

Random Walks on Periodic and Random Lattices. II. Random Walk Properties via Generating Function Techniques

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We investigate the random walk properties of a class of two-dimensional lattices with two different types of columns and discuss the dependence of the properties on the densities and detailed arrangements of the columns. We show that the row and column components of the mean square displacement are asymptotically independent of the details of the arrangement of columns. We reach the same conclusion for some other random walk properties (return to the origin and number of distinct sites visited) for various periodic arrangements of a given relative density of the two types of columns. We also derive exact asymptotic results for the occupation probabilities of the two types of distinct sites on our lattices which validate the basic conjecture on bond and step ratios made in the preceding paper in this series.

KEY WORDS: Random walks; periodic lattices; random lattices; generating function techniques.

1. INTRODUCTION

This is the third in a series of papers on random walks in a class of lattices that might serve as models for the study of transport properties in a variety of anisotropic and disordered systems. We consider two-dimensional lattices in which the transition probabilities may be different for sites lying in different columns. A special case of our model, already analyzed in detail in Refs. 1 and 2 (hereafter referred to as A and B) is one in which the walker can always step to nearest neighbor sites in any row but can step to nearest neighbor sites in a column only for certain specified columns. In this paper we

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allow the walker to step vertically as well as horizontally on any column, but we distinguish between two types of columns. The details of this distinction are described in Section 2.

There are three important questions that arise when one considers these two-dimensional lattices:

1. For a given spatial arrangement of the two types of columns, what is the dependence of random walk properties on the relative density of the columns and the detailed characteristics of each type of column?
2. For a given relative density of the two types of columns, how do random walk properties depend on the detailed arrangement of the columns?
3. Is it possible to define an anisotropic, translationally invariant lattice for which certain random walk properties of physical interest are identical to those of the lattices we consider?

The specific random walk properties that we consider in answering these questions are the mean square displacement, the probability of return to the origin, and the distinct number of sites visited, in n steps. The first of these is treated in Section 3. For this property we are able to answer the questions posed above completely because we are able to calculate the mean square displacement for *any* arrangement of columns. For the probability of return to the origin and the distinct number of sites visited we provide a partial answer to the questions posed. This is done in Section 4. We conclude in Section 5 with a result for the asymptotic behavior of the random walk that provides a simple interpretation for some of the results obtained here and for some conjectures made in B.

2. THE MODEL

Consider a random walker on a two-dimensional lattice of q rows and m columns with $N = mq$ sites. In this lattice we distinguish between lattice points that lie on “strong” columns (indicated by a double vertical line in Fig. 1) and those that lie on “weak” columns (indicated by a single vertical line on Fig. 1). From a lattice point lying on a weak column, the walker can step with probability p_1 to either nearest neighbor in the horizontal direction and with probability p_2 to each vertical nearest neighbor, with $2p_1 + 2p_2 = 1$. From a lattice point lying on a strong column, the nearest neighbor transition probabilities are $p_1 - \epsilon$ and $p_2 + \epsilon$ in the horizontal and vertical directions, respectively. These transition probabilities are shown in Fig. 1. An isotropic, translationally invariant, two-dimensional lattice is recovered if we set $\epsilon = 0$ and $p_1 = p_2 = \frac{1}{4}$. The “sparse” lattices considered in A and B correspond to the choice $p_2 = 0$ and thus $p_1 = \frac{1}{2}$. We shall indicate the density of strong

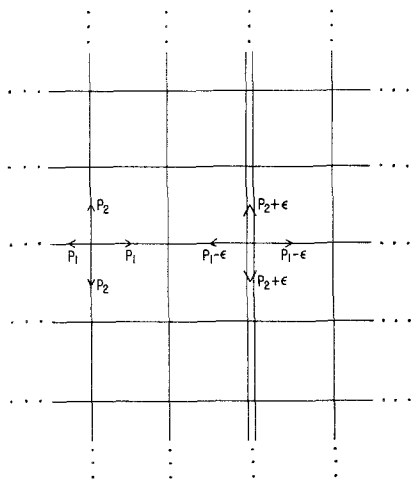


Fig. 1. Section of a two-dimensional lattice with weak (single line) and strong (double line) columns. The transition probabilities at a typical lattice point on each type of column are indicated.

columns by α ; e.g., if there is one strong column for every $k - 1$ weak columns, then $\alpha \equiv 1/k$.

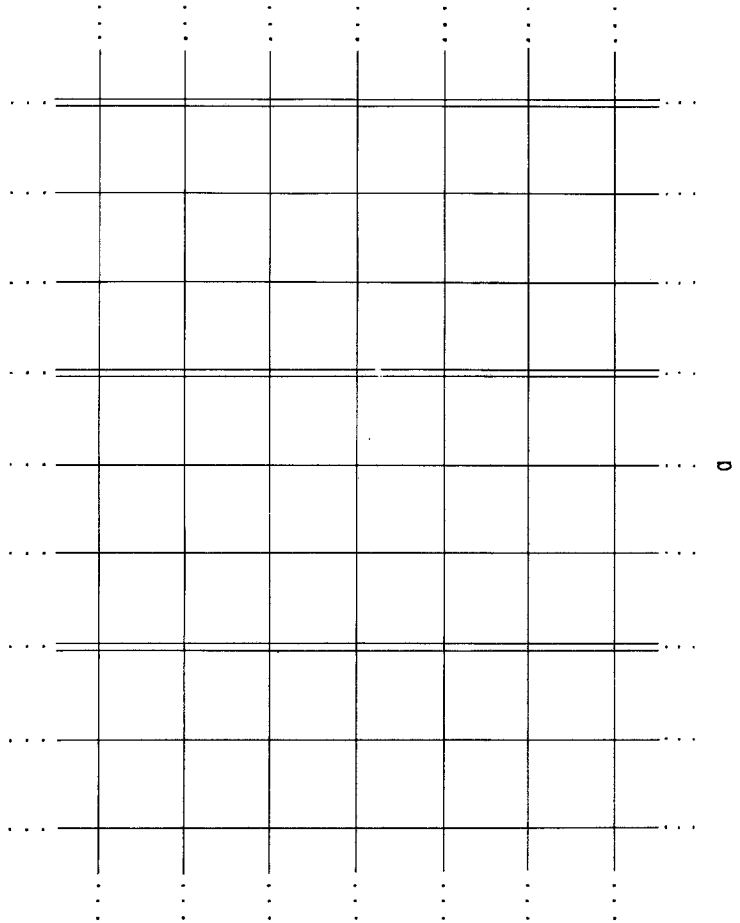
In this paper we will consider three types of arrangements of strong and weak columns. In the simplest arrangement, which we call “singly periodic,” every k th column is strong and the other columns are weak. This arrangement is illustrated in Fig. 2a. In the “clumped periodic” arrangement there are r adjacent strong columns followed by $(k - 1)r$ weak columns, so that the density of strong columns is still α . This arrangement is shown in Fig. 2b. The third arrangement consists of a random distribution of strong columns among the weak columns in such a way that the density of the former is still α .

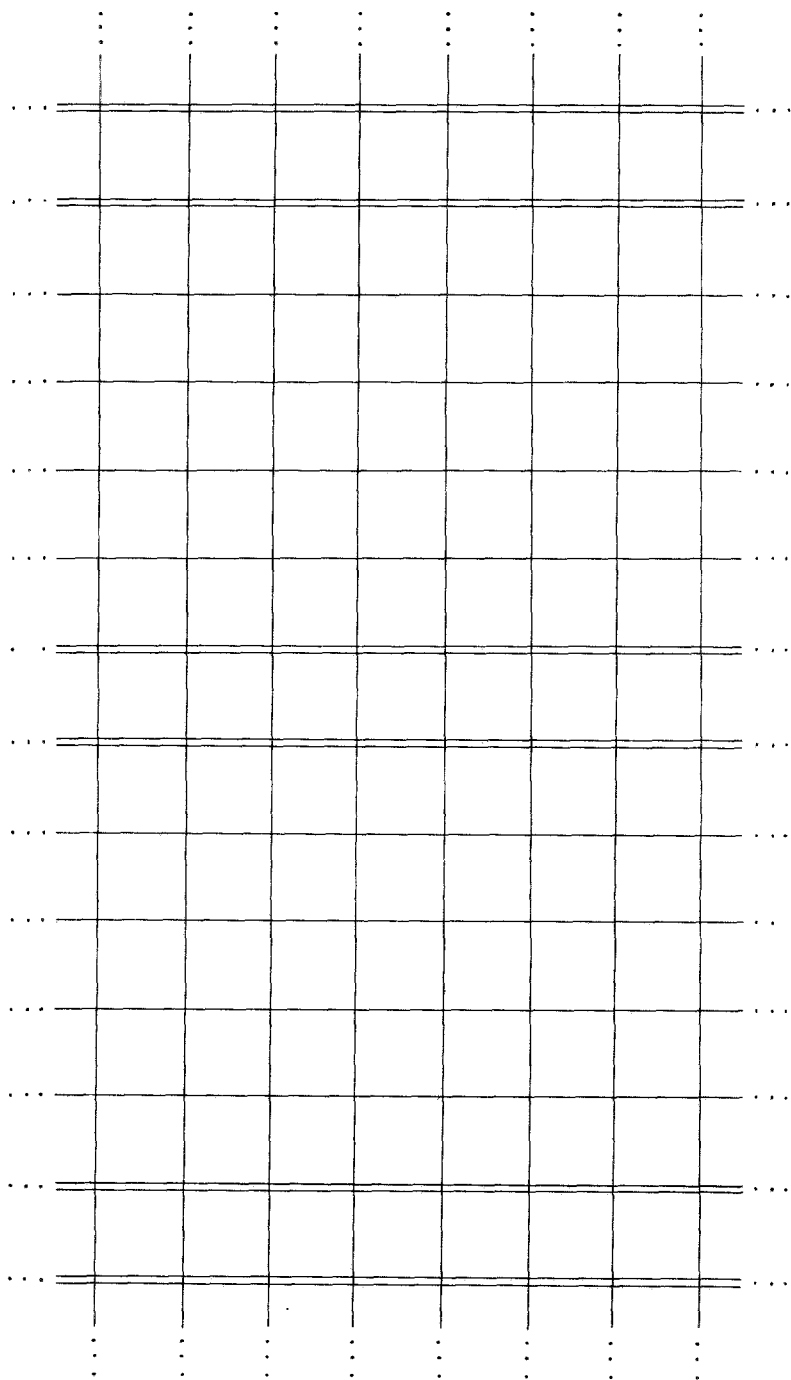
3. MEAN SQUARE DISPLACEMENT

One of the important measures of the anisotropy of transport properties in our periodic and random lattices is the difference in the mean square displacements along the rows (x direction) and the columns (y direction). We denote the mean square displacement in the x direction after n steps by $\langle x_n^2 \rangle$ and in the y direction by $\langle y_n^2 \rangle$. In this section we derive explicit asymptotic (large- n) expressions for $\langle x_n^2 \rangle$ and for the total mean square displacement $\langle x_n^2 \rangle + \langle y_n^2 \rangle$ from which $\langle y_n^2 \rangle$ can then be readily obtained.

Regardless of the arrangement and density α of the strong columns and the relative strengths of the columns, the total mean square displacement for symmetric nearest neighbor walks is given by

$$\langle l_n^2 \rangle \equiv \langle x_n^2 \rangle + \langle y_n^2 \rangle = n \tag{3.1}$$





b

Fig. 2. Periodic arrangements of strong and weak columns. (a) Singly periodic lattice with $k = 3$. (b) Clumped periodic lattice with $k = 3$ and $r = 2$.

To show this, we begin with the equation satisfied by the probability $P_n(l|l_0)$ that the walker is at site l after n steps, having started at site l_0 ,

$$P_n(l|l_0) = \sum_{l'} a(l, l') P_{n-1}(l'|l_0) \quad (3.2)$$

Here $a(l, l')$ is the transition probability from site l' to site l in one step. For the walks considered here, $a(l, l')$ is nonzero only for $|l - l'| = 1$. The mean square displacement is

$$\langle l_n^2 \rangle = \sum_l (l - l_0)^2 P_n(l|l_0) \quad (3.3)$$

To obtain an equation for it we multiply (3.2) by $(l - l_0)^2$ and sum over l . This gives

$$\langle l_n^2 \rangle = \sum_l \sum_{l'} (l - l_0)^2 a(l, l') P_{n-1}(l'|l_0) \quad (3.4)$$

On the right side of (3.4) we write $(l - l_0)^2$ as $(l - l')^2 + (l' - l_0)^2 + 2(l - l') \cdot (l' - l_0)$. The first term yields

$$\sum_l \sum_{l'} (l - l')^2 a(l, l') P_{n-1}(l'|l_0) = \sum_{l'} P_{n-1}(l'|l_0) = 1 \quad (3.5)$$

The third term gives

$$2 \sum_l \sum_{l'} (l - l') \cdot (l' - l_0) a(l, l') P_{n-1}(l'|l_0) = 0 \quad (3.6)$$

where we have used the fact that for a symmetric walk $\sum_l (l - l') a(l, l') = 0$. The second term gives

$$\sum_l \sum_{l'} (l' - l_0)^2 a(l, l') P_{n-1}(l'|l_0) = \sum_{l'} (l' - l_0)^2 P_{n-1}(l'|l_0) = \langle l_{n-1}^2 \rangle \quad (3.7)$$

Collecting (3.5)–(3.7) in (3.4) leads to

$$\langle l_n^2 \rangle = 1 + \langle l_{n-1}^2 \rangle \quad (3.8)$$

and since $\langle l_1^2 \rangle = 1$, we immediately obtain (3.1) as the solution of the above difference equation.

It is of great interest to determine whether the *components* $\langle x_n^2 \rangle$ and $\langle y_n^2 \rangle$ of the mean square displacement depend on the detailed arrangement of strong and weak columns or whether it is only their density that matters. In B it was conjectured that the density of strong columns completely determines the asymptotic behavior of $\langle x_n^2 \rangle$ and $\langle y_n^2 \rangle$. We here prove this conjecture to be correct.

In A it was shown that an equivalence between the asymptotic behavior of the components of the mean square displacement of a sparsely periodic lattice and an anisotropic, translationally invariant lattice can be established.

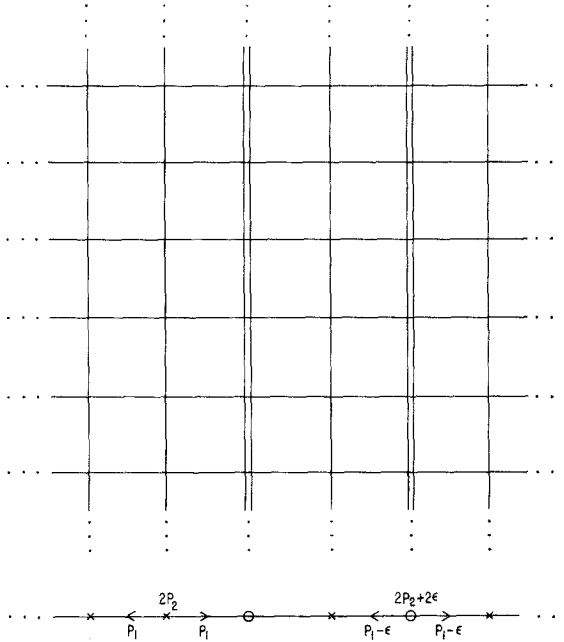


Fig. 3. A section of a two-dimensional lattice with weak and strong columns and its projection onto a one-dimensional lattice. A \times denotes a weak partial trap with stepping probabilities p_1 and pausing probability $2p_2$. A circle denotes a strong partial trap with stepping probabilities $p_1 - \epsilon$ and pausing probability $2p_2 + 2\epsilon$. The pausing probabilities for the projected random walk correspond to the column stepping probabilities for the random walk on the two-dimensional lattice.

We here generalize this result in two ways. We consider a more general class of lattices than those considered in A and we make this identification for lattices with random as well as periodic distributions of strong columns.

As discussed in A for the sparsely periodic lattice, the projection of the two-dimensional walk on the x axis is a symmetric, one-dimensional random walk with "partial traps." By "partial traps" we mean sites at which the walker can pause with a finite probability at every step. In the lattices we consider here, the pausing probabilities at the partial traps (which we shall call their strengths) and their location depend on the distribution of weak and strong columns in the original two-dimensional lattice. This is illustrated in Fig. 3.

3.1. Singly Periodic Distribution of Strong Columns

Consider the two-dimensional lattice in which every k th vertical column is strong and the other columns are weak (see Fig. 2a). The corresponding

one-dimensional system has a strong partial trap every k sites and weak partial traps at all other sites. Since the distribution of strong partial traps is periodic, the overall system is periodic and one can find the mean square displacement $\langle x_n^2 \rangle$ using standard Fourier transform and defect techniques.^(1,3,4) The calculation is carried out in Appendix A and the asymptotic (large- n) results are

$$\langle x_n^2 \rangle \sim \frac{2p_1}{1 + \alpha\epsilon/(p_1 - \epsilon)} n \quad (3.9a)$$

$$\langle y_n^2 \rangle \sim \frac{2p_2 + \alpha\epsilon/(p_1 - \epsilon)}{1 + \alpha\epsilon/(p_1 - \epsilon)} n \quad (3.9b)$$

independent of initial condition, where $\langle y_n^2 \rangle$ is obtained from (3.9a) and (3.1). Note that these results reduce to those of B when $p_1 = \frac{1}{2}$ and $p_2 = 0$ and to those of A when one further sets $\epsilon = \frac{1}{4}$.

It is instructive to compare (3.9) to the corresponding mean square displacement results for a translationally invariant, anisotropic, two-dimensional lattice, i.e., a lattice in which all sites are identical but the probabilities of stepping in the $\pm x$ direction (p_1') and in the $\pm y$ direction (p_2') are different ($p_1' \neq p_2'$). For such a lattice one readily obtains asymptotically

$$\langle x_n^2 \rangle \sim [p_1'/(p_1' + p_2')]n \quad (3.10a)$$

$$\langle y_n^2 \rangle \sim [p_2'/(p_1' + p_2')]n \quad (3.10b)$$

The results (3.10) for the translationally invariant lattice and (3.9) for our periodically disordered lattice are identical if we make the identifications

$$p_1' = \frac{p_1}{1 + \alpha\epsilon/(p_1 - \epsilon)} \quad (3.11a)$$

$$p_2' = \frac{p_2 + \alpha\epsilon/2(p_1 - \epsilon)}{1 + \alpha\epsilon/(p_1 - \epsilon)} \quad (3.11b)$$

We will show later that with this same identification, other random walk properties are also identical for the periodically disordered and the translationally invariant anisotropic lattices.

3.2. Random Distribution of Strong Columns

We now treat a two-dimensional lattice in which the strong columns are distributed at random with a density α , i.e., on the average one out of every k columns is strong. The corresponding (projected) one-dimensional system has a density α of strong partial traps which are randomly distributed, and a density $1 - \alpha$ of weak partial traps. Since this system is not periodic, standard Fourier transform methods cannot be applied in any simple way to find the

mean square displacement of a walker on this system. We thus proceed in a somewhat different manner. The probability that the walker is at site l after n steps, having started the walk at site l_0 , satisfies the equation

$$P_n(l|l_0) = \sum_{l'} p(l, l')P_{n-1}(l'|l_0) + \sum_{l'} q(l, l')P_{n-1}(l'|l_0) \tag{3.12}$$

where

$$p(l, l') = p_1 \delta_{l \pm 1, l'} + 2p_2 \delta_{l, l'} \tag{3.13a}$$

$$q(l, l') = \epsilon \sum_{l_j} \{2\delta_{l', l_j} \delta_{l, l'} - \delta_{l', l_j} \delta_{l+1, l'} - \delta_{l', l_j} \delta_{l-1, l'}\} \tag{3.13b}$$

Here $p(l, l')$ is the transition probability from site l' to site l in a regular one-dimensional lattice in which the probability of stepping to a nearest neighbor is p_1 and the probability of remaining at a site is $2p_2$. The defect matrix $q(l, l')$ represents the modification in the transition probabilities due to the strong partial traps. At these sites, denoted by $\{l_j\}$, the transition probability to nearest neighboring sites is $[p(l_j \pm 1, l_j) + q(l_j \pm 1, l_j)] = p_1 - \epsilon$ and the probability $[p(l_j, l_j) + q(l_j, l_j)]$ of remaining at site l_j is $2p_2 + 2\epsilon$.

We define the generating function⁽³⁾ for our random one-dimensional lattice as

$$G_{ll'}(z) \equiv \sum_{n=0}^{\infty} z^n P_n(l|l') \tag{3.14}$$

The equation satisfied by this generating function is found from (3.12) by multiplying by z^n and summing over n :

$$G_{ll_0}(z) = \sum_{l'} [p(l, l') + q(l, l')]G_{l'l_0}(z) + \delta_{l, l_0} \tag{3.15}$$

The generating function $G_{ll_0}(z)$ can be expressed in terms of the generating function $U_{ll_0}(z)$ of the regular ($\epsilon = 0$) lattice as

$$G_{ll_0}(z) = U_{ll_0}(z) + z \sum_{l'} U_{ll'}(z)F_{l'l_0}(z) \tag{3.16}$$

where

$$U_{ll'}(z) = \left\{ \frac{(1 - 2zp_2) - [(1 - 2zp_2)^2 - (2zp_1)^2]^{1/2}}{2zp_1} \right\}^{|l-l'|} \times [(1 - 2zp_2)^2 - (2zp_1)^2]^{-1/2} \tag{3.17}$$

and

$$F_{l'l_0}(z) = \sum_{l''} q(l', l'')G_{l''l_0}(z) \tag{3.18}$$

We introduce the Fourier transform $f_{l_0}(\phi, z)$ of an arbitrary function $f_{l_0}(z)$ by the definition

$$f_{l_0}(\phi, z) \equiv \sum_{l=-\infty}^{\infty} f_{l_0}(z) e^{i(l-l_0)\phi} \tag{3.19}$$

The Fourier transform of Eq. (3.16) then is

$$\hat{G}_{l_0}(\phi, z) = \hat{U}_{l_0}(\phi, z) + z \sum_l e^{i(l-l_0)\phi} \sum_{l'} U_{ll'}(z) F_{l'l_0}(z) \tag{3.20}$$

The generating function for the mean square displacement as defined in Eq. (A8) of Appendix A is then given by

$$X(z) = -\frac{\partial^2}{\partial \phi^2} \hat{G}_{l_0}(\phi, z)|_{\phi=0} \tag{3.21}$$

and the mean square displacement $\langle x_n^2 \rangle \equiv \langle l_n^2 \rangle$ is the coefficient of z^n in the expansion of $X(z)$ in powers of z .

In Appendix A we point out that for large n the main contribution to $\langle x_n^2 \rangle$ comes from the coefficient of $1/(1-z)^2$ in an expansion of $X(z)$ in powers of $(1-z)$. To obtain the asymptotic mean square displacement it is thus sufficient to evaluate (3.21) explicitly to order $(1-z)^{-2}$. From (3.17) it can directly be seen that the contribution of the regular lattice portion of (3.20) to (3.21) is

$$-\frac{\partial^2}{\partial \phi^2} \hat{U}_{l_0}(\phi, z)|_{\phi=0} = \frac{2p_1}{(1-z)^2} + O(1-z)^{-1} \tag{3.22}$$

The contribution due to the strong partial traps can be expressed as

$$-\frac{\partial^2}{\partial \phi^2} z \sum_l e^{i(l-l_0)\phi} \sum_{l'} U_{ll'}(z) F_{l'l_0}(z)|_{\phi=0} = -\frac{2\epsilon z}{1-z} \sum_{l_j} G_{l_j l_0}(z) \tag{3.23}$$

The sum $\sum_{l_j} G_{l_j l_0}(z)$ is considered in detail in Appendix B. We there obtain the result

$$\sum_{l_j} G_{l_j l_0} = \frac{p_1}{(1-z)[k(p_1 - \epsilon) + \epsilon]} + O(1) \tag{3.24}$$

Combining the results of (3.20)–(3.24) finally yields

$$X(z) = \frac{1}{(1-z)^2} \frac{2p_1}{1 + \alpha\epsilon(p_1 - \epsilon)^{-1}} + O(1-z)^{-1} \tag{3.25}$$

Using Darboux’s theorem,⁽⁶⁾ we then obtain

$$\langle x_n^2 \rangle \sim \frac{2p_1}{1 + \alpha\epsilon/(p_1 - \epsilon)} n \tag{3.26}$$

Equation (3.26) is identical to Eq. (3.9a). We have thus established the important result that the asymptotic mean square displacements in the x and y directions are *independent* of the arrangement of strong and weak connections and depend *only* on their density.

4. PROBABILITY OF RETURN TO THE ORIGIN AND NUMBER OF DISTINCT SITES VISITED

Two properties that are of interest in random walk models are the probability $P_n(l_0|l_0)$ of return to the origin l_0 in n steps and the number S_n of distinct sites visited in n steps. The former is closely related to a quantity that is of considerable experimental interest in the study of disordered materials, namely, the probability for an excitation or electron originally located at site l_0 to be at the site at a later time t .⁽⁶⁾ The second property, S_n , is of experimental interest in problems involving traps, since in some cases time-dependent trapping probabilities can be related to S_n .⁽⁷⁾

It is clearly of interest to determine the dependence of these properties on the arrangements of weak and strong columns. For this purpose it would be desirable to obtain $P_n(l_0|l_0)$ and S_n for arbitrary arrangements. Unfortunately, we have been unable to carry out analytic calculations for random arrangements of strong columns. We have, however, been able to obtain results for a variety of periodic arrangements of columns. These results are generalizations of those obtained in A. We find that for a particular class of *periodic arrangements* the properties $P_n(l_0|l_0)$ and S_n in fact do *not* depend on the details of the arrangements but depend *only* on the density of strong and weak columns. This is in accord with the conjecture made in B. The further conjecture made there, that this independence of the details of the arrangements also holds for random ones, must remain a conjecture at this time.

We shall also show that one can identify an anisotropic, translationally invariant lattice with each lattice considered here in such a way that the $P_n(l_0|l_0)$ as well as the S_n for both these lattices are asymptotically identical. Furthermore, this identification is the same as that made via the components of the mean square displacement in Section 3.

It should be noted that if one could produce a proof for the conjecture made in B that $P_n(l_0|l_0)$ and S_n only depend on the density α of strong columns even for random arrangements of such columns, then the whole apparatus of the generating function technique for translationally invariant, anisotropic lattices⁽³⁾ could be used to obtain these random walk properties for lattices with random arrangements of strong columns.

It is important to note that the two properties that we deal with here are obtained from the same generating function. We will evaluate the necessary terms of this generating function for two different arrangements of strong columns, namely, for the singly periodic and for the clumped periodic arrangements discussed in Section 2.

The labeling of sites that we choose to use is shown in Fig. 4. The lattice site (i, j) in the i th row and j th column is indexed $(i - 1)m + j$, where $1 \leq i \leq q$ and $1 \leq j \leq m$; q is the number of rows and m is the number of

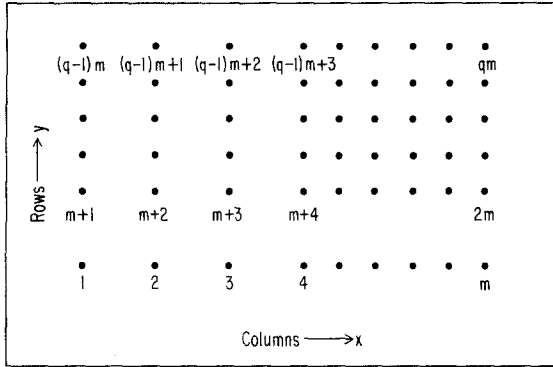


Fig. 4. Labeling of lattice sites.

columns of the lattice. For computational convenience we impose periodic boundary conditions on the rows (i.e., sites in the q th row are nearest neighbors to those in the first row) and reflecting boundary conditions on the columns [i.e., a walker on a site in the first or m th column can jump to a nearest neighboring site in the same column or to the nearest neighbor site in the second or $(m - 1)$ th column]. In the limit $q, m \rightarrow \infty$, which we shall take at the end of the calculation, the boundary conditions chosen are unimportant.

An arrangement of connections is specified by the set of variables $\{x_1, x_2, \dots, x_m\}$, where

$$x_i = x_{i+jm} = \begin{cases} 1 & \text{if } i\text{th column is strongly connected} \\ 0 & \text{if } i\text{th column is weakly connected} \end{cases} \quad (4.1)$$

The singly periodic arrangement corresponds to the choices $x_1 = 1, x_2 = x_3 = \dots = x_k = 0, x_{k+1} = 1, x_{k+2} = \dots = x_{2k} = 0, \dots, x_{m-k} = 1, x_{m-k+1} = \dots = x_{m-1} = 0, x_m = 1$. In the multiply periodic arrangement $x_1 = x_2 = \dots = x_r = 1, x_{r+1} = \dots = x_{kr} = 0, x_{kr+1} = \dots = x_{(k+1)r} = 1, \dots, x_{m-r} = x_{m-r+1} = \dots = x_m = 1$.² In the limit $m \rightarrow \infty$ the density of strong connections in both of these arrangements is α .

As in A, we begin with the equation for the probability $P_n(l_0|l_0)$ that the walker is at site l after n steps, given that she was initially at l_0 ,

$$P_n(l|l_0) = \sum_{l'} p_{ll'} P_{n-1}(l'|l_0) \quad (4.2)$$

² We choose m so that $m - 1$ is a multiple of k in the singly periodic case and so that $m - r$ is a multiple of kr in the clumped periodic case.

where the stepping probabilities $p_{ll'}$ are given by

$$\begin{aligned}
 p_{ll'} &= 0 && \text{if } l \text{ and } l' \text{ are not nearest neighbors} \\
 p_{l,l\pm 1} &= (p_1 - \epsilon x_{l\pm 1}) && \text{provided } l \pm 1 \text{ is not} \\
 &&& \text{in the first or } m\text{th column} \\
 p_{l,l\pm m} &= (p_2 + \epsilon x_l) && \text{provided } l \text{ is not} \\
 &&& \text{in the first or } m\text{th column} \\
 p_{l+1,l} &= (2p_1 - 2\epsilon x_1) && \text{if } l \text{ is in the first column} \\
 p_{l-1,l} &= (2p_1 - 2\epsilon x_m) && \text{if } l \text{ is in the } m\text{th column} \\
 p_{l,l\pm m} &= (p_2 + \epsilon) && \text{if } l \text{ is in the first or } m\text{th column}
 \end{aligned} \tag{4.3}$$

In matrix form we can write (4.2) as

$$\mathbf{P}_n(l_0) = \mathbf{T} \mathbf{P}_{n-1}(l_0) \tag{4.4}$$

where the transition probability matrix \mathbf{T} has elements $p_{ll'}$. Because of the periodic boundary conditions in the vertical direction, \mathbf{T} is a $q \times q$ cyclic matrix whose elements are $m \times m$ matrices \mathbf{U} and \mathbf{V} :

$$\mathbf{T} = \begin{bmatrix} \mathbf{U} & \mathbf{V} & 0 & 0 & \dots & 0 & 0 & \mathbf{V} \\ \mathbf{V} & \mathbf{U} & \mathbf{V} & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \dots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \mathbf{V} & \mathbf{U} & \mathbf{V} \\ \mathbf{V} & 0 & 0 & 0 & \dots & 0 & \mathbf{V} & \mathbf{U} \end{bmatrix} \tag{4.5}$$

The matrix \mathbf{U} represents walks within a given row, while \mathbf{V} corresponds to walks along the columns. The specific form of these matrices depends on the arrangement of strong and weak columns, so that we will consider each case separately later in this section.

The generating function $G_{l_0 l_0}(z; q, m)$ for the walker to return to the origin l_0 is defined by

$$G_{l_0 l_0}(z; q, m) = \sum_{n=0}^{\infty} P_n(l_0 | l_0) z^n \tag{4.6}$$

This generating function is for walks that begin and end at the particular site l_0 . This initial value problem is quite difficult to solve. We shall instead perform an average over initial positions. Such an averaged generating function is not only simpler to evaluate, but indeed corresponds to the physical situation in experiments where the initial position of the walker can be anywhere in the system. In any case one expects the asymptotic behavior

where $\Psi(1)$ is given by Eq. (4.14) evaluated at $z = 1$. We note that when $p_2 = 0$, $p_1 = \frac{1}{2}$, and $\epsilon = \frac{1}{4}$, $\Psi(1)$ reduces to the result in (4.9) of A. We also show there that the asymptotic formula $P_{2n} \sim \Psi(1)/2n$ is remarkably accurate even for small n when k is small, i.e., the asymptotic result is valid once the walker has sampled the structure of the lattice.

The asymptotic probability of return to the origin in $2n$ steps in an anisotropic, translationally invariant lattice with transition probabilities p_1' and p_2' in the x and y directions is⁽³⁾

$$P_{2n} \sim \frac{1}{2n} \frac{1}{4\pi(p_1'p_2')^{1/2}} + O\left(\frac{1}{n^2}\right) \quad (4.16)$$

If we use Eqs. (3.11a) and (3.11b) for the relations between the stepping probabilities p_i' for an anisotropic, translationally invariant lattice and the p_i for our lattice, then Eq. (4.15) becomes identical with (4.16). This is an important result, since we have now been able to make the *same* identification for such different properties as the components of the mean square displacement and the probability of return to the origin. Since we found in Section 3 that the components of the mean square displacement are independent of the arrangement of strong columns, the above result strengthens the conjecture made in B that the leading term in (4.15) is also independent of the arrangement of strong columns and is completely determined by their density.

The average number S_n of distinct sites visited in an n -step walk has the generating function⁽³⁾

$$R(z) = \sum_{n=0}^{\infty} S_n z^n \quad (4.17)$$

which is simply related to $G(z)$ of Eq. (4.13) by

$$R(z) = [(1 - z)^2 G(z)]^{-1} \quad (4.18)$$

For small values of n and k , Eq. (4.18) can be used in conjunction with Eq. (4.13) to find exact values of S_n . The generating function $R(z)$ is regular inside the unit circle and has branch point singularities at $z = \pm 1$. Expansions about these singularities are analogous to that given in Eq. (4.13). Asymptotic expansions for S_n can be obtained from Darboux's theorem; the leading order term in this expansion can alternatively be derived from the Hardy-Littlewood-Karamata Tauberian theorem. Following the prescription set out by Montroll and Weiss,⁽⁴⁾ we find

$$S_n \sim 4\pi(p_1'p_2')^{1/2}n/\ln n \quad (4.19)$$

with p_1' and p_2' given in (3.4). Once again we can thus make the same identification made earlier between the singly periodic and the translationally invariant anisotropic lattices.

4.2. Clumped Periodic Distribution of Strong Columns

In Appendix C we present in detail the calculation of the generating function $G(z)$ for the clumped periodic lattice. The main difference between this calculation and the one for the singly periodic case lies in the more complicated determinant $\det \mathbf{D}_m$ that occurs in the former. In Appendix C we carry out the detailed evaluation of the generating function only for the case $p_1 = \frac{1}{2}$, $p_2 = 0$, and $\epsilon = \frac{1}{4}$. We find that in this case $G(z)$ is given by Eq. (4.13) with (4.14), i.e., we have proved that for this choice of p_1 , p_2 , and ϵ the properties P_{2n} and S_n for the clumped periodic lattice are identical to those of the singly periodic lattice *with the same density of strong columns*. The more general case of arbitrary p_1 , p_2 , and ϵ can be dealt with in an analogous manner.

5. OCCUPATION THEOREM

We conclude this paper by presenting an argument based on the theory of Markov chains that helps to explain the independence of the mean square displacement of the random walker on the details of the arrangement of strong and weak columns. This argument also provides a basis for the conjecture made in B that the other random walk properties that we have considered are also independent of the detailed arrangement for random as well as periodic arrangements for a given density α .

Consider the defining equation (3.2) in the asymptotic ($n \rightarrow \infty$) limit. In this limit $P_n(l|l_0)$ becomes independent of n , so that we write

$$P(l|l_0) = \sum_{l'} a(l, l')P(l'|l_0) \tag{5.1}$$

where $P(l|l_0)$ is the conditional probability of being at site l in the limit $n \rightarrow \infty$. It is a straightforward matter to show that Eq. (5.1) is satisfied for any possible arrangement of columns by making the reasonable assumption that $P(l|l_0)$ can only take on two values, depending on whether site l lies on a strong or weak vertical column. Let $P(l|l_0) = A$ when l lies on a strong column and let $P(l|l_0) = B$ when l lies on a weak column. If site l lies on a strong column, then, depending on the arrangement of columns, one of the four situations depicted in Fig. 5 results. We use the stepping probabilities shown in Fig. 1, i.e., from a lattice point lying on a weak column the walker can step with probability p_1 to either nearest neighbor in the horizontal direction and with probability p_2 to each vertical neighbor, with $2p_1 + 2p_2 = 1$. From a lattice point lying on a strong column, the nearest neighbor transition probabilities are $p_1 - \epsilon$ and $p_2 + \epsilon$ in the horizontal and vertical directions, respectively.

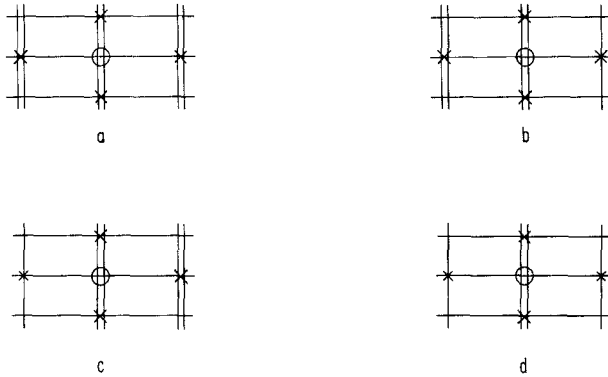


Fig. 5. Possible arrangements of columns around a lattice point l on a strong column. Site l is indicated by a circle and its nearest neighbors are indicated by a \times .

Equation (5.1) then reduces to the identity $A = A$ for Fig. 5a and to the relation

$$A = \frac{p_1}{p_1 - \epsilon} B \quad (5.2)$$

for Figs. 5b–5d. Relation (5.2) is in fact just the detailed balance condition for the random walk on the rows. If lattice site l lies on a weak column, then again four configurations are possible. One of these yields the identity $B = B$ and the other three yield (5.2). Note that $A > B$ if $\epsilon > 0$, i.e., sites on strong columns have a higher asymptotic probability of occupation than those on weak columns. To obtain explicit values for A and B we use the normalization condition

$$NA + N(k - 1)B = 1 \quad (5.3)$$

where Nk is the total number of lattice sites. Equations (5.2) and (5.3) give

$$A = \frac{1}{N} \frac{\alpha p_1}{p_1 - \epsilon + \alpha \epsilon} \quad (5.4)$$

and

$$B = \frac{1}{N} \frac{\alpha(p_1 - \epsilon)}{p_1 - \epsilon + \alpha \epsilon} \quad (5.5)$$

These results correspond precisely to those obtained in Eq. (A25) of Appendix A. Thus we have proved that the asymptotic probability of occupation of a site for a given density of strong columns depends only on whether that site is on a strong or weak column *and not on the nature of the arrangement of the columns*. This is a crucial result that was used in Section 3 [cf. Eqs. (A21)–(A26)] to prove the independence of the mean square displacement from the arrangement of columns.

It should be noted that the results (5.4) and (5.5) for the occupancy probabilities of sites on strong and weak columns are in complete agreement with the results obtained in B for the corresponding probabilities $P(i)$ and $P_1(n)$. If we set $p_1 = \frac{1}{2}$ and $\epsilon = \frac{1}{4}$, then Eqs. (5.4) and (5.5) reduce to Eqs. (36) and (37) of B. *The results presented in this paper on occupation probabilities thus validate the conjecture (4) of B on the relation between the ratio of steps along the rows and columns to the ratio of the number of bonds (in irreducible lattice fragments) along the rows and columns.*

The results of this paper on the mean square displacements and on occupation probabilities could, with sufficient tedious analysis, be extended to the three-dimensional lattices considered in B.

APPENDIX A

The equation that describes a random walker on a periodically disordered lattice is

$$P_n(l, \gamma|\gamma_0) = \sum_{\gamma'=1}^k \sum_{l'=-\infty}^{\infty} p_{\gamma\gamma'}(l-l')P_{n-1}(l', \gamma'|\gamma_0) \tag{A1}$$

Here $P_n(l, \gamma|\gamma_0)$ is the probability that the walker is at the γ th site ($\gamma = 1, 2, \dots, k$) of the l th unit cell ($-\infty < l < \infty$) after n steps, having started at site γ_0 of the zeroth unit cell, and $p_{\gamma\gamma'}(l-l')$ is the probability of stepping from site γ' in unit cell l' to site γ in unit cell l in one step. We wish to evaluate

$$\langle x_n^2 \rangle = \sum_{\gamma=1}^k \sum_{l=-\infty}^{\infty} [lk + (\gamma - \gamma_0)]^2 P_n(l, \gamma|\gamma_0) \tag{A2}$$

In terms of the partial moments $B_{\gamma\gamma_0}^{(j)}(n)$, where

$$B_{\gamma\gamma_0}^{(j)}(n) = \sum_{l=-\infty}^{\infty} l^j P_n(l, \gamma|\gamma_0) \tag{A3}$$

we have

$$\langle x_n^2 \rangle = k^2 \sum_{\gamma=1}^k B_{\gamma\gamma_0}^{(2)}(n) + 2k \sum_{\gamma=1}^k (\gamma - \gamma_0) B_{\gamma\gamma_0}^{(1)}(n) + \sum_{\gamma=1}^k (\gamma - \gamma_0)^2 B_{\gamma\gamma_0}^{(0)}(n) \tag{A4}$$

It is also convenient to define the single-step partial moments $A_{\gamma\gamma'}^{(j)}$:

$$A_{\gamma\gamma'}^{(j)} = \sum_{l=-\infty}^{\infty} l^j p_{\gamma\gamma'}(l) \tag{A5}$$

On multiply Eq. (A1) by l^j [expressing l as $(l-l') + l'$] and summing over l by changing summations over l and l' on the right-hand side to sums over l' and $l-l'$, we find a set of difference equations:

$$\begin{aligned} \mathbf{B}^{(0)}(n) &= \mathbf{A}^{(0)}\mathbf{B}^{(0)}(n-1) \\ \mathbf{B}^{(1)}(n) &= \mathbf{A}^{(1)}\mathbf{B}^{(0)}(n-1) + \mathbf{A}^{(0)}\mathbf{B}^{(1)}(n-1) \\ \mathbf{B}^{(2)}(n) &= \mathbf{A}^{(2)}\mathbf{B}^{(0)}(n-1) + 2\mathbf{A}^{(1)}\mathbf{B}^{(1)}(n-1) + \mathbf{A}^{(0)}\mathbf{B}^{(2)}(n-1) \end{aligned} \tag{A6}$$

where $\mathbf{B}^{(j)}(n) = (B_{\gamma\gamma'}^{(j)}(n))$, $\mathbf{A}^{(j)} = (A_{\gamma\gamma'}^{(j)})$. Because of the sum rule

$$\sum_{\gamma=1}^k \sum_{l=-\infty}^{\infty} p_{\gamma\gamma'}(l) = 1 \tag{A7}$$

$\mathbf{A}^{(0)}$ is a stochastic matrix with column sums = 1. Also, since $P_0(\gamma, l | \gamma_0) = \delta_{l0} \delta_{\gamma\gamma_0}$, we have $\mathbf{B}^{(0)}(0) = \mathbf{I}$, $\mathbf{B}^{(1)}(0) = \mathbf{B}^{(2)}(0) = 0$. To proceed, generating functions are introduced:

$$X(z) = \sum_{n=0}^{\infty} \langle x_n^2 \rangle z^n \tag{A8}$$

and

$$\mathbf{G}^{(j)}(z) = \sum_{n=0}^{\infty} \mathbf{B}^{(j)}(n) z^n \tag{A9}$$

From Eq. (A4) we have

$$X(z) = k^2 \sum_{\gamma=1}^k G_{\gamma\gamma_0}^{(2)}(z) + 2k \sum_{\gamma=1}^k (\gamma - \gamma_0) G_{\gamma\gamma_0}^{(1)}(z) + \sum_{\gamma=1}^k (\gamma - \gamma_0)^2 G_{\gamma\gamma_0}^{(0)}(z) \tag{A10}$$

On multiplying Eq. (A6) by z^n , summing over n from 0 to ∞ , and solving successively for $\mathbf{G}^{(0)}(z)$, $\mathbf{G}^{(1)}(z)$, and $\mathbf{G}^{(2)}(z)$, we find

$$\begin{aligned} \mathbf{G}^{(0)}(z) &= [\mathbf{I} - z\mathbf{A}^{(0)}]^{-1} \\ \mathbf{G}^{(1)}(z) &= z\mathbf{G}^{(0)}(z)\mathbf{A}^{(1)}\mathbf{G}^{(0)}(z) \\ \mathbf{G}^{(2)}(z) &= z\mathbf{G}^{(0)}(z)\mathbf{A}^{(2)}\mathbf{G}^{(0)}(z) + 2z^2\mathbf{G}^{(0)}(z)\mathbf{A}^{(1)}\mathbf{G}^{(0)}(z)\mathbf{A}^{(1)}\mathbf{G}^{(0)}(z) \end{aligned} \tag{A11}$$

Without loss of generality, k can be chosen to be odd and unit cells taken with defect sites at the middle of the cells [$\gamma = (k + 1)/2$].

Up to this point the calculation has proceeded identically as in A, and has been reproduced here for the sake of completeness. The matrices $\mathbf{A}^{(j)}$ that we consider here are generalizations of those in A and are given by

$$\mathbf{A}^{(0)} = \begin{bmatrix} 2p_2 & p_1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 & p_1 \\ p_1 & 2p_2 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 2p_2 & p_1 - \epsilon & 0 & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & p_1 & 2p_2 + 2\epsilon & p_1 & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 & p_1 - \epsilon & 2p_2 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & 2p_2 & p_1 & \cdot \\ p_1 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & p_1 & 2p_2 & \cdot \end{bmatrix} \rightarrow (k + 1)/2 \tag{A12a}$$

↑
(k + 1)/2

$$\mathbf{A}^{(1)} = \begin{bmatrix} & p_1 \\ \bigcirc & \\ & -p_1 \end{bmatrix}; \quad \mathbf{A}^{(2)} = \begin{bmatrix} & p_1 \\ \bigcirc & \\ & p_1 \end{bmatrix} \tag{A12b}$$

Substituting (A12) in (A11) and (A11) in (A10), we obtain

$$X(z) = \frac{k^2 z p_1}{1 - z} (G_{k\gamma_0}^{(0)} + G_{1\gamma_0}^{(0)}) [1 + 2z p_1 (G_{1k}^{(0)} - G_{11}^{(0)})] + 2kz p_1 \sum_{\gamma=1}^k (\gamma - \gamma_0) (G_{\gamma 1}^{(0)} G_{k\gamma_0}^{(0)} - G_{\gamma k}^{(0)} G_{1\gamma_0}^{(0)}) + \sum_{\gamma=1}^k (\gamma - \gamma_0)^2 G_{\gamma\gamma_0}^{(0)} \tag{A13}$$

In deriving this equation we have used the results $G_{1k}^{(0)} = G_{k1}^{(0)}$ and $G_{kk}^{(0)} = G_{11}^{(0)}$. These are special cases of the relationship $G_{\gamma\gamma_0}^{(0)} = G_{k+1-\gamma, k+1-\gamma_0}^{(0)}$, which follows from the symmetry of the walk:

$$P_n(l, \gamma | \gamma_0) = P_n(-l, k + 1 - \gamma | k + 1 - \gamma_0) \tag{A14}$$

$G^{(0)}(z)$ can be interpreted as the generating function for random walks on a k -ring, the transition probability matrix of the walk being $\mathbf{A}^{(0)}$. Now we make the decomposition

$$\mathbf{A}^{(0)} = \mathbf{A}^{(0,p)} + \mathbf{\Delta} \tag{A15}$$

where

$$\mathbf{A}^{(0,p)} = \begin{bmatrix} 2p_2 & p_1 & 0 & \cdot & \cdot & p_1 \\ p_1 & 2p_2 & p_1 & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdot & 2p_2 & p_1 \\ p_1 & 0 & 0 & \cdot & p_1 & 2p_2 \end{bmatrix} \tag{A16a}$$

$$\mathbf{\Delta} = \begin{bmatrix} & -\epsilon & \\ \bigcirc & 2\epsilon & \bigcirc \\ & -\epsilon & \\ & \uparrow & \\ & (k+1)/2 & \end{bmatrix} \leftarrow (k+1)/2 \tag{A16b}$$

$\mathbf{A}^{(0,p)}$ is the transition probability matrix for walks on the perfect k -ring; $\mathbf{\Delta}$ is a defect matrix with only three nonzero elements. It is a simple exercise to derive an expression for $\mathbf{G}^{(0)}(z)$ in terms of the Green's function $\mathbf{U}^R(z)$, where⁽⁴⁾

$$\mathbf{U}^R(z) = [\mathbf{I} - z\mathbf{A}^{(0,p)}]^{-1} \tag{A17}$$

$\mathbf{U}^R(z)$ is the generating function for walks on a perfect k -ring with matrix elements given by

$$U_{\gamma\gamma'}^R(z) = \frac{1}{[(1 - 2zp_2)^2 - (2zp_1)^2]^{1/2}} \left[\frac{x^{|\gamma-\gamma'|} + x^{k-|\gamma-\gamma'|}}{1 - x^k} \right] \tag{A18}$$

where

$$x = \frac{1 - 2zp_2 - [(1 - 2zp_2)^2 - (2zp_1)^2]^{1/2}}{2zp_1} \quad (\text{A19})$$

The generating function $\mathbf{G}^{(0)}(z)$ for the defective lattice can be determined from the perfect lattice generating function $\mathbf{U}^R(z)$ using the defect technique.⁽⁴⁾ The result is

$$G_{\gamma\gamma'}^{(0)} = U_{\gamma\gamma'}^R + \epsilon z G_{(k+1)/2, \gamma'}^{(0)} [2U_{\gamma, (k+1)/2}^R - U_{\gamma, (k+3)/2}^R - U_{\gamma, (k-1)/2}^R] \quad (\text{A20a})$$

where

$$G_{(k+1)/2, \gamma'}^{(0)} = \frac{U_{(k+1)/2, \gamma'}^R}{1 - 2z\epsilon(U_{\gamma'\gamma'}^R - U_{\gamma', \gamma'+1}^R)} \quad (\text{A20b})$$

Since $\mathbf{A}^{(0)}$ is stochastic, it has a nondegenerate maximum eigenvalue of unity and it follows from Eq. (A1) that $G_{\gamma\gamma'}^{(0)}(z)$ is a regular function of z except for a finite number of poles, the closest to the origin being a simple one at $z = 1$. It then follows from Eq. (A13) and Darboux's theorem that

$$\langle x_n^2 \rangle \sim Cn + D \quad \text{as } n \rightarrow \infty \quad (\text{A21})$$

where C is the coefficient of $1/(1-z)^2$ in $X(z)$, while D is equal to C plus the coefficient of $1/(1-z)$ in $X(z)$. Thus

$$\begin{aligned} C &= k^2 p_1 \lim_{z \rightarrow 1} [(1-z)(G_{k\gamma_0}^{(0)} + G_{1\gamma_0}^{(0)})][1 + \lim_{z \rightarrow 1} 2p_1(G_{1k}^{(0)} - G_{11}^{(0)})] \\ &+ 2kp_1 \sum_{\gamma=1}^k (\gamma - \gamma_0) \{ \lim_{z \rightarrow 1} [(1-z)G_{\gamma 1}^{(0)}] \lim_{z \rightarrow 1} [(1-z)G_{k\gamma_0}^{(0)}] \\ &- \lim_{z \rightarrow 1} [(1-z)G_{\gamma k}^{(0)}] \lim_{z \rightarrow 1} [(1-z)G_{1\gamma_0}^{(0)}] \} \end{aligned} \quad (\text{A22})$$

In order to evaluate this expression, we use the following expansions:

$$U_{\gamma\gamma'}^R(z) \sim \left\{ k(1-z) \left[1 + \frac{(1-z)^{1/2}}{p_1^{1/2}} (1 - 2p_1^{-1}) + O(1-z) \right] \right\}^{-1} \quad (\text{A23a})$$

and

$$\frac{U_{\gamma, \gamma+n}^R(z)}{U_{\gamma\gamma}^R(z)} = 1 + \frac{1-z}{2p_1} \eta(\eta - k) + O(1-z)^2 \quad (\text{A23b})$$

from which we find

$$\lim_{z \rightarrow 1} [(1-z)U_{\gamma, \gamma+n}^R(z)] = 1/k \quad (\text{A24a})$$

$$\lim_{z \rightarrow 1} [U_{\gamma, \gamma+n}^R(z) - U_{\gamma\gamma}^R(z)] = -\eta(k - \eta)/2kp_1 \quad (\text{A24b})$$

Then from Eq. (A20)

$$\lim_{z \rightarrow 1} (G_{1k}^{(0)} - G_{11}^{(0)}) = \lim_{z \rightarrow 1} (U_{1k}^R - U_{11}^R) = -(k - 1)/2kp_1 \quad (\text{A25a})$$

$$\lim_{z \rightarrow 1} [(1 - z)G_{\gamma\gamma'}^{(0)}] = \frac{1}{k} \frac{p_1 - \epsilon}{p_1 - \epsilon + \alpha\epsilon} \quad \text{provided } \gamma \neq \frac{k+1}{2} \quad (\text{A25b})$$

$$\lim_{z \rightarrow 1} [(1 - z)G_{(k+1)/2, \gamma'}^{(0)}] = \frac{1}{k} \frac{p_1}{p_1 - \epsilon + \alpha\epsilon} \quad (\text{A25c})$$

Finally, on substituting Eqs. (A24) and (A25) into Eq. (A22), we find

$$C = \frac{2p_1}{1 + \alpha\epsilon/(p_1 - \epsilon)} \quad (\text{A26})$$

which yields Eq. (3.9a). Equation (3.9b) then follows directly from (3.1).

APPENDIX B

To evaluate the matrix elements $G_{i,j_0}(z)$ occurring in Eq. (3.23) we consider a finite ring of Nk sites with N strong partial traps distributed randomly among $N(k - 1)$ weak partial traps. The density of strong partial traps is thus $1/k$ independent of the number of lattice sites in the ring. At the end of the calculation we will take the limit $N \rightarrow \infty$. We consider the equation

$$g_{i_0}(z) = U_{i_0}^R(z) + z \sum_{l'=1}^{Nk} \sum_{l''=1}^{Nk} U_{il''}^R(z) q(l', l'') g_{l''i_0}(z) \quad (\text{B1})$$

where $q(l, l')$ is defined in Eq. (3.13b) and $U_{i_0}^R(z)$ is the perfect Nk -ring generating function [cf. Eq. (A17) with k everywhere replaced by Nk]. Equation (B1) defines the matrix $\mathbf{g}(z)$ and in the limit $N \rightarrow \infty$ we have

$$\lim_{N \rightarrow \infty} g_{i_0}(z) = G_{i_0}(z) \quad (\text{B2})$$

Now consider Eq. (B1) at the strong partial trap sites $\{l_j\}$. Successively setting l equal to the l_j yields the following set of N simultaneous algebraic equations in the N unknowns $g_{l_j, i_0}(z)$:

$$\begin{aligned} A_{i_1 l_1} g_{l_1 i_0} + A_{i_1 l_2} g_{l_2 i_0} + \dots + A_{i_1 l_N} g_{l_N i_0} &= U_{i_1 l_0}^R \\ A_{i_2 l_1} g_{l_1 i_0} + A_{i_2 l_2} g_{l_2 i_0} + \dots + A_{i_2 l_N} g_{l_N i_0} &= U_{i_2 l_0}^R \\ \vdots & \\ A_{i_{N-1} l_1} g_{l_1 i_0} + A_{i_{N-1} l_2} g_{l_2 i_0} + \dots + A_{i_{N-1} l_N} g_{l_N i_0} &= U_{i_{N-1} l_0}^R \end{aligned} \quad (\text{B3})$$

where

$$A_{i_l l_i} \equiv 1 - 2z\epsilon(U_0^R - U_1^R) \quad (\text{B4a})$$

$$A_{i_l l_j} \equiv \epsilon(2U_{i_l l_j}^R - U_{i_l, l_j, l_j+1}^R - U_{i_l, l_j, l_j-1}^R), \quad i \neq j \quad (\text{B4b})$$

$$U_0^R \equiv U_{i_l}^R, \quad U_1^R \equiv U_{i_l, l \pm 1}^R \quad (\text{B4c})$$

Equation (B3) can be solved by the method of determinants. For example, consider the solution for $g_{i_1 l_0}$:

$$g_{i_1 l_0} = \begin{vmatrix} U_{i_1 l_0}^R & A_{i_1 l_2} & \cdots & A_{i_1 l_N} \\ U_{i_2 l_0}^R & A_{i_2 l_2} & \cdots & A_{i_2 l_N} \\ \vdots & \vdots & & \vdots \\ U_{i_N l_0}^R & A_{i_N l_2} & \cdots & A_{i_N l_N} \end{vmatrix} \times \begin{vmatrix} A_{i_1 l_1} & \cdots & A_{i_1 l_N} \\ \cdot & & \cdot \\ \vdots & & \vdots \\ A_{i_N l_1} & & A_{i_N l_N} \end{vmatrix}^{-1} \quad (\text{B5})$$

It is convenient for the following calculations to divide each element in (B5) by U_0^R and thus to rewrite $g_{i_1 l_0}$ in the form

$$g_{i_1 l_0} = |\text{Num}|/|\text{Den}| \quad (\text{B6})$$

where

$$|\text{Num}| \equiv \begin{vmatrix} U_{i_1 l_0}'^R & A'_{i_1 l_2} & \cdots & A'_{i_1 l_N} \\ U_{i_2 l_0}'^R & A'_{i_2 l_2} & \cdots & A'_{i_2 l_N} \\ \vdots & \vdots & & \vdots \\ U_{i_N l_0}'^R & A'_{i_N l_2} & \cdots & A'_{i_N l_N} \end{vmatrix} \quad (\text{B7a})$$

$$|\text{Den}| \equiv \begin{vmatrix} A'_{i_1 l_1} & \cdots & A'_{i_1 l_N} \\ \vdots & & \vdots \\ A'_{i_N l_1} & \cdots & A'_{i_N l_N} \end{vmatrix} \quad (\text{B7b})$$

and where

$$U_{i l_0}'^R \equiv U_{i l_0}^R / U_0^R \quad (\text{B8a})$$

$$A'_{i l_j} \equiv A_{i l_j} / U_0^R \quad (\text{B8b})$$

As discussed in the text and in Appendix A, for our purposes it is sufficient to evaluate the $g_{i l_j}$ to $O(1 - z)^{-1}$ when we consider an expansion in powers of $(1 - z)$. From Eq. (A22b) we have

$$U_{i l_0}'^R = 1 - \frac{l_i(Nk - l_i)}{2p_1} \Lambda + O(\Lambda^2) \quad (\text{B9})$$

where

$$\Lambda \equiv (1 - z) \quad (\text{B10})$$

Hence

$$A'_{i l_i} = \Lambda Nk \left(1 - \frac{\epsilon z}{p_1}\right) + \frac{\epsilon z}{p_1} \Lambda + O(\Lambda^2) \equiv a\Lambda + O(\Lambda^2) \quad (\text{B11a})$$

$$A'_{i l_j} = \frac{\epsilon z}{p_1} \Lambda + O(\Lambda^2) \equiv b\Lambda + O(\Lambda^2), \quad i \neq j \quad (\text{B11b})$$

Using (B9) and (B11) in (B7), we obtain

$$\begin{aligned}
 |\text{Num}| &= \begin{vmatrix} 1 & b & b & b & \dots & b \\ 1 & a & b & b & \dots & b \\ 1 & b & a & b & \dots & b \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 1 & b & b & b & \dots & a \end{vmatrix} \Lambda^{N-1} + O(\Lambda^N) \\
 &= (a - b)^{N-1} \Lambda^{N-1} + O(\Lambda^N)
 \end{aligned} \tag{B12}$$

For the denominator of (B6) as given in (B7b) we obtain

$$\begin{aligned}
 |\text{Den}| &= \begin{vmatrix} a & b & b & \dots & b \\ b & a & b & \dots & b \\ \vdots & \vdots & \vdots & & \vdots \\ b & b & b & \dots & a \end{vmatrix} \Lambda^N + O(\Lambda^{N+1}) \\
 &= (a - b)^{N-1} [a + (N - 1)b] \Lambda^N + O(\Lambda^{N+1})
 \end{aligned} \tag{B13}$$

Therefore, substituting (B12) and (B13) into (B6), we obtain

$$g_{i_1 i_0} = \left[Nk \left(1 - \frac{\epsilon z}{p_1} \right) + N \frac{\epsilon z}{p_1} \right]^{-1} \Lambda^{-1} + O(\Lambda^0) \tag{B14}$$

where we have used the definitions of a and b given in (B11).

To construct the sum of generating functions that occurs on the right-hand side of Eq. (3.23), we note that the leading term in (B14) is independent of l_1 . Hence we have

$$\sum_{l_j} g_{l_j l_0} = N g_{i_1 l_0}$$

and using Eq. (B2), we obtain

$$\sum_{l_j} G_{l_j l_0} = \lim_{N \rightarrow \infty} N g_{i_1 l_0} = \left[k \left(1 - \frac{\epsilon z}{p_1} \right) + \frac{\epsilon z}{p_1} \right]^{-1} \Lambda^{-1} + O(\Lambda^0) \tag{B15}$$

which is the result given in Eq. (3.24).

APPENDIX C

C1. Singly Periodic Distribution of Strong Columns

Expansion of the determinant of \mathbf{D}_m given in Eq. (4.12) about its bottom row leads to the recurrence relation

$$\det \mathbf{D}_m = [w - 2(p_2 + \epsilon)c] \det \mathbf{E}_{m-1} - [p_1(2p_1 - 2\epsilon)] \det \mathbf{E}_{m-2} \tag{C1}$$

where $\det \mathbf{E}_{m-1}$ and $\det \mathbf{E}_{m-2}$ are determinants obtained by deleting one and two rows and columns from \mathbf{D}_m , respectively. As mentioned in Section 4, $(m-1)$ is a multiple r of k . Let $E_r^{k-j_1}$ be the determinant obtained by deleting $kj_2 + j_1$ rows and columns from \mathbf{E}_{m-1} , where $0 \leq j_1 \leq k-1$ and $0 \leq j_2 \leq r-1$. Thus, e.g., $\det \mathbf{E}_{m-1} = E_r^k$. Because $\det \mathbf{E}_{m-1}$ is a continuant, it is possible to develop a recurrence relation between $E_{j_2}^{j_1}$ and $E_{j_2}^{j_1 \pm 1}$. Using this recurrence relation, it can be shown⁽¹⁾ that E_r^j satisfies a second-order linear difference equation with the solution

$$E_r^j = A_j \lambda_1^r + B_j \lambda_2^r \tag{C2}$$

where $\lambda_{1,2}$ are the roots of the quadratic equation $P_k(\lambda) = 0$ and

$$P_k(\lambda) = \begin{vmatrix} 1 & -(w-2p_2c) & p_1^2 & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & 1 & -(w-2p_2c) & p_1^2 & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 & -(w-2p_2c) & p_1^2 \\ p_1(p_1-\epsilon) & \cdot & \cdot & \cdot & \cdot & 0 & \lambda & -\lambda(w-2p_2c) \\ -(w-2p_2c-2\epsilon c) & p_1(p_1-\epsilon) & \cdot & \cdot & \cdot & 0 & 0 & \lambda \end{vmatrix} \tag{C3}$$

The coefficients A_j and B_j can be found from $\det \mathbf{E}_1$ and $\det \mathbf{E}_2$, but we will not need to know their values for our calculation, as will become clear below. By systematic expansion of the determinant (C3) and use of the Chebyshev polynomials (Ref. 10, p. 183) $U_k(\lambda)$ defined by

$$U_k(\lambda) \equiv \begin{vmatrix} 2\lambda & 1 & 0 & 0 & \cdot & \cdot & \cdot & 0 \\ 1 & 2\lambda & 1 & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & 1 & 2\lambda & 1 & \cdot & \cdot & \cdot & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdot & \cdot & \cdot & \cdot & 1 & 2\lambda & 1 \\ 0 & \cdot & \cdot & \cdot & \cdot & 0 & 1 & 2\lambda \end{vmatrix} \tag{C4}$$

it can be shown that

$$P_k(\lambda) = \lambda^2 - X_k(w, c)\lambda + p_1^{2k-2}(p_1 - \epsilon)^2 = 0 \tag{C5}$$

where

$$X_k(w, c) = p_1^k U_k + (2\epsilon p_1^{k-1} - p_1^k) U_{k-2} - 2\epsilon c p_1^{k-1} U_{k-1} \tag{C6}$$

and

$$U_k \equiv U_k\left(\frac{w - 2p_2c}{2p_1}\right) \tag{C7}$$

The two roots of Eq. (C5) are given by

$$\lambda_{1,2} = \frac{1}{2}X_k(w, c) \pm \frac{1}{2}[X_k^2(w, c) - 4p_1^{2k-2}(p_1 - \epsilon)^2]^{1/2} \tag{C8}$$

Hence from Eqs. (C1), (C2), and (C8) we obtain

$$\begin{aligned} \det \mathbf{D}_m &= [w - 2(p_2 + \epsilon)c](A_k \lambda_1^r + B_k \lambda_2^r) - [2(p_1 - \epsilon)p_1](A_{k-1} \lambda_1^r + B_{k-1} \lambda_2^r) \\ &= \{A_k[w - 2(p_2 + \epsilon)c] - A_{k-1}[2(p_1 - \epsilon)p_1]\} \lambda_1^r \\ &\quad + O\left[\left(\frac{\lambda_2^r}{\lambda_1}\right)\right], \quad \lambda_1 > \lambda_2 \end{aligned} \tag{C9}$$

In the limit $m \rightarrow \infty$, i.e., $r \rightarrow \infty$,

$$(\log \det \mathbf{D}_m)/m \rightarrow \log \lambda_1 \tag{C10}$$

Taking the limit $m \rightarrow \infty$ of (A9) and using (C10), we obtain the result

$$\begin{aligned} G(z) &\equiv \lim_{m \rightarrow \infty} G(z; m) \\ &= \frac{w}{k\pi} \int_0^\pi \frac{\partial X_k / \partial w}{[X_k^2 - 4p_1^{2k-2}(p_1 - \epsilon)^2]^{1/2}} d\Theta \\ &= \frac{w}{k\pi} \int_0^\pi \int_0^\pi \frac{\partial X_k}{\partial w} \frac{d\Theta d\Theta'}{X_k - 2p_1^{k-1}(p_1 - \epsilon) \cos \Theta'} \\ &= \frac{w}{k\pi} \int_0^\pi \int_0^\pi \int_0^\infty \frac{\partial X_k}{\partial w} \exp\{-t[X_k - 2p_1^{k-1}(p_1 - \epsilon) \cos \Theta']\} d\Theta d\Theta' dt \end{aligned} \tag{C11}$$

with $X_k \equiv X_k(w, c)$ of Eq. (C6). Using the following integral representation of the Bessel function $I_j(x)$ of imaginary argument (Ref. 10, p. 14)

$$I_j(x) = \frac{1}{\pi} \int_0^\pi \cos(j\Theta) e^{x \cos \Theta} d\Theta \tag{C12}$$

we obtain

$$G(z) = \frac{w}{k\pi} \int_0^\pi \int_0^\infty \frac{\partial X_k}{\partial w} e^{-tX_k} I_0(2tp_1^{k-1}(p_1 - \epsilon)) dt d\Theta_1 \tag{C13}$$

The Θ_1 integral is evaluated by Laplace's⁽¹¹⁾ method. Thus (C13) reduces to

$$\begin{aligned} G(z) &= \frac{w}{k\pi} \int_0^\infty \frac{\partial X_k}{\partial w} \Big|_{\Theta_1=0} \left[\frac{-\pi}{2t(\partial^2 X_k / \partial \Theta_1^2) |_{\Theta_1=0}} \right]^{1/2} \\ &\quad \times [\exp(-tX_k |_{\Theta_1=0})] I_0(2tp_1^{k-1}(p_1 - \epsilon)) dt \end{aligned} \tag{C14}$$

It can easily be shown by using the relations between the derivatives of Chebyshev polynomials (Ref. 10, p. 183) and (C6) that

$$X_k|_{\Theta_1=0} = p_1^k U_k(w') + p_1^{k-1}(2\epsilon - p_1)U_{k-2}(w') - 2\epsilon p_1^{k-1}U_{k-1}(w') \quad (C15a)$$

$$\begin{aligned} \frac{\partial^2 X_k}{\partial \Theta_1^2} \Big|_{\Theta_1=0} &= p_2 p_1^{k-1} U_k'(w') + p_2 p_1^{k-2} (2\epsilon - p_1) U_{k-2}'(w') \\ &\quad + 2\epsilon p_1^{k-1} U_{k-1}(w') - 2\epsilon p_1^{k-2} p_2 U_{k-1}'(w') \end{aligned} \quad (C15b)$$

$$\frac{\partial X_k}{\partial w} \Big|_{\Theta_1=0} = \frac{1}{2p_1} [p_1^k U_k'(w') + (2\epsilon p_1^{k-1} - p_1^k) U_{k-2}'(w') - 2\epsilon p_1^{k-1} U_{k-1}'(w')] \quad (C15c)$$

where $w' = (w - 2p_2)/2p_1$ and $U_k'(x) \equiv (d/dx)U_k(x)$.

We now proceed to examine the singularities of $G(z)$ with respect to z . The integral in (C14) can be split into two parts as follows:

$$G(z) = \int_0^T f(t) dt + \int_T^\infty f(t) dt \quad (C16)$$

Here $f(t)$ denotes the integrand in (C14) and T is an arbitrarily large but finite positive number. The first integral is an analytic function of $z = w^{-1}$. The second integral diverges at $z = 1$ and gives the logarithmic divergence often encountered in two-dimensional lattice problems. To show this, we substitute in the second integral in (C16) the following asymptotic expansion for the Bessel functions $I_j(x)$ (Ref. 10, p. 86):

$$I_j(x) = (2\pi x)^{-1/2} e^x [1 - (4j^2 - 1)/8x + O(1/x^2)] \quad (C17)$$

This yields

$$\begin{aligned} G(z) &= \int_0^T f(t) dt + S(k, p_1, \epsilon) \left\{ \int_T^\infty \frac{\exp[2tp_1^{k-1}(p_1 - \epsilon) - tX_k|_{\Theta_1=0}]}{t} \right. \\ &\quad \left. \times \left[1 + \frac{1}{16tp_1^{k-1}(p_1 - \epsilon)} + O\left(\frac{1}{t^2}\right) \right] dt \right\} \end{aligned} \quad (C18)$$

where

$$S(k, p_1, \epsilon) = \frac{w}{2k\pi} \left[-2 \frac{\partial^2 X_k}{\partial \Theta_1^2} \Big|_{\Theta_1=0} \right]^{-1/2} [p_1^{k-1}(p_1 - \epsilon)]^{-1/2} \frac{\partial X_k}{\partial w} \Big|_{\Theta_1=0} \quad (C19)$$

Inserting the explicit expression for $X_k|_{\Theta_1=0}$ from (C6) gives

$$\begin{aligned} G(z) &= \int_0^T f(t) dt + S(k, p_1, \epsilon) \\ &\quad \times \left\{ \int_T^\infty \frac{e^{-TC}}{t} \left[1 + \frac{1}{8tp_1^{k-1}(p_1 - \epsilon)} + O\left(\frac{1}{t^2}\right) \right] dt \right\} \end{aligned} \quad (C20)$$

where

$$C = (t/T)\{\frac{1}{3}p^{k-2}[p_1(2k + 1) - 2\epsilon k](1 - z)\} \tag{C21}$$

We define the first integral in (C20) as $\Phi(z)$, which is a regular function of z at $z = 1$ as pointed out earlier. Defining the functions

$$\phi_m(x) \equiv \int_1^\infty t^{-m} e^{-xt} dt \tag{C22}$$

we then have

$$G(z) = \Phi(z) + S(k, p_1, \epsilon) \left[\phi_1(TC) + \frac{1}{8p_1^{k-1}(p_1 - \epsilon)} \phi_2(TC) + \dots \right] \tag{C23}$$

The functions $\phi_m(x)$ are simply related to the incomplete gamma functions. They have a branch point singularity at $x = 0$ and it can be shown that

$$\phi_m(x) = - \sum_{\substack{j=0 \\ j \neq m-1}}^\infty \frac{(-1)^j x^j}{j!(j + 1 - m)!} + \frac{(-1)^{m-1} x^{m-1}}{(m-1)!} + \frac{(-1)^m}{(m-1)!} x^{m-1} \log x \tag{C24}$$

Thus

$$\phi_1(TC) \sim -\log(TC) \sim -\log(1 - z) \tag{C25a}$$

and

$$\phi_m(TC) \sim -(TC)^{m-1} \log TC \sim -(1 - z)^{m-1} \log(1 - z) \tag{C25b}$$

As $z \rightarrow 1$, the dominant contribution therefore results from $\phi_1(TC)$ and is equal to $-\log(1 - z)$.

We now evaluate $S(k, p_1, \epsilon)$ in powers of $(1 - z)$. Expanding the derivatives of the Chebyshev polynomials in (C15) in powers of $(1 - z)$, we obtain

$$\frac{\partial X_k}{\partial w} \Big|_{\theta_1=0} = kp_1^{k-2}[k(p_1 - \epsilon) + \epsilon] + O(1 - z) \tag{C26a}$$

$$\frac{\partial^2 X_k}{\partial \theta_1^2} \Big|_{\theta_1=0} = 2kp_1^{k-2} \left(\frac{kp_1}{2} + kp_1(\epsilon - p_1) + \epsilon \frac{1 - k}{2} \right) + O(1 - z) \tag{C26b}$$

Substituting (C26) in (C19) gives

$$S(k, p, \epsilon) = \frac{1}{4\pi} \left\{ \frac{p_1[p_2 + \alpha\epsilon/2(p_1 - \epsilon)]}{[1 + \alpha\epsilon/(p_1 - \epsilon)]^2} \right\}^{-1/2} + O(1 - z) \tag{C27}$$

Combining Eqs. (C23), (C25), and (C27), we obtain the result quoted in Eqs. (4.13) and (4.14).

C2. Clumped Periodic Distribution of Strong Columns

As mentioned in the text, the clumped periodic distribution of strong columns corresponds to the choices $x_1 = x_2 = \dots = x_r = 1$, $x_{r+1} = \dots = x_{kr} = 0$, $x_{kr+1} = \dots = x_{(k+1)r} = 1, \dots, x_{m-r} = x_{m-r+1} = \dots = x_m = 1$. Sub-

Once again we can use the Laplace method to evaluate the Θ_1 integration, with the result

$$G(z) = \lim_{r \rightarrow \infty} \frac{w}{kr\pi} \frac{\partial X_{kr}}{\partial w} \Big|_{\Theta_1=0} \left[\frac{\pi}{2 \partial^2 X_{kr} / \partial \Theta_1^2} \Big|_{\Theta_1=0} \right]^{1/2} \times \int_0^\infty \frac{e^{-tX_{kr}(w)}}{\sqrt{t}} I_0 \left(\frac{2t}{2^{(k+1)r}} \right) dt \tag{C33}$$

The integral in (C33) can be split into two parts, in a manner similar to Eq. (C16). The first part is a finite integral of the integrand in (C33) from zero to a large but finite value T of the variable t . This part is an analytic function of z as $z \rightarrow 1$ and will be denoted by $\Phi(z)$. The second part is an integral from T to infinity of the integrand. Proceeding as in Eqs. (C17)–(C25), it is straightforward to show that the second part has a logarithmic singularity as $z \rightarrow 1$. Thus we write

$$G(z) = \Phi(z) - \Psi'(z) \ln(1 - z) \tag{C34}$$

where

$$\Psi'(z) = \lim_{r \rightarrow \infty} \frac{w}{kr\pi} \frac{\partial X_{kr}}{\partial w} \Big|_{\Theta_1=0} \left[2^{3-(r+1)k} \frac{\partial^2 X_{kr}}{\partial \Theta_1^2} \Big|_{\Theta_1=0} \right]^{-1/2} \tag{C35}$$

The explicit forms for the derivatives of X_{kr} occurring in (C35) are

$$\frac{\partial^2 X_{kr}}{\partial \Theta_1^2} \Big|_{\Theta_1=0} = \frac{kr^2}{2^{rk+r-1}} + O(1 - z) \tag{C36a}$$

$$\frac{\partial X_{kr}}{\partial w} \Big|_{\Theta_1=0} = \frac{2k(k+1)r^2}{2^{rk+r-1}} + O(1 - z) \tag{C36b}$$

Combining Eqs. (C35) and (C36), we obtain

$$\Psi'(z) = \frac{1}{2\pi} \frac{k+1}{\sqrt{k}} [1 + O(1 - z)] \tag{C37}$$

which is identical to the result (4.14) if we set $p_1 = \frac{1}{2}$, $p_2 = 0$, and $\epsilon = \frac{1}{4}$.

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