square lattices and the distribution of primes.

We have shown in Appendix C that the generating function for the average number of lattice points visited at least r times, $S_n^{(r)}$, is

$$S^{(r)}(z) = \left\{1 - \frac{1}{P(0, z)}\right\}^{r-1} \frac{1}{(1 - z)^2 P(0, z)}, \qquad \text{(III.16)}$$

while that of

$$\Delta_n^{(r)} = S_n^{(r)} - S_{n-1}^{(r)}$$

is

$$\Delta^{(r)}(z) = \left\{1 - \frac{1}{P(0, z)}\right\}^{r-1} \frac{1}{(1 - z)P(0, z)}, \quad r \geq 2. \qquad \text{(III.17)}$$

The average number of lattice points visited *exactly*

r times after n steps, $V_n^{(r)}$ is given by

$$V_n^{(r)} = S_n^{(r)} - S_n^{(r+1)}. \qquad \text{(III.18)}$$

Its generating function is

$$V^{(r)}(z) = \sum_0^\infty V_n^{(r)} z^r$$
$$= \frac{1}{(1-z)^2[P(0,z)]^2}\left\{1 - \frac{1}{P(0,z)}\right\}^{r-1}. \qquad \text{(III.19)}$$

By applying the above Tauberian theorem to Eq. (III.17) we can generalize (III.15c) to find $S_n^{(r)}$, the average number of points occupied at least r times in a walk of n steps on a three-dimensional lattice. If we set $z = e^{-y}$ and let $y \to 0$ we find

$$\Delta^{(r)}(e^{-y}) \sim \left\{1 - \frac{1}{P(0,1)}\right\}^{r-1} \frac{1}{P(0,1)y}, \qquad \text{(III.20)}$$

so that in the notation of the Tauberian theorem $\sigma = 1$ and

$$L(x) = \frac{1}{P(0,1)}\left\{1 - \frac{1}{P(0,1)}\right\}^{r-1}$$
$$= \text{constant}. \qquad \text{(III.21)}$$

Hence, since for $r > 1$

$$S_n^{(r)} = \Delta_1^{(r)} + \Delta_2^{(r)} + \cdots + \Delta_n^{(r)},$$

Eq. (III.16) implies that as $n \to \infty$

$$S_n^{(r)} \sim \frac{n}{P(0,1)}\left\{1 - \frac{1}{P(0,1)}\right\}^{r-1}. \qquad \text{(III.22)}$$

Noting that the quantity $f = 1 - [P(0,1)]^{-1}$ is the probability that a random walker who starts from the origin ever returns to the origin, we can write

$$S_n^{(r)} \sim n(1-f)f^{r-1}. \qquad \text{(III.23)}$$

The values of f for the three cubic lattices are sc 0.34056, bcc 0.28223, and fcc 0.25632.

As $n \to \infty$, the average number of points occupied on a 3-D lattice exactly r times in an n step walk is

$$V_n^{(r)} = S_n^{(r)} - S_n^{(r+1)} \sim n(1-f)^2 f^{r-1}. \qquad \text{(III.24)}$$

If one wishes to find correction terms to the asymptotic formulas (III.15) for S_n, the number of points visited at least once in an n step walk, he must proceed in a more systematic manner. In the 3-D case it is shown in Appendix D that

$$P(0,z) = u_0 - u_1(1-z)^{\frac{1}{2}} + u_2(1-z)$$
$$- u_3(1-z)^{\frac{3}{2}} + \cdots. \qquad \text{(III.25)}$$

The numbers u_0 for the various cubic lattices are given in Eq. (D.3) of that appendix.[9] It was also shown that

$$u_1 = \begin{cases} (3/\pi)(\frac{3}{2})^{\frac{1}{2}} = 1.1695454 & \text{sc}, \qquad \text{(III.26a)} \\ 1/2^{\frac{1}{2}}\pi = 0.2250791 & \text{bcc}, \qquad \text{(III.26b)} \\ 3^{\frac{1}{2}}/4\pi = 0.4134967 & \text{fcc}. \qquad \text{(III.26c)} \end{cases}$$

The values of u_2 and u_3 have not been calculated for the bcc and fcc; however, for the sc lattice,[11]

$$u_2 = 1.384761, \qquad \text{(III.27a)}$$

$$u_3 = \frac{9}{4\pi}\left(\frac{3}{2}\right)^{\frac{1}{2}} = 0.877159. \qquad \text{(III.27b)}$$

Equation (III.25) can be substituted into the generating function $S(z)$ [see Eq. (III.10)] to obtain

$$S(z) = [u_0(1-z)^2]^{-1}$$
$$+ (u_1/u_0^2)(1-z)^{-\frac{3}{2}} + [(u_1^2 - u_2u_0)/u_0^3](1-z)^{-1}$$
$$+ [(u_1^3 - 2u_0u_1u_2 + u_3u_0^2)/u_0^4](1-z)^{-\frac{1}{2}} + \cdots. \qquad \text{(III.28)}$$

Now the coefficient of z^n in the series expansion of $(1-z)^m$ is

for $m = -2$: $(n+1)$, (III.29a)

for $m = -\frac{3}{2}$: $(2n+1)!/2^{2n}n!\,n!$, (III.29b)

for $m = -1$: 1, (III.29c)

for $m = -\frac{1}{2}$: $(2n-1)!/2^{2n-1}n!\,(n-1)!$. (III.29d)

One can use Stirling's expansion for large n to find

$$\frac{(2n+1)!}{2^{2n}n!\,n!} \sim 2\left(\frac{n}{\pi}\right)^{\frac{1}{2}}$$
$$\times \left[1 + \frac{3}{8n} - \frac{7}{128n^2} + \cdots\right], \qquad \text{(III.30a)}$$

$$\frac{(2n-1)!}{2^{2n-1}n!\,(n-1)!} \sim \frac{1}{(n\pi)^{\frac{1}{2}}}$$
$$\times \left[1 - \frac{1}{8n} + \frac{1}{128n^2} - \cdots\right]. \qquad \text{(III.30b)}$$

Then

$$S_n \sim \frac{n}{u_0} + \frac{2u_1}{u_0^2}\left(\frac{n}{\pi}\right)^{\frac{1}{2}} + (u_1^2 - u_2u_0 + u_0^2)/u_0^3$$
$$+ (3u_1u_0^2 + 4u_1^3 - 8u_0u_1u_2$$
$$+ 4u_3u_0^2)/[4u_0^4(\pi n)^{\frac{1}{2}}] + O(1/n). \qquad \text{(III.31)}$$

In the case of the bcc lattice

$$S_n \sim \frac{4\pi^3 n}{[\Gamma(\frac{1}{4})]^4} + \frac{16\pi^5}{[\Gamma(\frac{1}{4})]^8}\left(\frac{2n}{\pi}\right)^{\frac{1}{2}} + O(1)$$
$$= 0.71777001n + 0.130846n^{\frac{1}{2}} + O(1). \qquad \text{(III.32)}$$

[11] A. Maradudin, E. Montroll, G. Weiss, R. Herman, and H. Milnes, "Green's Functions for Monatomic Simple Cubic Lattices," Acad. Roy. Belg. Cl. Sci. Mem. Coll. in 4° (2) 14 (1960) No. 7.

In the case of the fcc lattice

$$S_n \sim \frac{2^{11/3} n \pi^4}{9\{\Gamma(\frac{1}{3})\}^6} + \frac{2^{19/3}\pi^7}{9\{\Gamma(\frac{1}{3})\}^{12}}\left(\frac{n}{3\pi}\right)^{1/2} + O(1)$$

$$= 0.74368182n + 0.258048n^{1/2} + O(1), \quad \text{(III.33)}$$

while with the extra information available for the sc lattice one finds in that case

$$S_n \sim 0.65946267n + 0.573921n^{1/2}$$

$$+ 0.449530 + 0.40732n^{-1/2} + \cdots . \quad \text{(III.34)}$$

A similar expression can be obtained for the number of points occupied at least once after n steps on a 1-D lattice walk in which the walker steps only to a nearest-neighbor point on each step (steps in either direction being equally probable). Then from (III.10)

$$S(z) = \frac{(1-z^2)^{\frac{1}{2}}}{(1-z)^2} = \frac{[2-(1-z)]^{\frac{1}{2}}}{(1-z)^{\frac{3}{2}}}$$

$$= 2^{\frac{1}{2}}\{(1-z)^{-\frac{3}{2}} - \tfrac{1}{4}(1-z)^{-\frac{1}{2}}$$

$$- \tfrac{1}{32}(1-z)^{\frac{1}{2}} - \tfrac{1}{128}(1-z)^{\frac{3}{2}} - \cdots\}, \quad \text{(III.35)}$$

so that

$$S_n \sim \frac{2^{\frac{1}{2}}(2n+1)!}{2^{2n} n!\, n!}\left\{1 - \frac{1}{4(2n+1)} - \frac{1}{32(4n^2-1)} - \cdots\right\}. \quad \text{(III.36)}$$

If n is chosen to be as small as 4 this yields 3.347 as compared with the exact value 3.375 given in Table II. By using Stirling's approximation [see Eq. (III.30)] for the factorials we find the somewhat simplified expression

$$S_n \sim \left(\frac{8n}{\pi}\right)^{\frac{1}{2}}\left\{1 + \frac{1}{4n} - \frac{3}{64n^2} + \cdots\right\}. \quad \text{(III.37)}$$

The generating function for the number of points which are occupied exactly once in an n step 1-D walk is, from (III.19) and (III.12a)

$$V^{(1)}(z) = [(1-z)P(z,0)]^{-2}$$

$$= (1-z^2)/(1-z)^2 = (1+z)/(1-z)$$

$$= 1 + 2z + 2z^2 + 2z^3 + \cdots . \quad \text{(III.38)}$$

Hence

$$V_1^{(1)} = 1 \quad \text{and} \quad V_n^{(1)} = 2 \quad \text{for} \quad n > 1. \quad \text{(III.39)}$$

The asymptotic expression for $V_n^{(1)}$ for large n on a 2-D square lattice can be obtained by finding the generating function for

$$D_n^{(1)} = V_n^{(1)} - V_{n-1}^{(1)},$$
$$D^{(1)}(z) = -1 + (1-z)^{-1}[P(z,0)]^2 \quad \text{(III.40)}$$

(here $D_n^{(1)}$ is analogous to Δ_n in the calculation of S_n). By employing (III.40) and our Tauberian theorem we find

$$V_n^{(1)} \sim n\pi^2/(\log n)^2 \quad \text{(III.41)}$$

to be the asymptotic number of points occupied exactly once in the 2-D case. The result has also been derived by Erdos and Taylor[5] by a different method.

The 1-D generating function for $S_n^{(2)}$, the number of points occupied at least twice in an n-step walk is

$$S^{(2)}(z) \equiv \{1 - (1-z^2)^{\frac{1}{2}}\}\frac{(1-z^2)^{\frac{1}{2}}}{(1-z)^2}$$

$$= S^{(1)}(z) - \left(\frac{1+z}{1-z}\right). \quad \text{(III.42a)}$$

Hence when $n \geq 2$

$$S_n^{(2)} = S_n^{(1)} - 2, \quad \text{(III.42b)}$$

which can be verified in Table II. Similarly,

$$S^{(3)}(z)$$
$$= [1 - 2(1-z^2)^{\frac{1}{2}} + (1-z^2)](1-z^2)^{\frac{1}{2}}/(1-z)^2$$
$$= (2-z^2)S^{(1)}(z) - 2(1+z)/(1-z)$$

Hence

$$S_n^{(3)} = 2S_n^{(1)} - S_{n-2}^{(1)} - 4 \quad \text{if} \quad n \geq 4. \quad \text{(III.42c)}$$

TABLE I. Values of $P(\mathbf{s}, 1)$ for a simple cubic lattice when $s^2 = s_1^2 + s_2^2 + s_3^2 < 15$. These numbers correspond to the symmetrical case with $P(s_1s_2s_3, 1) = P(s_2s_1s_3, 1) = \cdots$, etc. This function is the lattice Green's function defined by (II.6) and (I.5) when $z = 1$.

(s_1, s_2, s_3)	$P(\mathbf{s}, 1)$	(s_1, s_2, s_3)	$P(\mathbf{s}, 1)$
001	0.516387	023	0.132451
002	0.257336	111	0.261470
003	0.165271	112	0.191792
011	0.331149	113	0.144196
012	0.215590	122	0.156953
013	0.153139	123	0.126946
022	0.168331	222	0.135908

TABLE II. $S_n^{(r)}$ = Average number of points occupied at least r times in a 1-D walk of n steps.

n/r	1	2	2	4	5
0	1	0	0	0	0
1	2	0	0	0	0
2	5/2	1/2	0	0	0
3	3	1	0	0	0
4	27/8	11/8	1/4	0	0
5	15/4	7/4	1/2	0	0
6	65/16	33/16	3/4	1/8	0
7	35/8	19/8	1	1/4	0

TABLE III. $V_n^{(r)}$ = Average number of points occupied exactly r times in a 1-D walk of n steps.

$n/^r$	1	2	3	4	5
0	1	0	0	0	0
1	2	0	0	0	0
2	2	1/2	0	0	0
3	2	1	0	0	0
4	2	9/8	1/4	0	0
5	2	5/4	1/2	0	0
6	2	21/16	5/8	1/8	0
7	2	11/8	3/4	1/4	0

Similarly

$$S_n^{(4)} = 4S_n^{(1)} - 3S_{n-2}^{(1)} - 6 \quad \text{if} \quad n \geq 6, \qquad \text{(III.42d)}$$

etc.

This scheme can be continued further and when these formulas are combined with (III.36) and (III.37), very accurate asymptotic expansions can be found for $S_n^{(r)}$ for 1-D walks, $r \ll n$.

IV. THE NUMBER OF VISITS TO A GIVEN LATTICE POINT DURING A WALK OF n STEPS

The probability that a point $\mathbf{s}$ is visited at least r times in an n-step walk is

$$\sum_{j=1}^{n} F_j^{(r)}(s) \quad \text{if} \quad \mathbf{s} \neq 0,$$

$$\sum_{j=1}^{n} F_j^{(r-1)}(0) \quad \text{if} \quad s = 0,$$

so that the probability that $\mathbf{s}$ is visited *exactly* r times is

$$\beta_n^{(r)}(\mathbf{s}) = \begin{cases} \sum_{j=1}^{n} [F_j^{(r)}(\mathbf{s}) - F_j^{(r+1)}(\mathbf{s})], & \text{if} \quad \mathbf{s} \neq 0, \\ \sum_{j=1}^{n} [F_j^{(r-1)}(0) - F_j^{(r)}(0)], & \text{if} \quad \mathbf{s} = 0. \end{cases} \qquad \text{(IV.1)}$$

The formulas for $\beta_n^{(r)}(0)$ are distinctive because the walker starts at the origin.

The generating function for $\beta^{(r)}(\mathbf{s}, z)$,

$$\beta^{(r)}(\mathbf{s}, z) \equiv \sum_{1}^{n} z^n \beta_n^{(r)}, \qquad \text{(IV.2)}$$

is easily seen from (I.20) to be

$$\beta^{(r)}(\mathbf{s}, z) = \begin{cases} (1-z)^{-1}F(\mathbf{s}, z)[1 - F(0, z)] \\ \qquad \times [F(0, z)]^{r-1}, \ \mathbf{s} \neq 0, \\ (1-z)[F(0, z)]^{r-1} \\ \qquad \times [1 - F(0, z)], \ \mathbf{s} = 0. \end{cases} \qquad \text{(IV.3)}$$

The mean number of times the point $\mathbf{s}$ has been visited after n steps is

$$M_n(\mathbf{s}) = \sum r\beta_n^{(r)}(\mathbf{s}). \qquad \text{(IV.4)}$$

This has the generating function

$$\begin{aligned} M(\mathbf{s}, z) &= \sum_{r=1}^{\infty} \sum_{n=1}^{\infty} r\beta_n^{(r)}(\mathbf{s}) z^n \\ &= \sum_{r=1}^{\infty} r\beta^{(r)}(\mathbf{s}, z) \\ &= \frac{F(\mathbf{s}, z)}{(1-z)[1 - F(0, z)]} \quad \text{if} \quad \mathbf{s} \neq 0 \\ &= (1-z)^{-1}P(\mathbf{s}, z). \end{aligned} \qquad \text{(IV.5)}$$

If $\mathbf{s} = 0$,

$$\begin{aligned} M(0, z) &= \{(1-z)[1 - F(0, z)]\}^{-1} \\ &= (1-z)^{-1}P(0, z). \end{aligned} \qquad \text{(IV.6)}$$

Hence (IV.5) is valid for all $\mathbf{s}$ including $\mathbf{s} = 0$.

The asymptotic form for $M_n(0)$ for 3-D lattices can be obtained by using the expression for $P(0, z)$ given in Appendix F. There it is shown that

$$P(0, z) \sim u_0 - [2(1-z)]^{\frac{1}{2}}/\pi\sigma_1\sigma_2\sigma_3 + \cdots, \qquad \text{(IV.7)}$$

where the u_0 and σ's are defined generally and evaluated for walks on cubic lattices where only steps to nearest-neighbor points (all with equal probability) are taken. By combining Eqs. (IV.6), (IV.7), and (III.29) we obtain

$$M_n(0) \sim u_0 - (2/\pi n)^{\frac{1}{2}}/\pi\sigma_1\sigma_2\sigma_3 + O(1/n). \qquad \text{(IV.8)}$$

The numerical results are

$$M_n(0) \sim \begin{cases} 1.51639 - 1.31969n^{-\frac{1}{2}} + \cdots & \text{sc}, \\ 1.39320 - 0.25397n^{-\frac{1}{2}} + \cdots & \text{fcc}, \\ 1.34466 - 0.46658n^{-\frac{1}{2}} + \cdots & \text{bcc}. \end{cases} \qquad \text{(IV.9)}$$

As $n \to \infty$

$$M_n(\mathbf{s}) \to P(\mathbf{s}, 1). \qquad \text{(IV.10)}$$

These functions have been tabulated for[11] sc lattices when $s^2 < 25$. Some values are given in Table I.

When $\mathbf{s}$ is large and $z \to 1$ we have from (I.18b) [where $\lambda^2 = \sum (s_j/\sigma_j)^2$]

$$\begin{aligned} P(\mathbf{s}, z) &\sim \frac{\exp\{-\lambda[2(1-z)^{\frac{1}{2}}]\}}{\lambda\sigma_1\sigma_2\sigma_3(2\pi)^2} \\ &\sim \frac{1}{\lambda\sigma_1\sigma_2\sigma_3(2\pi)^2}\{1 - \lambda[2(1-z)]^{\frac{1}{2}} + \cdots\}. \end{aligned} \qquad \text{(IV.11)}$$

Hence, from (IV.5), (IV.7), and (III.29), when s

and n are both large, but still with $s \ll n^{\frac{1}{2}}$,

$$M_n(\mathbf{s}) \sim \frac{1}{\lambda\sigma_1\sigma_2\sigma_3(2\pi)^2} \times \left\{1 - \lambda\left(\frac{2}{\pi n}\right)^{\frac{1}{2}} + \cdots\right\}. \tag{IV.12}$$

Employing the σ values given in Appendix D for the walks involving only steps to nearest-neighbor lattice points on cubic lattices we find

$$M_n(\mathbf{s}) \sim \begin{cases} \dfrac{3}{4s\pi^2}\left[1 - s\left(\dfrac{6}{\pi n}\right)^{\frac{1}{2}} + \cdots\right] \text{sc} \\ \dfrac{1}{4s\pi^2}\left[1 - s\left(\dfrac{2}{\pi n}\right)^{\frac{1}{2}} + \cdots\right] \text{bcc} \\ \dfrac{3}{8s\pi^2}\left[1 - s\left(\dfrac{3}{\pi n}\right)^{\frac{1}{2}} + \cdots\right] \text{fcc}. \end{cases} \tag{IV.13}$$

A word of caution should be given concerning these results. One would expect that $M_n(\mathbf{s})$ should appear with some ordering with respect to nearest neighbors. However the bcc results are not between the sc and fcc. This is because all lattices were obtained by restricting walks on a fundamental sc lattice. If the unit cells of each of the lattices were made the same size and s reexpressed as a length the results would fall properly in order.

V. LATTICE WALKS FOR CONTINUOUS TIME VARIABLE

The preceding results can be used as a basis for the analysis of continuous time random walks on discrete lattices. In this theory we shall be interested in functions like $\bar{P}(\mathbf{s}, t)$ and $\bar{F}(\mathbf{s}, t)$ (the probability of being at $\mathbf{s}$ at time t) and the probability density for reaching $\mathbf{s}$ for the first time at time t, respectively. We shall assume that jumps are made at random times $t_1, t_2, t_3, \cdots$ where the random variables

$$T_1 = t_1, \quad T_2 = t_2 - t_1, \cdots, \quad T_n = t_n - t_{n-1}, \cdots \tag{V.1}$$

have a common density $\psi(t)$. It will be convenient to define a further class of probability densities $\{\psi_n(t)\}$ by

$$\psi_0(t) = \delta(t), \tag{V.2}$$

$$\psi_n(t) = \int_0^t \psi(\tau)\psi_{n-1}(t - \tau)\, d\tau, \quad n = 1, 2, 3, \cdots. \tag{V.3}$$

These are the probability densities for the occurrence of the nth step at time t. The most significant property of the $\psi_n(t)$ is the fact that their Laplace transforms are

$$\int_0^\infty e^{-ut}\psi_n(t)\, dt = [\psi^*(u)]^n, \tag{V.4}$$

where

$$\psi^*(u) = \int_0^\infty e^{-ut}\psi(t)\, dt. \tag{V.5}$$

In terms of the $F_n(\mathbf{s})$ defined in Sec. 1, $\bar{F}(\mathbf{s}, t)$ is given by

$$\bar{F}(\mathbf{s}, t) = \sum_{n=0}^\infty F_n(\mathbf{s})\psi_n(t) \tag{V.6}$$

and its Laplace transform is

$$\begin{aligned} \bar{F}^*(\mathbf{s}, u) &= \int_0^\infty \bar{F}(\mathbf{s}, t)e^{-ut}\, dt \\ &= \sum_{n=0}^\infty F_n(\mathbf{s})[\psi^*(u)]^n \\ &= F[\mathbf{s}, \psi^*(u)], \end{aligned} \tag{V.7}$$

where $F(\mathbf{s}, z)$ is the generating function of Eq. (I.17).

The function $\bar{P}(\mathbf{s}, t)$ is almost as simply related to the generating function $P(\mathbf{s}, z)$. Let $Q(\mathbf{s}, t)$ be the probability density for the random walk to reach $\mathbf{s}$ at time t (not necessarily for the first time) and let

$$\begin{aligned} \Psi(t) &= \text{probability that walker remains fixed in time interval } (0, t) \\ &= 1 - \int_0^t \psi(x)\, dx = \int_t^\infty \psi(x)\, dx. \end{aligned} \tag{V.8}$$

Then

$$\bar{P}(\mathbf{s}, t) = \int_0^t Q(\mathbf{s}, \tau)\Psi(t - \tau)\, d\tau, \tag{V.9}$$

or, in terms of Laplace transforms,

$$\bar{P}^*(\mathbf{s}, u) = Q^*(\mathbf{s}, u)[1 - \psi^*(u)]/u. \tag{V.10}$$

But $Q(s, t)$ is given by

$$Q(\mathbf{s}, t) = \sum_{n=0}^\infty P_n(\mathbf{s})\psi_n(t) \tag{V.11}$$

or

$$\begin{aligned} Q^*(\mathbf{s}, u) &= \sum_{n=0}^\infty P_n(\mathbf{s})[\psi^*(u)]^n \\ &= P[\mathbf{s}, \psi^*(u)], \end{aligned} \tag{V.12}$$

so that only the generating functions already discussed need be calculated.

Moments for various quantities of interest are easily derived from the formulas above. For example the first moment and variance of the first-passage time to s are

$$\bar{t} = -\frac{\partial F[\mathbf{s}, \psi^*(u)]}{\partial u}\bigg]_{u=0^+} = \langle n(\mathbf{s})\rangle \bar{T}, \qquad \text{(V.13a)}$$

$$\overline{t^2} - \bar{t}^2 = [\langle n^2(\mathbf{s})\rangle - \langle n(\mathbf{s})\rangle^2]\bar{T}^2 + \langle n(\mathbf{s})\rangle[\overline{T^2} - \bar{T}^2], \qquad \text{(V.13b)}$$

where $\overline{T^n}$ is the nth moment of the time between steps and $\langle n(s)\rangle$ and $\langle n^2(s)\rangle$ are given by (II.2) and (II.3).

Continuous analogues of other discrete results are obtained in the same manner. For example, the probability density for the random walker to reach s for the rth time is

$$\overline{F^{(r)}}(\mathbf{s}, t) = \sum_{n=0}^{\infty} F_n^{(r)}(\mathbf{s})\psi_n(t) \qquad \text{(V.14a)}$$

or

$$\overline{F^{(r)}}^*(\mathbf{s}, u) = F^{(r)}[\mathbf{s}, \psi^*(u)], \qquad \text{(V.14b)}$$

where $F^{(r)}(\mathbf{s}, z)$ is given by (I.20).

We can also consider the statistics of the number of distinct steps visited after a time t. Let $S(t)$ be the average number of lattice points visited at least once in time t. Then

$$S(t) = \sum_{\mathbf{s}} \int_0^t F^{(r)}(\mathbf{s}, \tau)\, d\tau. \qquad \text{(V.15a)}$$

Hence the Laplace transform of $S(t)$ is

$$\mathfrak{L}\{S(t)\} = \frac{\psi^*(u)}{u[1 - \psi^*(u)]P(0, \psi^*(u))}. \qquad \text{(V.15b)}$$

To find the large t behavior of $S(t)$ it is necessary to use the expansion

$$\psi^*(u) = 1 - u\bar{T} + o(u) \qquad \text{(V.16)}$$

in Eq. (V.5), together with the asymptotic forms of Eq. (III.12) for the behavior of $P(0, z)$ in the neighbor hood of $z = 1$. In this way, we find that in one dimension

$$\mathfrak{L}\{S(t)\} = (2/\bar{T})^{\frac{1}{2}}u^{-\frac{3}{2}} + O(u^{-1}) \qquad \text{(V.17)}$$

in the neighborhood of $u = 0$. But, by a Tauberian theorem[7] this implies that

$$S(t) = (8t/\pi\bar{T})^{\frac{1}{2}} + O(1). \qquad \text{(V.18)}$$

In three dimensions the result is

$$S(t) = (t/\bar{T})/P(0, 1) + O(1). \qquad \text{(V.19)}$$

The results are in agreement with (III.15a) and (III.15b) since the number of steps n is just $t/\bar{T}$ in the case of steps at regular time intervals.

VI. EFFECT OF TRAPS ON PROBABILITY OF RETURN TO THE ORIGIN ON A 1-D LATTICE

Another type of random walk problem is concerned with effect of traps on the probability of a walker eventually returning to the origin. We shall limit ourselves here to a discussion of the 1-D case while an analysis of the 2-D and 3-D problems, which are much more difficult, will be given elsewhere.

It has been shown[2] that in the presence of one trap at l_1 and another at l_2 with $l_2 < 0 < l_1$ the probability that a walker initially at the origin is trapped before return to the origin is

$$(l_1 - l_2)/2l_1(-l_2) = \tfrac{1}{2}(l_1^{-1} - l_2^{-1}).$$

This probability is not changed by the addition of any number of new traps *which are not located in the interval* $l_2 < 0 < l_1$.

Let c be the concentration of independently located traps. Then, if it is known that the origin is not a trap, the probability that a trap exists at l_1 and at l_2 and none in between is

$$c(1 - c)^{-l_2-1}(1 - c)^{l_1-1}c.$$

Hence the probability of our walker being trapped before returning to the origin is

$$\sum_{l_1=1}^{\infty} \sum_{l_2=-1}^{-\infty} c^2(1 - c)^{l_1-l_2-2}(\tfrac{1}{2})(l_1^{-1} - l_2^{-1})$$
$$= c^2(1 - c)^{-1}\left\{\sum_{l=1}^{\infty} (1 - c)^{l-1}\right\}\left\{\sum_{l_1=1}^{\infty} (1 - c)^{l_1}/l_1\right\}$$
$$= -[c/(1 - c)] \log c.$$

Then as a function of concentration of traps, the probability of a walker returning to the origin before being trapped is

$$F(c) = 1 + [c/(1 - c)] \log c.$$

APPENDIX A. ASYMPTOTIC FORM OF $\varphi(s, z)$ AS $s \to \infty$

The Green's function

$$\varphi(\mathbf{s}, z) = \frac{1}{(2\pi)^k} \int_{-\pi}^{\pi} \cdots \int \frac{\exp i\mathbf{s}\cdot\boldsymbol{\vartheta}\, d^k\boldsymbol{\vartheta}}{1 - z\lambda(\boldsymbol{\vartheta})} \qquad \text{(A.1)}$$

can be expressed as

$$\varphi(\mathbf{s}, z) = \frac{1}{(2\pi)^k} \int_0^{\infty} e^{-\alpha}\, d\alpha \int_{-\pi}^{\pi} \cdots \int e^{i\mathbf{s}\cdot\boldsymbol{\vartheta}} \times e^{\alpha z\lambda(\boldsymbol{\vartheta})}\, d^k\boldsymbol{\vartheta}. \qquad \text{(A.2)}$$

When s is very large the main contribution to the $\boldsymbol{\vartheta}$ integration comes from small values of $|\boldsymbol{\vartheta}|$. In this range in a symmetrical random walk (see I.4)

$$\lambda(\boldsymbol{\vartheta}) = 1 - \tfrac{1}{2}\sum \sigma_i^2\vartheta_i^2 + \tfrac{1}{4}\sum_{ij}\mu_{ij}\vartheta_i^2\vartheta_j^2 - \cdots. \tag{A.3}$$

If we let $s_i\vartheta_i = \varphi_i$ and $\lambda_i = s_i/\sigma_i$, then $\varphi(s, z)$ becomes

$$\varphi(s, z) = \frac{1}{(2\pi)^k}\int_0^\infty e^{-\alpha(1-z)}\, d\alpha$$
$$\times \int_{-\pi s_1}^{\pi s_1}\cdots\int_{-\pi s_k}^{\pi s_k} e^{i(\varphi_1+\varphi_2+\cdots)}e^{-\frac{1}{2}\alpha z\sum \lambda_i^{-2}\varphi_i^2}$$
$$\times \{1 + \tfrac{1}{4}\alpha z \sum (\mu_{ij}/s_i^2s_j^2)\varphi_i^2\varphi_j^2 + \cdots\}\, d^k\varphi/s_1\cdots s_k. \tag{A.4}$$

As all $s_i \to \infty$ the limits on the φ integration can be extended to $\pm\infty$ with errors of only $O[\exp(-cs_i^2)]$ appearing.

If we let

$$R_n(a) = \int_{-\infty}^{\infty} e^{i\varphi}e^{-\frac{1}{2}a\varphi^2}\varphi^n\, d\varphi, \tag{A.5}$$

then

$$\varphi(s, z) \sim (2\pi)^{-k}\int_0^\infty e^{-\alpha(1-z)}\, d\alpha\left\{\prod_{\nu=1}^k R_0(\alpha z\lambda_\nu^{-2})\right\}$$
$$\times\left\{1 + \tfrac{1}{4}\alpha z\sum_{i=1}^k (\mu_{ii}/s_i^4)(R_4/R_0)_{\alpha z\lambda_i^{-2}}\right.$$
$$\left. + \tfrac{1}{4}\alpha z \sum{}' \frac{\mu_{ij}}{s_i^2s_j^2}\left(\frac{R_2}{R_0}\right)_{\alpha z\lambda_i^{-2}}\left(\frac{R_2}{R_0}\right)_{\alpha z\lambda_j^{-2}} + \cdots\right\},$$

where as usual the prime in the summation indicates that the terms with $i = j$ are to be omitted.

From standard integral tables one finds

$$R_0(a) = (2\pi/a)^{\frac{1}{2}}\exp(-1/2a),$$
$$(R_2/R_0)_a = a^{-1}(1 - a^{-1}),$$
$$(R_4/R_0)_a = a^{-2}(3 - 6a^{-1} + a^{-2}).$$

Then, if we let

$$S_n(z) = \int_0^\infty \alpha^{-\frac{1}{2}n}e^{-\alpha(1-z)}\exp\left(-\frac{1}{2\alpha z}\sum\lambda_\nu^2\right)d\alpha,$$

we find

$$\varphi(\mathbf{s}, z) \sim \frac{(2\pi z)^{-\frac{1}{2}k}}{\sigma_1\cdots\sigma_k}\left[S_k + \sum_{i=1}^k \frac{\mu_{ii}}{4z\sigma_i^4}\right.$$
$$\times(3S_{k+2} - 6z^{-1}\lambda_i^2S_{k+4} + z^{-2}\lambda_i^4S_{k+6})$$
$$+ \tfrac{1}{4}\sum{}'\frac{\mu_{ij}}{z\sigma_i^2\sigma_j^2}[S_{k+2} - z^{-1}(\lambda_i^2 + \lambda_j^2)S_{k+4}$$
$$\left. + z^{-2}\lambda_i^2\lambda_j^2S_{k+6}] + \cdots\right].$$

In the special case $z = 1$, we see that

$$S_n(1) = (2/\lambda^2)^{\frac{1}{2}(n-2)}\Gamma(\tfrac{1}{2}n - 1)$$

where

$$\lambda^2 = \sum\lambda_\nu^2 = \sum_{\nu=1}^k s_\nu^2/\sigma_\nu^2.$$

Generally,

$$S_n(z) = 2\left(\frac{2}{\lambda}\right)^{\frac{1}{2}n-1}[z(1-z)]^{\frac{1}{4}(n-2)}K_{\frac{1}{2}n-1}\left(\left[\frac{\lambda^2}{z}(1-z)\right]^{\frac{1}{2}}\right)$$

where K_ν is the νth modified Bessel Function of the second kind. When $z = 1$

$$\varphi(\mathbf{s}, 1) = \frac{\Gamma(\frac{1}{2}k - 1)}{2\sigma_1\cdots\sigma_k\pi^{\frac{1}{2}k}\lambda^{k-2}}\left\{1 - \frac{(1-\frac{1}{2}k)}{2\lambda^2}\sum_{i=1}^k\frac{\mu_{ii}}{\sigma_i^4}\right.$$
$$\times\left[3 - 6k\left(\frac{\lambda_i}{\lambda}\right)^2 + k(k+2)\left(\frac{\lambda_i}{\lambda}\right)^4\right]$$
$$- (1/2\lambda^2)(1 - \tfrac{1}{2}k)\sum{}'\frac{\mu_{ij}}{\sigma_i^2\sigma_j^2}[1 - k(\lambda_i^2 + \lambda_j^2)/2\lambda^2$$
$$\left. + k(k+2)\lambda_i^2\lambda_j^2/\lambda^4] + O(\lambda^{-4})\right\}.$$

If $\varphi_1(\mathbf{s}, z)$ is defined [see Eq. (I.9)] as

$$\varphi_1(\mathbf{s}, z)$$
$$= \frac{1}{(2\pi)^k}\int_{-\pi}^{\pi}\cdots\int\frac{\exp(i\boldsymbol{\vartheta}\cdot\mathbf{s})\, d^k\boldsymbol{\vartheta}}{1 - z + \frac{1}{2}z(\sigma_1^2\vartheta_1^2 + \cdots + \sigma_k^2\vartheta_k^2)},$$

then as $\mathbf{s} \to \infty$ and $z \to 1$ when $k \geq 3$, then [see Eq. (I.186)]

$$\varphi_1(\mathbf{s}, z) \sim \frac{\Gamma(\frac{1}{2}k - 1)}{2\sigma_1\cdots\sigma_k\pi^{\frac{1}{2}k}\lambda^{k-2}},$$

which is the leading term in $\varphi(\mathbf{s}, 1)$. Hence if we let

$$\varphi(\mathbf{s}, z) = \varphi_1(\mathbf{s}, z) + \varphi_2(\mathbf{s}, z)$$

where $\varphi_2(s, z)$ is defined as $\varphi(\mathbf{s}, z) - \varphi_1(\mathbf{s}, z)$, we see that when $k \geq 3$

$$\lim_{\mathbf{s}\to\infty}\frac{\varphi_1(\mathbf{s}, 1)}{\varphi_2(\mathbf{s}, 1)} = 0.$$

APPENDIX B. CALCULATION OF 2-D $\varphi(0, 1)$ FOR $N \times N$ LATTICE AS $N \to \infty$

The expression for $\varphi(0, 1)$ in a finite lattice is (Eq. I.16)

$$\varphi(0, 1) = N^{-2}\sum_{r_1=1}^{N-1}\sum_{r_2=1}^{N-1}\left\{1 - \lambda\left(\frac{2\pi r}{N}\right)\right\}^{-1}$$
$$= 4N^{-2}\sum_{1}^{[(N-1)/2]}\sum_{1}^{[(N-1)/2]}\{1 - \lambda\}^{-1}$$
$$+ O(1/N). \tag{B.1}$$

As $N \to \infty$ this sum approaches a divergent integral, the divergence being related to the smallness of $1 - \lambda(2\pi\mathbf{r}/N)$ as $(2\pi\mathbf{r}/N) \to 0$. Hence one would expect the main contribution to (0, 1) to result from small integral values of r_1 and r_2. In this range one can approximate λ by [see Eq. (I.4)]

$$\lambda(2\pi\mathbf{r}/N) \sim 1 - (2\pi^2/N^2)(\sigma_1^2 r_1^2 + \sigma_2^2 r_2^2) + \cdots . \quad \text{(B.2)}$$

We now restrict ourselves to $\sigma_1 = \sigma_2$, the more general case being amenable to a similar analysis.

The range of summation in (B.1) is divided into two parts; the first part containing those lattice points (r_1, r_2) such that $(r_1^2 + r_2^2)^{\frac{1}{2}} < \alpha N$ where α is small enough so that (B.2) is a good approximation of λ for all these points, and the second containing the remainder of the lattice points. It can be shown that the contribution of the second set to $\varphi(0, 1)$ remains bounded as $N \to \infty$. The contribution of the first set is

$$4N^{-2} \sum_{1<(r_1^2+r_2^2)^{\frac{1}{2}}<\alpha N}\sum (N^2/2\pi^2\sigma_1^2)(r_1^2 + r_2^2)^{-1}.$$

When N is sufficiently large, the sum is well approximated by the corresponding integral, which we express in polar coordinates

$$\sum_{1<(r_1^2+r_2^2)^{\frac{1}{2}}<\alpha N} (r_1^2 + r_2^2)^{-1} \sim \int_1^{\alpha N} \frac{2\pi j\, dj}{j^2} = \frac{\pi}{2} \log \alpha N.$$

Hence, as $N \to \infty$ for fixed α,

$$\varphi(0, 1) \sim (1/\pi\sigma_1^2) \log N.$$

In the unsymmetric case $\sigma_1 \neq \sigma_2$, one finds

$$\varphi(0, 1) \sim (1/\pi\sigma_1\sigma_2) \log N.$$

The above ideas can, with a little effort, be made completely rigorous.

APPENDIX C. GENERATING FUNCTION FOR AVERAGE NUMBER OF POINTS VISITED AT LEAST r TIMES IN AN n-STEP WALK

Let $S_n^{(r)}$ be the average number of lattice points visited at least r times in an n-step walk. Then

$$\mathrm{S}_n^{(r)} = F_1^{(r-1)}(0) + \cdots + F_n^{(r-1)}(0)$$
$$+ \sum_{\mathbf{s}}{}' \{F_1^{(r)}(\mathbf{s}) + F_2^{(r)}(\mathbf{s}) + \cdots + F_n^{(r)}(\mathbf{s})\}, \quad \text{(C.1)}$$

where the primed summation proceeds over all lattice points except the origin. As usual $F_j^{(r)}(\mathbf{s})$ is the probability that the walker arrives at $\mathbf{s}$ for the rth time on the jth step. The sum

$$F_1^{(r)}(s) + F_2^{(r)}(s) + \cdots + F_n^{(r)}(s)$$

represents the probability that the point $\mathbf{s}$ has been occupied *at least* r times in n steps. The reason

$$F_1^{(r-1)}(0) + \cdots + F_n^{(r-1)}(0)$$

is chosen to represent $(r - 1)$ returns to the origin instead of r is that the walker started at the origin, so visiting the origin r times means *returning* to it $r - 1$ times.

It is convenient to define a quantity

$$\Delta_k^{(r)} = S_k^{(r)} - S_{k-1}^{(r)}. \quad \text{(C.2)}$$

Since $S_0^{(1)} = 1$ and $S_1^{(1)} = 2$ while $S_0^{(r)} = S_1^{(r)} = 0$ for $r > 1$,

$$\Delta_1^{(1)} = 1 \quad \text{and} \quad \Delta_1^{(r)} = 0 \quad \text{if} \quad r > 1. \quad \text{(C.3)}$$

Also

$$S_n^{(r)} = \delta_{r,1} + \Delta_1^{(r)} + \Delta_2^{(r)} + \cdots + \Delta_n^{(r)}. \quad \text{(C.4)}$$

Through the use of an appropriate Tauberian Theorem we will be able to find the asymptotic properties of $S_n^{(r)}$ in terms of the properties of the generating function

$$\Delta^{(r)}(z) = \sum_{n=1}^{\infty} z^n \Delta_n^{(r)}. \quad \text{(C.5)}$$

Note that

$$\Delta_n^{(r)} = F_n^{(r-1)}(0) + \sum_{\mathbf{s}}{}' F_n^{(r)}(\mathbf{s})$$
$$= [F_n^{(r-1)}(0) - F_n^{(r)}(0)] + \sum_{\mathbf{s}} F_n^{(r)}(\mathbf{s}). \quad \text{(C.6)}$$

Hence if we multiply this equation by z^n and sum from $n = 1$ to ∞ we find

$$\Delta^{(r)}(z) = \{F^{(r-1)}(0, z) - F^{(r)}(0, z)\} + \sum_{\mathbf{s}} F^{(r)}(\mathbf{s}, z).$$

From Eq. (I.20) we obtain

$$\Delta^{(r)}(z) = \{F(0, z)\}^{r-1}\{1 - F(0, z) + \sum_{\mathbf{s}} F(\mathbf{s}, z)\},$$

while Eq. (I.18) implies

$$\Delta^{(r)}(z) = \left\{1 - \frac{1}{P(0, z)}\right\}^{r-1} \times \left\{\frac{1}{P(0, z)} + \sum_{\mathbf{s}} \left[\frac{P(\mathbf{s}, z) - \delta_{\mathbf{s},0}}{P(0, z)}\right]\right\}.$$

Finally from (I.14b)

$$\Delta^{(r)}(z) = \left\{1 - \frac{1}{P(0, z)}\right\}^{r-1} \{(1 - z)P(0, z)\}^{-1}.$$

From this expression and (C.4) one finds

$$S^{(r)}(z) = \left\{1 - \frac{1}{P(0, z)}\right\}^{r-1} \{(1 - z)^2 P(0, z)\}^{-1}. \quad \text{(C.7)}$$

APPENDIX D. THE ASYMPTOTIC FORM OF $P(0, z)$ AS $z \to 1$ FOR 3-D LATTICES

The generating function

$$P(0, z) = \frac{1}{(2\pi)^3} \iiint_{-\pi}^{\pi} \frac{d^3\varphi}{1 - z\lambda(\varphi)} \quad \text{(D.1)}$$

can be expressed as

$$\frac{1}{(2\pi)^3}\iiint_{-\pi}^{\pi}\frac{d^3\varphi}{1-\lambda(\varphi)}$$

$$-\frac{(1-z)}{(2\pi)^3}\iiint_{-\pi}^{\pi}\frac{\lambda(\varphi)\,d^3\varphi}{[1-\lambda(\varphi)][1-z\lambda(\varphi)]}=u_0-\delta. \quad \text{(D.2)}$$

The first part, u_0 has been found by G. N. Watson[9] for simple, body-centered, and face-centered cubic lattices. His results are

$$\begin{aligned}&\text{sc} \quad 1.5163860591,\\&\text{bcc} \quad (4\pi^3)^{-1}[\Gamma(\tfrac{1}{4})]^4 = 1.3932039297,\\&\text{fcc} \quad 9\{\Gamma(\tfrac{1}{3})\}^6 2^{-11/3}\pi^{-4} = 1.3446610732.\end{aligned} \quad \text{(D.3)}$$

We shall be concerned with the determination of δ as $z \to 1$.

The main contribution to δ as $z \to 1$ comes from values of φ close to the origin. We can write

$$\lambda(\varphi) = 1 - \tfrac{1}{2}(\sigma_1^2\varphi_1^2 + \sigma_2^2\varphi_2^2 + \sigma_3^2\varphi_3^2) + O(\varphi^4). \quad \text{(D.4)}$$

For example in the case of steps to the nearest-neighbor lattice points only on cubic lattices one finds from (I.5) that

$$\text{sc} \quad \sigma_1 = \sigma_2 = \sigma_3 = (\tfrac{1}{3})^{\frac{1}{2}}, \quad \text{(D.5a)}$$

$$\text{bcc} \quad \sigma_1 = \sigma_2 = \sigma_3 = 1, \quad \text{(D.5b)}$$

$$\text{fcc} \quad \sigma_1 = \sigma_2 = \sigma_3 = (\tfrac{2}{3})^{\frac{1}{2}}. \quad \text{(D.5c)}$$

As $\varphi \to 0$ and $z \to 1$ the integrand of δ becomes

$$2/\{(\sigma_1^2\varphi_1^2 + \sigma_2^2\varphi_2^2 + \sigma_3^2\varphi_3^2) \times [(1-z) + \tfrac{1}{2}(\varphi_1^2\sigma_1^2 + \varphi_2^2\sigma_2^2 + \varphi_3^2\sigma_3^2) + \cdots]\}.$$

It can be shown that as $z \to 1$ the range of integration can be made infinite in δ if one is concerned only with terms first order in $(z-1)$. Then, if we let $x_i = \sigma_i\varphi_i$ and calculate δ using polar coordinates with $r^2 = x_1^2 + x_2^2 + x_3^2$ we find

$$\delta \sim \frac{1-z}{\sigma_1\sigma_2\sigma_3\pi^2}\int_0^\infty \frac{dr}{(1-z)+\frac{1}{2}r^2} = \frac{[\frac{1}{2}(1-z)]^{\frac{1}{2}}}{\sigma_1\sigma_2\sigma_3\pi},$$

so that

$$P(0,z) \sim u_0 - [2(1-z)]^{\frac{1}{2}}/\sigma_1\sigma_2\sigma_3\pi + O(1-z). \quad \text{(D.6)}$$

It is much harder to calculate the term of $O(1-z)$. It has only been done for the simple cubic lattice. Since

$$1/\sigma_1\sigma_2\sigma_3 = \begin{cases} 3^{\frac{3}{2}} & \text{sc},\\ 1 & \text{bcc},\\ (\frac{3}{2})^{\frac{3}{2}} & \text{fcc}.\end{cases} \quad \text{(D.7)}$$

we find that for bcc

$$P(0,z) \sim \frac{1}{4\pi^3}\{\Gamma(\tfrac{1}{4})\}^4 - \frac{1}{\pi}[\tfrac{1}{2}(1-z)]^{\frac{1}{2}} + \cdots; \quad \text{(D.8a)}$$

for fcc

$$P(0,z) \sim \frac{9\{\Gamma(\frac{1}{3})\}^6}{2^{11/3}\pi^4} - \frac{3^{\frac{3}{2}}}{4\pi}(1-z)^{\frac{1}{2}} + \cdots. \quad \text{(D.8b)}$$

More terms have been obtained for the sc lattice[11]:

$$P(0,z) \sim 1.516386 - \frac{3}{\pi}\left(\frac{3}{2}\right)^{\frac{1}{2}}(1-z)^{\frac{1}{2}}$$

$$+ 1.384761(1-z) - \frac{9}{4\pi}\left(\frac{3}{2}\right)^{\frac{1}{2}}(1-z)^{\frac{3}{2}} + \cdots. \quad \text{(D.9)}$$