

Random Walks on Lattices

by

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1. INTRODUCTION

TYPICAL PROBLEMS

We shall be concerned principally with counting the number of ways certain events can occur on lattices, where, by a lattice, we mean a periodic collection of points. These problems have importance to many branches of chemistry and solid-state physics since the lattice may be thought of as a mathematical model of a crystal, with the points of the lattice corresponding to atoms of the crystal.

The most important problem to be dealt with is that of random walks on periodic space lattices. The random walk problem will be emphasized here because, as we shall see, many of the features of this problem also arise in other lattice problems. The random walk problem on a crystal lattice arises in many different physical situations. For example, suppose the crystal lattice has an interstitial defect, i.e., there is one atom which is a little different from its neighbors and, thus, may move from one point to another. In this case, the diffusion constant for impurities in the crystal depend on the random walk in lattices. For another example, consider the process of photosynthesis, where energy from

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a light source causes a molecule to go into an "excited" state, and this excitation is passed from molecule to molecule until it reaches a "trap" where the important features of the process start. In this case, the existence of a molecule in an "excited" state corresponds to the random walker. Another type of situation involving random walks is the annealing of metal alloys. While the alloy is hot, the structure is porous, but as it cools it assumes a crystalline lattice structure. In doing so, however, some of the atoms assume the wrong positions and, consequently, they must move into their correct positions. In this situation, as the atoms move to form an equilibrium state, the important question is the number of new positions occupied by an atom during a certain number of steps.

A second important lattice statistics problem is that involving dimers, or diatomic molecules. Here we consider the situation in which dimers are absorbed on the surface of a lattice, each dimer thereby occupying two adjacent lattice sites. We are interested here in the number of different possible configurations of dimers on the lattice surface.

Another lattice statistics problem, one which appears in the theory of phase transitions, is the so-called Ising problem (see [3], p.121). The Ising problem turns out to be equivalent not only to the dimer problem but also to the mathematical problem of counting the number of ways of drawing closed graphs on a lattice which has a specific number of fixed bonds.

The problem of vibration in chemical lattices, which at first glance does not seem to have much combinatorial significance, actually turns out to be very similar to the random walk problem.

A final problem is that of the motion of electrons in a lattice. As a model of the crystal in this case, we could use nodes (atoms) with wires

connecting them so that we can think of the electrons as traveling along the wires. This problem, too, is very similar to the random walk problem.

Thus, the above-mentioned problems are some of the more important lattice statistics problems. Before proceeding to discuss the most important of these, the random walk problem, we give a formal definition of a 3D (i.e., 3 dimensional) lattice. Consider a set of three non-coplanar unit vectors i_1, i_2 , and i_3 . The endpoints of the vectors

$$\underline{s} = (s_1, s_2, s_3) = s_1 i_1 + s_2 i_2 + s_3 i_3$$

which are generated by letting the s 's range through the integers $0, \pm 1, \pm 2, \dots$ form a *space lattice of three dimensions*. Periodic lattices of arbitrary dimensionality can be defined in a similar manner.

2. RANDOM WALKS ON LATTICES

THE POLYA PROBLEM

There will be three general types of questions which we shall be interested in concerning random walks on lattices:

1) What is the probability that the random walker travels from a starting point \underline{a} to a point \underline{b} in n steps? If $\underline{b} = \underline{a}$, then we have the classical Polya problem, i.e., to determine the probability that the walker returns to his starting point.

2) The first passage time problem, i.e., what is the probability that a walker arrives at a point \underline{s} for the first time after n steps?

3) What are the number of distinct lattice points visited by the random walker after n steps?

The present section will be devoted primarily to answering the first of these three questions.

We consider first the case of a finite $N \times N \times \dots \times N$ lattice with periodic boundary conditions. That is, the lattice will have N^d lattice points (where d is the dimensionality) and it will be a torus. In the 1D case, this would correspond to a ring of regularly spaced points. In the 2D case, it corresponds to a square grid of points wrapped into the form of a torus, etc.

Define

$$P_t(\underline{s}) = \text{prob. that walker is at } \underline{s} \text{ after } t \text{ steps}$$

$$F_t(\underline{s}) = \text{prob. that walker is at } \underline{s} \text{ for first time after } t \text{ steps.}$$

Without loss of generality, we can assume that the walker starts at the origin. Thus

$$P_0(\underline{s}) = \delta_{0,\underline{s}} = \begin{cases} 1 & \text{if } \underline{s} = \underline{0} \\ 0 & \text{if } \underline{s} \neq \underline{0}. \end{cases}$$

Further, we assume that the walker takes steps at regular time intervals, i.e., $t = 0, 1, 2, \dots$.

With our periodic boundary conditions, it follows that, letting $\underline{s} = (s_1, s_2, \dots, s_d)$,

$$\begin{aligned} P_t(s_1, s_2, \dots, s_d) &= P_t(s_1+N, s_2, \dots, s_d) \\ &= P_t(s_1, s_2+N, \dots, s_d) \\ &= \text{etc.} \end{aligned}$$

Finally we make the assumption that the random walk is a stationary random process, i.e., the transition probability that the walker goes from \underline{s}' to

\underline{s} at a given time t is independent of t , i.e.,

$$\Pr\{\underline{s}' \rightarrow \underline{s} \text{ at time } t\} = p(\underline{s}-\underline{s}'),$$

where we make the additional assumption that this probability depends only on the distance vector $\underline{s}-\underline{s}'$.

Under the above assumptions, it follows that the random walk constitutes a Markov chain and thus all properties of Markov chains hold.

Furthermore, it is obvious that

$$\sum_{\underline{s}} P_t(\underline{s}) = 1 \quad (1)$$

and

$$\sum_{\underline{s}} p(\underline{s}) = 1. \quad (2)$$

We now see that we have the difference equation

$$P_t(\underline{s}) = \sum_{\underline{s}'} p(\underline{s}-\underline{s}')P_{t-1}(\underline{s}'). \quad (3)$$

Define the generating function

$$P(\underline{s}, z) = \sum_{t \geq 0} z^t P_t(\underline{s}), \quad (4)$$

then, by substituting the difference equation in (4), we have

$$\begin{aligned} P(\underline{s}, z) &= \sum_{t \geq 1} z \sum_{\underline{s}'} p(\underline{s}-\underline{s}')P_{t-1}(\underline{s}')z^{t-1} + \delta_{\underline{s}, \underline{0}} \\ &= z \sum_{\underline{s}'} p(\underline{s}-\underline{s}')P(\underline{s}', z) + \delta_{\underline{s}, \underline{0}} \end{aligned}$$

which implies

$$P(\underline{s}, z) - z \sum_{\underline{s}'} p(\underline{s}-\underline{s}')P(\underline{s}', z) = \delta_{\underline{s}, \underline{0}}. \quad (5)$$

This last is a Green's function type of equation.

A simple expression for $\sum_{\underline{s}} P(\underline{s}, z)$ follows from (5) by summing over all \underline{s} and recalling (2):

$$\begin{aligned} \sum_{\underline{s}} P(\underline{s}, z) &= 1 + z \sum_{\underline{s}, \underline{s}'} p(\underline{s}-\underline{s}')P(\underline{s}', z) \\ &= 1 + z \sum_{\underline{s}''} p(\underline{s}'') \sum_{\underline{s}} P(\underline{s}-\underline{s}'', z); \quad [\underline{s}'' = \underline{s}-\underline{s}'] \\ &= 1 + z \sum_{\underline{s}''} p(\underline{s}'') \sum_{\underline{s}} P(\underline{s}, z) \\ &= 1 + z \sum_{\underline{s}} P(\underline{s}, z) \end{aligned}$$

so that

$$\sum_{\underline{s}} P(\underline{s}, z) = \frac{1}{1-z}. \quad (6)$$

Another function which is of importance in this study is the finite Fourier transform

$$u\left(z, \frac{2\pi \underline{r}}{N}\right) = \sum_{\underline{s}} P(\underline{s}, z) e^{2\pi i \underline{r} \cdot \underline{s} / N} \quad (7)$$

where

$$\underline{r} = (r_1, r_2, \dots, r_d), \quad 1 \leq r_i \leq N-1.$$

This is just as good as a function to discuss as the generating function, since, by taking the Fourier inverse, we can get the generating function

from $u(z, (2\pi\underline{r}/N))$. Further, let us denote the finite Fourier transform of the transition probabilities by

$$\lambda \left(\frac{2\pi\underline{r}}{N} \right) \equiv \sum_{\underline{s}} p(\underline{s}) e^{2\pi i \underline{r} \cdot \underline{s} / N} . \quad (8)$$

This is called the *structure function*. It follows that

$$u - zu\lambda = 1$$

and hence

$$u = \frac{1}{1 - z\lambda} . \quad (9)$$

Notice that the structure function is a very basic function since it can be calculated immediately once we are given the transition probabilities. Thus the structure function is the function that tells the difference between a random walk on two separate lattices, or between one type of random walk and another type on the same lattice. For example, in the 1D case where we have the probability of a step to the left or to the right equal to $\frac{1}{2}$, then the structure function would be

$$\frac{1}{2} [e^{2\pi i r / N} + e^{-2\pi i r / N}] = \cos \frac{2\pi r}{N} \quad (10)$$

Now, once we know the structure function, then we can get the function $u(z, (2\pi\underline{r}/N))$, and thus by Fourier inversion we can get the generating function

$$P(\underline{s}, z) = \frac{1}{N^d} \sum_{r_1=0}^{N-1} \dots \sum_{r_d=0}^{N-1} \frac{e^{-2\pi i \underline{r} \cdot \underline{s} / N}}{1 - z\lambda \left(\frac{2\pi\underline{r}}{N} \right)} . \quad (11)$$

Therefore, from this we get

$$P_t(\underline{s}) = \frac{1}{N^d} \sum_{r_1=0}^{N-1} \dots \sum_{r_d=0}^{N-1} \left[\lambda \left(\frac{2\pi \underline{r}}{N} \right) \right]^t e^{-2\pi i \underline{r} \cdot \underline{s} / N} \quad (12)$$

Hence, it follows that for a given random walk, all we need study is its structure function. From this structure function, we can get all other interesting functions and probabilities.

We can extend these notions to the case of the infinite lattice, i.e., as $N^d \rightarrow \infty$. In this case, we must convert the above sums into integrals. We do so by letting

$$\frac{1}{N} = \frac{1}{2\pi} \cdot \frac{2\pi}{N}$$

$$\theta_j = \frac{2\pi r_j}{N}$$

Then

$$d\theta_j = \frac{2\pi}{N}$$

and we get

$$P(\underline{s}, z) = \frac{1}{(2\pi)^d} \int \dots \int_0^{2\pi} \frac{e^{-i\theta \underline{s}} d^d \theta}{1 - z\lambda(\theta)} \quad (13)$$

$$P_t(\underline{s}) = \frac{1}{(2\pi)^d} \int \dots \int_0^{2\pi} (\lambda(\theta))^t e^{i\theta \underline{s}} d^d \theta \quad (14)$$

[Note that the limits of the integrals could also be $(-\pi, \pi)$.]

In the above notation we see that

$$\lambda(\underline{\theta}) = \sum_{\underline{s}} p(\underline{s}) e^{i\theta \cdot \underline{s}} = \sum_{\underline{s}} p(\underline{s}) \left[1 + i\theta \cdot \underline{s} - \frac{\theta^2 \cdot \underline{s}^2}{2!} + \dots \right] \approx 1 + i\theta \sum p(\underline{s}) \underline{s} - \frac{\theta^2}{2} \sum \underline{s}^2 p(\underline{s}) \quad (15)$$

when $\underline{\theta}$ is very small, i.e., when \underline{r} is close to the origin.

We now want to relate the probabilities $P_t(\underline{s})$ of reaching a point \underline{s} on the t -th step to the probabilities $F_t(\underline{s})$ of reaching \underline{s} for the first time on step t . It is easy to see that

$$P_t(\underline{s}) = \delta_{\underline{s}, \underline{0}} \delta_{t,0} + \sum_{j=1}^t F_j(\underline{s}) P_{t-j}(\underline{0}). \quad (16)$$

The generating function for $F_t(\underline{s})$ is

$$F(\underline{s}, z) = \sum_{t=1}^{\infty} z^t F_t(\underline{s}). \quad (17)$$

Now

$$\sum_{t \geq 1} z^t P_t(\underline{s}) = \sum_{t \geq 1} \delta_{\underline{s}, \underline{0}} \delta_{t,0} z^t + \sum_{t \geq 1} \sum_{j=1}^t z^j F_j(\underline{s}) P_{t-j}(\underline{0}) z^{t-j}$$

or

$$P(\underline{s}, z) - \delta_{\underline{s}, \underline{0}} = P(\underline{0}, z) F(\underline{s}, z)$$

and hence

$$F(\underline{s}, z) = \frac{P(\underline{s}, z) - \delta_{\underline{s}, \underline{0}}}{P(\underline{0}, z)} = \begin{cases} 1 - \frac{1}{P(\underline{0}, z)} & \text{if } \underline{s} = \underline{0} \\ \frac{P(\underline{s}, z)}{P(\underline{0}, z)} & \text{if } \underline{s} \neq \underline{0} \end{cases}. \quad (18)$$

Therefore we see that we can get the generating function $F(\underline{s}, z)$ once we know the generating function $P(\underline{s}, z)$.

Further, we can get information about the Polya problem from these first probabilities. Indeed

Prob. that walker returns to origin = $F_1(\underline{0}) + F_2(\underline{0}) + F_3(\underline{0}) + \dots$

$$= F(\underline{0}, 1)$$

$$= 1 - \frac{1}{P(\underline{0}, 1)} \quad (19)$$

$$\begin{cases} = 1 & \text{if } P(\underline{0}, 1) = \infty \\ < 1 & \text{if } P(\underline{0}, 1) < \infty \end{cases}$$

Thus, the walker will be certain to return to the origin if $P(\underline{0}, 1) = \infty$ and the probability of return will be *less* than one if $P(\underline{0}, 1)$ is finite.

Now consider equation (11) which is an expression for $P(\underline{s}, z)$ for a finite lattice. If $\underline{r} = \underline{0}$ then $\lambda(2\pi\underline{r}/N)$ and $e^{-2\pi i \underline{r} \cdot \underline{s}/N}$ will equal one. Therefore,

$$P(\underline{s}, z) = \frac{1}{N^d(1-z)} + \phi(\underline{s}, z)$$

where the correction term $\phi(\underline{s}, z)$ is a sum omitting the origin $\underline{r} = \underline{0}$.

Hence if $z=1$, then $P(\underline{s}, z)$ will diverge, i.e., $P(\underline{0}, 1) = \infty$. Therefore, for a *finite* lattice, no matter what dimension, the random walker is certain to return to the origin.

Now we consider the Polya problem for an infinite lattice. From (13) we see that

$$P(\underline{0}, 1) = \frac{1}{(2\pi)^d} \int \cdots \int_0^{2\pi} \frac{d^d \theta}{1 - \lambda(\theta)} .$$

But from (15) it follows that as $\underline{\theta} \rightarrow \underline{0}$ then

$$1 - \lambda(\theta) \sim \frac{1}{2} \theta^2 \mu^2 ,$$

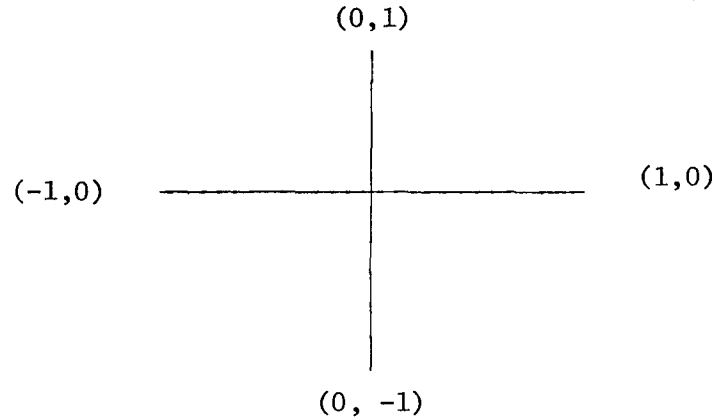
where $\mu = \sum_{\underline{s}} p(\underline{s}) \underline{s}$. The integral can be expressed as the sum of two

components, the first being over a d D sphere of a small radius, a , whose center is at the origin, and the second the integral over the d D hypercube of volume $(2\pi)^d$ with the central small sphere excluded. In a region not including the origin, the integrand is well behaved; no divergence can come from the second component of the integral. We calculate the contribution of the integral over a spherical shell about the origin of our $\underline{\theta}$ space in the neighborhood of $\underline{\theta}=0$ but omit the contribution of the sphere of radius ϵ and then let $\epsilon \rightarrow 0$. As long as the exterior radius, r , of the shell is small, the integrand depends only on r so we can use polar coordinates in our integration and $d^d\theta$ is proportional to $r^{d-1}dr$. Our required integral is then proportional to

$$I(\epsilon) = \int_{\epsilon}^a \frac{r^{d-1}}{r^2} dr = \int_{\epsilon}^a r^{d-3} dr = \begin{cases} \epsilon^{-2} - a^{-2} & \text{if } d = 1 \\ -\log \epsilon/a & \text{if } d = 2 \\ \frac{a^{d-2} - \epsilon^{d-2}}{d-2} & \text{if } d \geq 3 \end{cases}$$

As $\epsilon \rightarrow 0$ so that the neighborhood of the origin is included in the integration, $I(\epsilon) \rightarrow \infty$ when $d = 1, 2$, while $I(\epsilon) < \infty$ when $d \geq 3$. Hence $P(0,1)$ diverges when $d = 1, 2$ and converges when $d \geq 3$. This is equivalent to Polya's result: A random walker who walks so that steps are only to nearest neighbor sites is certain to return to his point of origin if he walks on a 1D or 2D lattice. A nonvanishing escape probability exists in infinite lattices of more than two dimensions.

Now consider the special case of a 2D square lattice in which steps can be made to nearest neighbors only, and all possible steps have equal probability. We wish to calculate the structure function. As the figure below shows,



there are only four possible step vectors, $\underline{s} = (s_1, s_2) = (1,0), (-1,0), (0,-1)$ and $(0,1)$. Thus each step vector \underline{s} has probability $p(\underline{s}) = \frac{1}{4}$ and, if $\underline{\theta} = (\theta_1, \theta_2)$, then the structure function is

$$\begin{aligned} \lambda(\underline{\theta}) &= \sum_{\underline{s}} p(\underline{s}) e^{i\underline{\theta} \cdot \underline{s}} \\ &= \frac{1}{4}(e^{i\theta_1} + e^{-i\theta_1} + e^{-i\theta_2} + e^{i\theta_2}) \\ &= \frac{1}{2}(c_1 + c_2) \end{aligned} \quad (20)$$

where we let

$$c_i = \cos \theta_i \quad i = 1, 2, \dots \quad (21)$$

Thus, from (10) and (21) we see that for a simple cubic lattice (S.C.) of $d=1,2$ dimensions we have

$$\begin{aligned} \lambda(\theta) &= c_1 \quad \text{for } d = 1 \\ &= \frac{1}{2}(c_1 + c_2) \quad \text{for } d = 2. \end{aligned}$$

Indeed it can be shown that, in general, for a simple cubic lattice of d dimensions, its structure function is

$$\lambda(\underline{\theta}) = \frac{1}{d} (c_1 + c_2 + \dots + c_d).$$

Further, for a 3D face-centered cubic lattice (F.C.C.), i.e., a cube with an extra point in the center, the structure function is

$$\lambda(\underline{\theta}) = \frac{1}{3}(c_1c_2+c_2c_3+c_1c_3) .$$

Likewise, for a 3D body-centered cubic lattice (B.C.C.), i.e., a cube with extra points on the faces, we have

$$\lambda(\underline{\theta}) = c_1c_2c_3.$$

Calculating the Polya probabilities for these examples proceeds as follows. We know that

$$\text{prob. of return to origin} = 1 - \frac{1}{P(0,1)} .$$

The integrals are

$$\begin{aligned} P(0,1) &= \left(\frac{1}{2\pi}\right)^3 \iiint_0^{2\pi} \frac{d^3\theta}{1-\frac{1}{3}(c_1+c_2+c_3)} && \text{for S.C. lattice} \\ &= \left(\frac{1}{2\pi}\right)^3 \iiint_0^{2\pi} \frac{d^3\theta}{1-\frac{1}{3}(c_1c_2+c_1c_3+c_2c_3)} && \text{for F.C.C. lattice} \\ &= \left(\frac{1}{2\pi}\right)^3 \iiint_0^{2\pi} \frac{d^3\theta}{1-c_1c_2c_3} && \text{for B.C.C. lattice.} \end{aligned}$$

Fortunately the values of these integrals have been calculated by G. N. Watson [9] and hence we have

$$\begin{aligned} \text{prob. return to origin} &\approx 0.34 && \text{S.C. lattice} \\ &\approx 0.28 && \text{B.C.C. lattice} \\ &\approx 0.256 && \text{F.C.C. lattice.} \end{aligned}$$

The number of nearest neighbors to a lattice point in a S.C. lattice is 6;

in a B.C.C. lattice, 8; and in a F.C.C., 12. Thus, it is not surprising that the return probability diminishes as the number of nearest neighbors increases, since more ways for escape exist.

3. FIRST PASSAGE TIMES

We now investigate the average number of steps required to return to the origin or to first reach a point of the lattice. We shall first do the analysis for a finite lattice and then see what happens as we let the number of lattice points become very large. In order to calculate the first passage time, we shall need certain moments; specifically, we let $\langle n(\underline{s}) \rangle$ be the average time to first reach point \underline{s} . In terms of $F(\underline{s}, z)$ this can be written

$$\langle n(\underline{s}) \rangle = \left. \frac{\partial F(\underline{s}, z)}{\partial z} \right|_{z=1}. \quad (22)$$

Recall that we can write

$$P(\underline{s}, z) = \frac{1}{N^d(1-z)} + \phi(\underline{s}, z) \quad (23)$$

where ϕ has no singularities at $z=1$. Thus, substituting (23) into (18), then from (22) we get:

(1) for $\underline{s} = \underline{0}$,

$$\begin{aligned} \langle n(\underline{0}) \rangle &= \left. \frac{\partial}{\partial z} \left[1 - \frac{1}{\frac{1}{N^d(1-z)} + \phi(\underline{0}, z)} \right] \right|_{z=1} \\ &= \left. \frac{\partial}{\partial z} [1 - N^d(1-z)] \right|_{z=1} \\ &= N^d \end{aligned} \quad (24)$$

and, (2) for $\underline{s} \neq \underline{0}$

$$\begin{aligned}
 \langle n(\underline{s}) \rangle &= \frac{\partial}{\partial z} \left\{ \frac{P(\underline{s}, z)}{P(\underline{0}, z)} \right\}_{z=1} \\
 &= \frac{\partial}{\partial z} \left\{ \frac{1+N^d(1-z)\phi(\underline{s}, z)}{1+N^d(1-z)\phi(\underline{0}, z)} \right\}_{z=1} \\
 &= \frac{\partial}{\partial z} \left\{ 1 + N^d(1-z)[\phi(\underline{s}, z) - \phi(\underline{0}, z)] + o(1-z)^2 \right\}_{z=1} \\
 &= N^d[\phi(\underline{0}, z) - \phi(\underline{s}, z)]. \tag{25}
 \end{aligned}$$

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.

As N becomes very large, it can be shown that

(a) For 1D, $\langle n(s) \rangle = s(N-s) \sim Ns$

(b) For 2D, $\frac{\langle n(\underline{s}) \rangle}{N^2} \sim \frac{\log \lambda}{\pi \sigma_1 \sigma_2}$

(c) For 3D, $\frac{\langle n(\underline{s}) \rangle}{N^3} \sim \phi(0,1) - \frac{1}{\pi \sigma_1 \sigma_2 \sigma_3 \lambda}$

where

$$\underline{s} = (s_1, s_2, \dots)$$

$$\sigma_i^2 = \sum_j s_j^2 p(\underline{s})$$

and

$$\lambda^2 = \frac{s_1^2}{\sigma_1^2} + \frac{s_2^2}{\sigma_2^2} + \dots$$

For the derivation of these and other results, reference should be made to [7].

4. NUMBER OF LATTICE POINTS VISITED

We now consider the question of how many distinct lattice points have been visited after n steps. This number obviously increases as the walker continues his walk. Indeed, we can determine this number by using the properties of the generating function $P(\underline{0}, z)$.

Let S_n be the expected number of distinct lattice points visited after n steps and recall that $F_t(\underline{s})$ is the probability that the walker first reaches point \underline{s} on the t -th step. Clearly,

$$S_0 = 1$$

$$S_n = 1 + \sum_{\underline{s} \neq \underline{0}} [F_1(\underline{s}) + F_2(\underline{s}) + \dots + F_n(\underline{s})], \quad n > 0,$$

so that

$$\Delta_n \equiv S_n - S_{n-1} = \sum_{\underline{s} \neq \underline{0}} F_n(\underline{s})$$

where the summation extends over all lattice points except the origin. It follows that

$$S_0 = 1, \quad S_1 = 2$$

$$S_n = 1 + \Delta_1 + \Delta_2 + \dots + \Delta_n, \quad n \geq 1.$$

Now we can relate the generating function $\Delta(z)$ of Δ_n to $P(\underline{0}, z)$ as follows:

$$\Delta(z) \equiv \sum_{n \geq 1} z^n \Delta_n = \sum_{\underline{s} \neq \underline{0}} z^n \sum_{n \geq 1} F_n(\underline{s})$$

$$\begin{aligned}
&= \sum_{\underline{s}} F(\underline{s}, z) - F(\underline{0}, z) \\
&= -1 + \frac{1}{(1-z)P(\underline{0}, z)} \tag{26}
\end{aligned}$$

where we have used (6).

When n is large the asymptotic properties of S_n can be derived from the asymptotic properties of $\Delta(z)$ as $z \rightarrow 1$ by employing the following Tauberian theorem:

Let the sum $A(y) = \sum a_n \exp(-ny)$ converge for $y > 0$ and let $a_n > 0$ for all n . If as $y \rightarrow 0$,

$$A(y) \sim \phi\left(\frac{1}{y}\right)$$

where $\phi(x) \equiv x^\sigma L(x)$ is a positive increasing function of x which tends to ∞ as $x \rightarrow \infty$, and if $\sigma \geq 0$ and $L(cx) \sim L(x)$ as $x \rightarrow \infty$; then as $n \rightarrow \infty$,

$$a_1 + a_2 + \dots + a_n \sim \frac{\phi(n)}{\Gamma(\sigma+1)} .$$

Using the asymptotic properties of $P(\underline{0}, z)$ as $z \rightarrow 1$, i.e.,

$$\begin{aligned}
P(\underline{0}, z) &= (1-z^2)^{-\frac{1}{2}} && \text{1D} \\
P(\underline{0}, z) &\sim \begin{cases} -\frac{1}{\pi} \log(1-z) & \text{2D} \\ P(\underline{0}, 1) + K(1-z)^{\frac{1}{2}} + \dots & \text{3D} \end{cases} && \text{(27)}
\end{aligned}$$

and inserting them in (26), letting $z = \exp(-y)$, we find that as $y \rightarrow 0$,

$$\Delta(s) \sim \begin{cases} (2y)^{\frac{1}{2}} & \text{1D} \\ (\frac{\pi}{y}) / \log(\frac{1}{y}) & \text{2D} \\ 1/yP(\underline{0}, 1) & \text{3D.} \end{cases}$$

The Tauberian theorem applies directly to our problem if we choose

$$\begin{aligned} 1D \quad \sigma &= \frac{1}{2}, & L(x) &= 2^{\frac{1}{2}} \\ 2D \quad \sigma &= 1, & L(x) &= \pi/\log x \\ 3D \quad \sigma &= 1, & L(x) &= 1/P(\underline{0},1) . \end{aligned}$$

Hence we obtain the results for the number of distinct lattice points visited after n steps as $n \rightarrow \infty$,

$$S_n \sim \begin{cases} (8n/\pi)^{\frac{1}{2}} & 1D \\ \pi n/\log n & 2D \\ n/P(\underline{0},1) & 3D \end{cases} \quad (28)$$

5. LATTICE WALKS WITH CONTINUOUS TIME VARIABLE

All the above work has been done under the assumption that the random walker takes steps at regular time intervals. We now wish to remove this assumption and consider the case where the time interval between steps has a continuous probability distribution. In this theory we are primarily interested in certain moments of the time variables.

To be specific, assume the steps are made at random times $0 = t_1 < t_2 < t_3 < \dots$ and that the variables

$$T_1 = t_1, \quad T_2 = t_2 - t_1, \quad T_3 = t_3 - t_2, \quad \dots ,$$

which correspond to the length of the time intervals, have a common probability density $\psi(t)$. Define the sequence $\{\psi_n(t)\}$ of probability densities recursively by

$$\begin{aligned}\psi_0(t) &= \delta(t), \\ \psi_n(t) &= \int_0^t \psi(\tau) \psi_{n-1}(t-\tau) d\tau, \quad n \geq 1.\end{aligned}\tag{29}$$

These are the probability densities of the occurrence of the n-th step at time t.

It turns out that the most interesting features in this theory can be gotten by considering the Laplace transforms of the densities. Indeed, the densities $\psi_n(t)$ have as Laplace transform

$$\begin{aligned}L\psi_n &= (L\psi_{n-1})L\psi = (L\psi_{n-2})(L\psi)^2 \\ &= \dots\dots = (L\psi)^n \\ &= [\psi^*(u)]^n\end{aligned}$$

where

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

Now the probabilities which we are interested in here are precisely

$$\bar{P}(\underline{s}, t) = \text{prob. walker is at } \underline{s} \text{ at time } t$$

$$\bar{F}(\underline{s}, t) = \text{prob. walker is at } \underline{s} \text{ for first time at time } t.$$

Since $\psi_n(t)$ is the probability that the n-th step is made at time t, and recalling that $F_n(\underline{s})$ is the probability that \underline{s} is reached for the first time after n steps, it follows that

$$\bar{F}(\underline{s}, t) = \sum_{n \geq 0} F_n(\underline{s}) \psi_n(t).$$

Hence its Laplace transform is

$$\begin{aligned} L\bar{F} \equiv \bar{F}(\underline{s}, u) &= \sum_{n \geq 0} F_n(\underline{s}) [\psi^*(u)]^n \\ &= F(\underline{s}, \psi^*(u)) \end{aligned}$$

where $F(\underline{s}, z)$ is the generating function for $F_t(\underline{s})$.

The above formulas can be used to easily derive the moments of various interesting quantities. For example, the expected first passage time to \underline{s} is

$$\begin{aligned} \bar{t} &= - \left. \frac{\partial}{\partial u} F(\underline{s}, \psi^*(u)) \right|_{u=0^+} \\ &= \sum_{n \geq 0} n F_n(\underline{s}) \frac{\partial \psi^*(u)}{\partial u} [\psi^*(u)]^{n-1} \Big|_{u=0^+} \\ &= \bar{T} \langle n(\underline{s}) \rangle \end{aligned}$$

since

$$\begin{aligned} \psi^*(0^+) &= 1 \\ \frac{\partial \psi^*}{\partial u} (0^+) &= \bar{T} . \end{aligned}$$

Further the variance of the first passage time to \underline{s} is

$$\overline{t^2} - \bar{t}^2 = [\langle n^2(\underline{s}) \rangle - \langle n(\underline{s}) \rangle^2] \bar{T}^2 + \langle n(\underline{s}) \rangle [\overline{T^2} - \bar{T}^2] ,$$

where \bar{T} and $\overline{T^2}$ are the moments of the times between steps.

Most of the formulas and results gotten for the discrete case can be calculated also for the case of continuous time intervals. As an example, for 1D we can use a Tauberian theorem for Laplace transforms to find that the average number of distinct points visited in time t is

$$S(t) \sim \left(\frac{8t}{\pi T} \right)^{\frac{1}{2}}.$$

Other results are obtained in a similar manner.

6. RANDOM WALKS IN PRESENCE OF DEFECTS

Until now we have been discussing random walks on perfectly periodic lattices. We now wish to investigate the effect of a small number of defective lattice points on the random walk. For example, we might be concerned with the effect of "traps" on the probability of the walker's going from the origin to a given lattice point. A typical problem of this sort is the process of photosynthesis, in which there are traps where the random walker "disappears".

Consider the case in which the lattice contains a few defective points. As discussed in Section 2, the probability that the walker is at point \underline{s} after t steps is determined by

$$P_{t+1}(\underline{s}) = \sum_{\underline{s}'} p(\underline{s}, \underline{s}') P_t(\underline{s}') \quad (30)$$

where $p(\underline{s}, \underline{s}')$ is the transition probability of a step from \underline{s} to \underline{s}' by a walker known to be at \underline{s} . However, this probability now depends on where \underline{s} is, so we cannot make the assumption that $p(\underline{s}, \underline{s}')$ is a function only of $(\underline{s}-\underline{s}')$. However, we can write

$$p(\underline{s}, \underline{s}') = p(\underline{s}-\underline{s}') + q(\underline{s}, \underline{s}'), \quad (31)$$

where the component $p(\underline{s}-\underline{s}')$ is that of the perfect lattice and $q(\underline{s}-\underline{s}')$ is a correction factor. We assume that $q(\cdot, \cdot)$ is non-vanishing for only a small number of points. Since the walker must certainly be at some point

after each step, then

$$\sum_{\underline{s}} p(\underline{s}, \underline{s}') = 1, \text{ for all } \underline{s}'.$$

However, for the perfect lattice we had

$$\sum_{\underline{s}} p(\underline{s} - \underline{s}') = 1,$$

and hence

$$\sum_{\underline{s}} q(\underline{s}, \underline{s}') = 0, \text{ for all } \underline{s}'.$$

Define the generating function $G(\underline{s}, z)$ for the system with defects as

$$G(\underline{s}, z) = \sum_{t \geq 0} P_t(\underline{s}) z^t. \quad (32)$$

As before, we get

$$\begin{aligned} G(\underline{s}, z) - z \sum_{\underline{s}'} p(\underline{s} - \underline{s}') G(\underline{s}', z) &= \delta_{\underline{s}, 0} + z \sum_{\underline{s}'} q(\underline{s}, \underline{s}') G(\underline{s}', z) \\ &\equiv F(\underline{s}) \end{aligned} \quad (33)$$

or equivalently

$$\theta G(\underline{s}, \cdot) = F(\underline{s})$$

where θ is the appropriate operator. We can use the standard Green's function technique to solve this, and we get

$$\begin{aligned} G(\underline{s}, z) &= \sum_{\underline{s}'} P(\underline{s} - \underline{s}', z) F(\underline{s}') \\ &= P(\underline{s}, z) + z \sum_{\underline{s}'} \sum_{\underline{s}''} P(\underline{s} - \underline{s}', z) q(\underline{s}', \underline{s}'') G(\underline{s}'', z). \end{aligned} \quad (34)$$

Now suppose that $q(\cdot, \cdot)$ is non-vanishing only at the defect points $\underline{s}^{(1)}, \underline{s}^{(2)}, \dots, \underline{s}^{(m)}$. If we can determine $G(\underline{s}^{(1)}, z), G(\underline{s}^{(2)}, z), \dots, G(\underline{s}^{(m)}, z)$, then we can use these in (34) to find $G(\underline{s}, z)$ in general.

From (34) we get

$$G(\underline{s}^{(1)}, z) = P(\underline{s}^{(1)}, z) + a_{11} G(\underline{s}^{(1)}, z) + a_{12} G(\underline{s}^{(2)}, z) + \dots$$

$$G(\underline{s}^{(2)}, z) = P(\underline{s}^{(2)}, z) + a_{21} G(\underline{s}^{(1)}, z) + a_{22} G(\underline{s}^{(2)}, z) + \dots$$

etc.

where

$$a_{ij} = z \sum_{\underline{s}'} P(\underline{s}^{(i)} - \underline{s}', z) q(\underline{s}', \underline{s}^{(i)}) \quad (35)$$

and hence

$$-P(\underline{s}^{(1)}, z) = (a_{11} - 1)G(\underline{s}^{(1)}, z) + a_{12} G(\underline{s}^{(2)}, z) + \dots$$

$$-P(\underline{s}^{(2)}, z) = a_{21} G(\underline{s}^{(1)}, z) + (a_{22} - 1)G(\underline{s}^{(2)}, z) + \dots$$

etc.,

so that if we know the transition probabilities at the defect points, then we can also find the values $G(\underline{s}^{(1)}, z), G(\underline{s}^{(2)}, z), \dots$

As an example, consider the case in which the lattice contains a single defect point $\underline{s}^{(1)}$. Solving the problem for this case is equivalent to solving it where the lattice contains an infinite number of defects which are spaced periodically. Suppose there is probability ϵ that a walker pauses at $\underline{s}^{(1)}$, i.e., $q(\underline{s}^{(1)}, \underline{s}^{(1)}) = \epsilon$. Suppose that on each step the walker normally goes to one of the nearest neighbors (with equal probability) and suppose that $\underline{s}^{(1)}$ has Z nearest neighbors. Then

$$\begin{aligned}
q(\underline{s}, \underline{s}^{(1)}) &= -\epsilon/Z \quad \text{if } \underline{s} \text{ is a nearest neighbor to } \underline{s}^{(1)} \\
&= 0 \quad \text{otherwise.}
\end{aligned}$$

Then,

$$G(\underline{s}, z) = P(\underline{s}, z) + zP(\underline{s}-\underline{s}^{(1)}, z) + \epsilon G(\underline{s}^{(1)}, z) - \frac{z\epsilon}{Z} \sum_{\{\underline{s}_j\}} P(\underline{s}-\underline{s}_j) G(\underline{s}^{(1)}, z)$$

where the sum in the last term is over all nearest neighbors of $\underline{s}^{(1)}$. We finally get

$$G(\underline{s}, z) = P(\underline{s}, z) + \epsilon \left\{ (z-1)P(\underline{s}-\underline{s}^{(1)}, z) + \delta_{\underline{s}, \underline{s}^{(1)}} \right\} G(\underline{s}^{(1)}, z)$$

$$G(\underline{s}^{(1)}, z) = P(\underline{s}^{(1)}, z) + \epsilon \{ (z-1)P(\underline{0}, z) + 1 \} G(\underline{s}^{(1)}, z)$$

and hence

$$\begin{aligned}
G(\underline{s}^{(1)}, z) &= \frac{P(\underline{s}^{(1)}, z)}{(1-\epsilon) + \epsilon(1-z)P(\underline{0}, z)} \\
G(\underline{s}, z) &= P(\underline{s}, z) - \frac{\epsilon(1-z)P(\underline{s}-\underline{s}^{(1)}, z)P(\underline{s}^{(1)}, z)}{(1-\epsilon) + \epsilon(1-z)P(\underline{0}, z)}.
\end{aligned} \tag{37}$$

Furthermore, as $\epsilon \rightarrow 1$,

$$\begin{aligned}
G(\underline{s}^{(1)}, z) &\rightarrow \frac{P(\underline{s}^{(1)}, z)}{(1-z)P(\underline{0}, z)} \\
G(\underline{s}, z) &\rightarrow P(\underline{s}, z) - \frac{P(\underline{s}-\underline{s}^{(1)}, z)P(\underline{s}^{(1)}, z)}{P(\underline{0}, z)}.
\end{aligned} \tag{38}$$

The case $\epsilon = 1$ corresponds to the situation in which the point $\underline{s}^{(1)}$ is a trap.

We proceed to apply the above results to the case in which a 1-dimensional lattice contains one trap at $\underline{s}^{(1)}$, and we wish to calculate the

Polya probability that the walker will eventually return to the origin. Before calculating this quantity, observe that we should expect this probability to increase as the distance, $|s^{(1)}|$, of $s^{(1)}$ from the origin increases.

From (19), the probability of eventual return to the origin is

$$F(0,1) = 1 - \frac{1}{P(0,1)} .$$

Now from (38) we have

$$\begin{aligned} G(0,z) &= P(0,z) - \frac{P(-s^{(1)},z)P(s^{(1)},z)}{P(0,z)} \\ &= P(0,z) \left[1 - \left(\frac{P(s^{(1)},z)}{P(0,z)} \right)^2 \right] . \end{aligned}$$

But by using (13) it can be shown that

$$P(s,z) = \frac{x|s|}{\sqrt{1-z^2}}$$

where

$$x = [1 - \sqrt{1-z^2}]/z .$$

It follows that

$$G(0,z) = \frac{1-x|2s^{(1)}|}{\sqrt{1-z^2}} .$$

Now as $z \rightarrow 1$, then

$$x|2s^{(1)}| \sim 1 - 2|s^{(1)}|\sqrt{1-z^2}$$

so that

$$G(0,1) = |2s^{(1)}|$$

and hence the probability of eventual return to the origin in the 1D case is

$$F(0,1) = 1 - \frac{1}{|2s^{(1)}|}.$$

Similarly, if we have two traps $s^{(2)} < 0 < s^{(1)}$ on a 1D lattice then the probability of return to the origin is

$$F(0,1) = 1 - \frac{1}{2} \left| \frac{1}{s^{(1)}} - \frac{1}{s^{(2)}} \right|.$$

Suppose for a 1D lattice we have a large number of traps and let the concentration be c , i.e., c is the number of traps divided by the total number of lattice points N . Then it can be shown that the probability of returning to the origin without being trapped is

$$1 - \frac{c}{1-c} \log \frac{1}{c}.$$

For 2D and 3D this last problem has not been solved.

7. LATTICE STATISTICS OF DNA MOLECULES

The problem we now consider is one which arises in the chemical analysis of DNA molecules. Some of the aspects of this problem are similar to those of the Ising problem. A full discussion of this problem can be found in [5].

The double-helix structure of a DNA molecule can be thought of simply as two intertwining strands with hydrogen bonds joining the opposing strands.

In fact, there are two such types of bonds joining the two strands, the so-called A-T and G-C bonds. Under chemical analysis, such as increases in temperature and immersion in solvent, these bonds tend to break. It is the breaking of these bonds which we wish to study. Empirical results show that when most of the bonds of the DNA molecules are of the A-T type, then the strands come apart at about 60° C; whereas, if most of the bonds are of the G-C type, then the strands separate at about 100° C. By the critical temperature, T_c , we shall mean the point at which $\frac{1}{2}$ of the bonds in the DNA molecule are broken.

For convenience, the DNA molecule can be drawn as a ladder whose rungs represent the hydrogen bonds joining the opposite strands. To make the analysis easier, we can even think of this chain of bonds as forming a circle.

For the j -th bond of the ladder define

$$\begin{aligned}\sigma_j &= +1 && \text{if } j\text{-th bond is intact} \\ &= -1 && \text{if } j\text{-th bond is broken.}\end{aligned}$$

Thus the state of bonding can be characterized by the sequence

$(\sigma_1, \sigma_2, \dots, \sigma_N)$ where N is the total number of bonds. We wish to consider probability distributions over these sequences, i.e., distributions of the form

$$P(\sigma_1, \sigma_2, \dots, \sigma_N) = \text{prob. } i\text{-th bond is in state } \sigma_i, \quad i = 1, \dots, N.$$

It is obvious that the number of bonds intact is

$$\sum_{j=1}^N \frac{1}{2}(1 + \sigma_j) = N(\sigma_1, \dots, \sigma_N)$$

and the number of bonds broken is

$$\sum_{j=1}^N \frac{1}{2}(1-\sigma_j) = \Psi(\sigma_1, \dots, \sigma_N).$$

It follows that the average number intact is

$$\langle \sum_{j=1}^N \frac{1}{2}(1+\sigma_j) \rangle_{Av} = \sum_{\sigma=\pm 1} \sum_{j=1}^N \left(\frac{1+\sigma}{2}\right) P(\sigma_1, \dots, \sigma_j).$$

Also note that if we assume that the bonds break independently then the distribution function factors:

$$P(\sigma_1, \dots, \sigma_N) = P(\sigma_1) \dots P(\sigma_N).$$

Now if we define the probability of a bond being intact as being proportional to $\exp(-J)$ and that of its being broken to $\exp J$, we can write

$$P(\sigma_j) = \frac{\exp(-J\sigma_j)}{2 \cosh J} = \text{prob. } j\text{-th bond is in state } \sigma_j.$$

Hence

$$\begin{aligned} \langle \sum_{j=1}^N \frac{1}{2}(1+\sigma_j) \rangle_{Av} &= N \sum_{\sigma=\pm 1} \left(\frac{1+\sigma}{2}\right) \frac{e^{-J\sigma}}{2 \cosh J} \\ &= \frac{Ne^{-J}}{2 \cosh J} \\ &= \frac{N}{2} [1 - \tanh J]. \end{aligned}$$

Now if we let J_1 be the parameter associated with the A-T bonds, and J_2 with the G-C bonds, then the number of bonds intact in a system with N_1 A-T bonds and N_2 G-C bonds is

$$\frac{1}{2}N\left(1 - \frac{N_1}{N} \tanh J_1 - \frac{N_2}{N} \tanh J_2\right);$$

or the fraction of bonds intact is

$$\frac{1}{2}(1 - c_1 \tanh J_1 - c_2 \tanh J_2)$$

where c_1 is the fraction of A-T bonds and c_2 is the fraction of G-C bonds.

Now consider the case where we have nearest neighbor correlations, i.e., we have a Markov situation in which

$$P(\sigma_1, \sigma_2, \sigma_3, \dots) = P(\sigma_1, \sigma_2)P(\sigma_2, \sigma_3) \dots$$

In this case, since $\sigma_j^2 = 1$, the most general form we can construct is

$$P(\sigma, \sigma') = \frac{1}{K} \exp\left\{-\frac{J}{2}(\sigma + \sigma') + U\sigma\sigma'\right\} \equiv \frac{1}{K} f(\sigma, \sigma')$$

where K is the normalizing constant

$$K = \sum_{\sigma_1=\pm 1} \dots \sum_{\sigma_N=\pm 1} \prod_{j=1}^N \exp\left\{-\frac{J}{2}(\sigma_j + \sigma_{j+1}) + U\sigma_j\sigma_{j+1}\right\}.$$

Hence

$$\begin{aligned} -\frac{\partial \log K}{\partial J} &= \frac{1}{K} \sum_{\sigma_1=\pm 1} \dots \sum_{\sigma_N=\pm 1} (\sigma_1 + \sigma_2 + \dots + \sigma_N) \prod_{j=1}^N \exp\{\dots\} \\ &= N \langle \sigma \rangle \end{aligned}$$

so that

$$\left\langle \sum_{j=1}^N \frac{1}{2}(1 + \sigma_j) \right\rangle_{Av} = \frac{1}{2}\left(N - \frac{\partial \log K}{\partial J}\right).$$

If we let F be the matrix

$$F = \begin{vmatrix} f(1,1) & f(1,-1) \\ f(-1,1) & f(-1,-1) \end{vmatrix} = \begin{vmatrix} e^{-J+U} & e^{-U} \\ e^{-U} & e^{J+U} \end{vmatrix}$$

then

$$\begin{aligned} K &= \text{trace } F^N \\ &= \lambda_1^N + \lambda_2^N \end{aligned}$$

where λ_1, λ_2 are the eigenvalues of the matrix F . Thus, as $N \rightarrow \infty$,

$$K \sim \lambda_{\max}^N$$

where

$$\lambda_{\max} = \max \{ \lambda_1, \lambda_2 \} .$$

Therefore

$$\langle \sum_j \frac{1}{2} (1 + \sigma_j) \rangle_{\text{Av}} = \frac{N}{2} \left(1 - \frac{\partial \log \lambda_{\max}}{\partial J} \right) .$$

Further, we get the fraction of bonds intact to be

$$f(J) = \frac{1}{2} \left[1 - \frac{\text{sign } J}{1 - (1 + e^{-4U} \text{csch } 2J)^{\frac{1}{2}}} \right] .$$

As the measure of correlation U vanishes, then $f(J)$ reduces to the random model result discussed before. On the other hand, as $U \rightarrow \infty$, we obtain what is called the strong zipper limit. In this case, with the very strong correlation the breaking of a bond forces the same to occur with the next bond so that the process proceeds like the opening of a zipper.

The following references are the principal papers which have been used for the material discussed above. For a more complete list of source material on lattice statistics, one should consult the bibliographical sections of these references, especially that of *Applied Combinatorial Mathematics*, edited by Beckenbach.

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