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Group Theory, Markov Chains, and Excluded Volume Effect in Polymers

F. T. Hioe[1] and C. Domb[2]

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A restricted walk of order r on a lattice is defined as a random walk in which polygons with r vertices or less are excluded. A study of restricted walks for increasing r provides an understanding of how the transition in properties is effected from random to self-avoiding walks which is important in our understanding of the excluded volume effect in polymers and in the study of many other problems. Here the properties of restricted walks are studied by the transition matrix method based on the theory of Markov chains. A group theoretical method is used to reduce the transition matrix governing the walk in a systematic manner and to classify the eigenvalues of the transition matrix according to the various representations of the appropriate group. It is shown that only those eigenvalues corresponding to two particular representations of the group contribute to the correlations among the steps of the walk. The distributions of eigenvalues for walks of various orders r on the two-dimensional triangular lattice and the three-dimensional face-centered cubic lattice are presented, and they are shown to have some remarkable features.

KEY WORDS: Restricted walk; self-avoiding walk; transition matrix; group representations.

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[1] Institute for Fundamental Studies, Department of Physics and Astronomy, University of Rochester, Rochester, New York.

[2] Physics Department, University of London King's College, London, England.

1. INTRODUCTION

The problem of self-avoiding walks on lattices, with its applications to the theory of polymer configurations and to the theory of the Ising and Heisenberg ferromagnets, has been studied extensively for many years.[3] Precise analytic information about the asymptotic properties of self-avoiding walks is very limited.[(3)] Much of the information about the properties of self-avoiding walks has been derived from the method of exact enumeration[(4)] and the method of Monte Carlo computations.[(5)] Of considerable importance is an understanding of how the transition in properties is effected from random to self-avoiding walks. In this respect, a good deal of understanding has been gained from the virial expansion method (see, e.g., Ref. 6) and the transition matrix method.[(7)] The transition matrix method for the study of short-range excluded volume effects was initiated by Montroll.[(8)] If we define a restricted walk of order r as a random walk in which polygons with r vertices or less are excluded, then a restricted walk of order r is a Markov process governed by a transition matrix with eigenvalues $\lambda_{1r}, \lambda_{2r},\ldots, \lambda_{Nr}$, N being the order of the matrix. The behavior of the number of walks c_{nr} of n steps and the mean-square length of walks of n steps $\langle R_{nr}^2\rangle$ can be readily shown to be as follows:

$$c_{nr} = a_{1r}\lambda_{1r}^n + a_{2r}\lambda_{2r}^n + \cdots + a_{Nr}\lambda_{nr}^N, \qquad \langle R_{nr}^2\rangle \simeq b_r n$$

For large n the largest eigenvalue λ_{1r} dominates and the behavior of c_{nr} becomes

$$c_{nr} \simeq a_{1r}\lambda_{1r}^n$$

However, in the transition from the restricted to self-avoiding walks, n and r increase simultaneously, and since the order of the transition matrix and hence the number of eigenvalues increases rapidly with increasing r, the distribution of the eigenvalues and their individual contribution to c_{nr} should be examined more carefully. In a previous paper[(7)] we studied the distribution of the eigenvalues of the "reduced" transition matrix for walks of various orders on the two-dimensional triangular lattice and on the three-dimensional face-centered cubic lattice, and the following picture emerges from our numerical data.

(a) The largest eigenvalue λ_{1r} (which is always real) is distinct and well separated from the others.

(b) The rest of the eigenvalues are rather symmetrically distributed about the origin.

(c) The contribution from $a_{1r}\lambda_{1r}^n$ to c_{nr} accounts for over 99% of the total contribution even when n is as small as r; significantly, the percentage

[3] See, e.g., Ref. 1. For a general review see Domb.[(2)]

contribution from $a_{1r}\lambda_{1r}^r$ to c_{rr} increases as r increases due to the increasing symmetry of the distribution of the rest of the eigenvalues with increasing r, with the result that they give a negligible net contribution to the value of c_{rr}.

(d) The largest eigenvalue satisfies approximately the relation

$$\lambda_{1r} \simeq \mu[1 + (g/r)]$$

and the origin of the n^g term in the asymptotic formula $c_n \simeq n^g\mu_n$ for the total number of self-avoiding walks of n steps is to be found in the relation

$$c_n \simeq \lambda_{11}\lambda_{12}\cdots\lambda_{1n} \simeq \mu^n \prod_{r=1}^{n} [1 + (g/r)]$$

Aside from the total number of n-step walks c_n, another quantity of considerable interest in attempting to understand the transition from random to self-avoiding walks is the correlation between two steps separated by, say, t steps. To study the correlations among the steps, we must study the "full" transition matrix for the walk. The transition matrix studied in Ref. 7 for the total number of walks is a particular reduced form of this full transition matrix, as will become clear in this paper. In Section 2 of this paper a group theoretical method is given which is used to reduce the full transition matrix in a systematic way and to classify its eigenvalues according to the various representations of the appropriate group. The reduced matrix studied in Ref. 7 for the total number of walks is shown to correspond to the "identity representation." In Section 3, we derive exact expressions for the correlations among the steps of a restricted walk in terms of the eigenvalues and eigenvectors of the full transition matrix, and we show that only those eigenvalues corresponding to the identity representation and those corresponding to what we call the "maximal representation" of the group contribute to the correlations. The distribution of eigenvalues corresponding to these two representations for walks of order $r \leqslant 7$ on the plane triangular lattice (for which the reduced transition matrices are of the order 260) and for walks of order $r \leqslant 5$ on the three-dimensional face-centered cubic lattice (for which the reduced matrices are of the order 170) are presented in Section 4. It will be seen that the distribution of eigenvalues corresponding to the maximal representation has the same remarkable features as the distribution of eigenvalues corresponding to the identity representation. The correlation between two steps separated by t steps is found to be principally characterized by the ratio $(\lambda_{j_1r}/\lambda_{1r})^t$, where λ_{j_1r} and λ_{1r} are respectively the largest eigenvalues corresponding to the maximal and the identity representations; these also turn out to be respectively the second largest and the largest eigenvalues of the full transition matrix. The behavior of the ratio $\lambda_{j_1r}/\lambda_{1r}$ is examined and a conjecture is made concerning the limiting value of this ratio as $r \to \infty$.

2. GROUP THEORY AND THE TRANSITION MATRIX FOR A RESTRICTED WALK

To construct the transition matrix corresponding to a restricted walk of order r, we begin by considering all possible $(r - 1)$-step self-avoiding walks. Let us denote these walks by $w(1), w(2),..., w(c_{r-1})$, where c_{r-1} is the total number of $(r - 1)$-step self-avoiding walks on the lattice considered, and let us denote the number of walks after n steps ending in types $w(1), w(2),..., w(c_{r-1})$ by $w_n(1)$, $w_n(2),...,$ $w_n(c_{r-1})$, respectively. Now the addition of a further step to a walk of type $w_{r-1}(1)$ in all possible ways leads either to some forbidden self-intersections, which we reject, or to a walk of type $w_r(k)$, or type $w_r(l)$, etc. Consideration in a similar way of the addition of a step to the types $w_{r-1}(2), w_{r-1}(3),..., w_{r-1}(c_{r-1})$ leads to a set of recurrence relations which can be conveniently expressed by the matrix equation

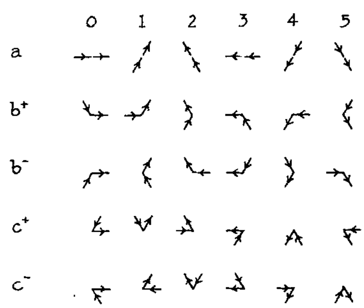
$$\mathbf{w}_r = \mathsf{A}\mathbf{w}_{r-1} \tag{1}$$

where the transition matrix A is of order c_{r-1}. The number of n-step walks ending in types $w(1), w(2), \ldots, w(c_{r-1})$ is then given by the components of $\mathbf{w}_n$

$$\mathbf{w}_n = \mathsf{A}^{n-r+1}\mathbf{w}_{r-1} \tag{2}$$

The matrix A will be referred to as the full transition matrix corresponding to the restricted walk of the given order. Clearly A has the symmetry property of the lattice considered and we now wish to show how A can be reduced in a systematic way.

First let us consider an example of walks which exclude triangles as well as immediate reversals on the plane triangular lattice. Starting with all the possible two-step walks ($c_2 = 30$), the corresponding matrix A can be constructed quite simply (A is a 30×30 matrix). Let us label the walks as follows:



(3)

so that $\to\nearrow$, for example will be denoted by $b^+(1)$, or to be more precise, we shall denote by $b_n{}^+(1)$ the walk after n steps the last two steps of which end in $\to\nearrow$

By making the substitutions

$$\begin{gathered} a(m) = \omega_s{}^m a(0), \qquad b^+(m) = \omega_s{}^m b^+(0), \qquad b^-(m) = \omega_s{}^m b^-(0) \\ c^+(m) = \omega_s{}^m c^+(0), \qquad \text{and} \qquad c^-(m) = \omega_s{}^m c^-(0), \end{gathered} \tag{4}$$

where $m = 0, 1, \ldots, 5$ and $\omega_s = e^{2\pi i s/6}$, $s = 0, 1, \ldots, 5$, it is easy to see that A is effectively reduced to six 5×5 matrices. But now it is not at all obvious whether the matrices can be reduced further. We might expect that b^+ and b^-, and c^+ and c^-, would have some kind of "reflection symmetry." It turns out that we can equate b^+ to b^- and c^+ to c^- only for $\omega = 1$ or -1. For other values of ω the relation between them is not simple.

To assist us in the search for the full symmetry of A, we draw upon the resources of group theory. It is the useful characteristic of group theory that it provides us with a systematic calculus for exploiting symmetry properties to the fullest extent. We now describe how the method of group theory can be applied to the reduction of A.

Starting with an arbitrary function ψ, group theory tells us how to resolve the function into a sum of functions, each of which belongs to a particular row of some irreducible representation, by the use of a projection operator (see, e.g., Ref. 9). Using the usual notations in group theory, a projection operator is defined by

$$P_i^{(\mu)} = (n_\mu/g) \sum_R D_{ii}^{(\mu)}(R^{-1}) O_R \tag{5}$$

where O_R is the symmetry operator corresponding to the element R of the group, $D^{(\mu)}(R)$ is the matrix corresponding to the μth representation of R, n_μ is the degree of the μth representation, g is the order of the group, and the summation of the right-hand side is taken over all elements of the group. The application of $P_i^{(\mu)}$ to any arbitrary function ψ projects out that part of the function that belongs to the ith row of the μth representation, that is,

$$P_i^{(\mu)} \psi = \psi_i^{(\mu)} \tag{6}$$

The significance of this result to the problem of reducing our transition matrix A will soon become clear.

We now come back to the problem of a walk excluding triangles on a plane triangular lattice. The walks given by (3) suggest that we should consider the symmetry group C_{6v}. Denoting a 60° rotation by ω, Table I gives the results when various symmetry operators of the group are applied to walks of types $a(0)$, $b^+(0)$, $b^-(0)$, $c^+(0)$, and $c^-(0)$. The character table of group C_{6v} is reproduced in Table II.

Table I. Operation by Elements of Group C_{6v}

E	$C_6(\omega)$	$C_6(\omega^5)$	$C_6^2(\omega^2)$	$C_6^2(\omega^4)$	C_6^3	$\sigma_v(0)$	$\sigma_v(\pi/3)$	$\sigma_v(2\pi/3)$	$\sigma_d(\pi/6)$	$\sigma_d(3\pi/6)$	$\sigma_d(5\pi/6)$
a_0	a_1	a_5	a_2	a_4	a_3	a_0	a_2	a_4	a_1	a_3	a_5
b_0^+	b_1^+	b_5^+	b_2^+	b_4^+	b_3^+	b_0^-	b_2^-	b_4^-	b_1^-	b_3^-	b_5^-
b_0^-	b_1^-	b_5^-	b_2^-	b_4^-	b_3^-	b_0^+	b_2^+	b_4^+	b_1^+	b_3^+	b_5^+
c_0^+	c_1^+	c_5^+	c_2^+	c_4^+	c_3^+	c_0^-	c_2^-	c_4^-	c_1^-	c_3^-	c_5^-
c_0^-	c_1^-	c_5^-	c_2^-	c_4^-	c_3^-	c_0^+	c_2^+	c_4^+	c_1^+	c_3^+	c_5^+

Table II. Character Table for the Symmetry Group C_{6v}

C_{6v}	E	C_6^3	$C_6^2(2)$	$c_6(2)$	$\sigma_v(3)$	$\sigma_d(3)$
A_1	1	1	1	1	1	1
A_2	1	1	1	1	-1	-1
B_2	1	-1	1	-1	1	-1
B_1	1	-1	1	-1	-1	1
E_1	2	2	-1	-1	0	0
E_2	2	-2	-1	1	0	0

Consider first the A_1 representation. Since it is a one-dimensional representation, $D_{11}^{(A_1)}(R) = \chi^{(A_1)}(R)$. Starting with an arbitrary 1×30 vector having components $a(0), a(1),..., a(5)$; $b^+(0),..., b^+(5)$; $b^-(0),..., b^-(5)$; $c^+(0),..., c^+(5)$; $c^-(0),..., c^-(5)$, application of the projection operator $P_1^{(A_1)}$ on this vector gives the following results (ignoring the numerical factor n_μ/g):

On $a(0)$:

$$P_1^{(A_1)}a(0) = 2[a(0) + a(1) + a(2) + a(3) + a(4) + a(5)].$$

On $b^+(0)$:

$$P_1^{(A_1)}b^+(0) = b^+(0) + b^+(1) + b^+(2) + b^+(3) + b^+(4) + b^+(5) + b^-(0) + b^-(1) + b^-(2) + b^-(3) + b^-(4) + b^-(5).$$

On $c^+(0)$:

$$P_1^{(A_1)}c^+(0) = c^+(0) + c^+(1) + c^+(2) + c^+(3) + c^+(4) + c^+(5) + c^-(0) + c^-(1) + c^-(2) + c^-(3) + c^-(4) + c^-(5).$$

We readily see that

$$\begin{aligned}
P_1^{(A_1)}a(0) &= P_1^{(A_1)}a(1) = \cdots = P_1^{(A_1)}a(5) \\
P_1^{(A_1)}b^+(0) &= P_1^{(A_1)}b^+(1) = \cdots = P_1^{(A_1)}b^+(5) \\
&= P_1^{(A_1)}b^-(0) = P_1^{(A_1)}b^-(1) = \cdots = P_1^{(A_1)}b^-(5) \\
P_1^{(A_1)}c^+(0) &= \cdots = P_1^{(A_1)}c^+(5) \\
&= P_1^{(A_1)}c^-(0) = \cdots = P^{(A_1)}c^-(5)
\end{aligned} \tag{7}$$

This means that the components of the eigenvectors of A corresponding to the A_1 representation must take the form given by (7).

Conversely, by making the substitutions

$$\begin{aligned}
a(1) &= a(1) = \cdots = a(5) \\
b^+(0) &= b^+(1) = \cdots = b^+(5) \\
&= b^-(0) = b^-(1) = \cdots = b^-(5) \\
c^+(0) &= c^+(1) = \cdots = c^+(5) \\
&= c^-(0) = c^-(1) = \cdots = c^-(5)
\end{aligned} \tag{8}$$

we should be able to obtain all the eigenvectors corresponding to the A_1 representation. But these substitutions also effectively reduce the 30×30 matrix A to a 3×3 matrix. If we consider in a similar way other representations, we are then provided with a systematic calculus for obtaining a set of reduced matrices the eigenvalues of which exhaust all possible eigenvalues of A (it will be noted that the eigenvalues corresponding to the E representations are doubly degenerate). It should be pointed out that in general the set of reduced matrices can be further reduced due to the "symmetry of constraints" which arises, because as far as excluding polygons of up to r vertices is concerned, some different types of walks may be considered as equivalent. Details of this kind of symmetry will not be discussed here.

It is now clear that this method can be applied to walks of any order. For walks on other lattices the appropriate symmetry group must be considered. For example, for walks on the square lattice the symmetry group C_{4v} must clearly be considered, and the general result in this case is very similar to that for the plane triangular lattice. The usefulness of the group theoretical method described above becomes more apparent and striking in the three-dimensional case, for while the substitutions, Eq. (4), for the two-dimensional case might have been guessed at without using group theory, the appropriate substitutions for the three-dimensional case, aside from the identity representation, are difficult to conceive intuitively.

The group theoretical method which we just outlined can be described more generally. Let us denote a particular type of walk by $a(1)$, and let a set of symmetry operators $O_{R_1}, O_{R_2}, \ldots, O_{R_g}$ of a group G of g elements generate all its possible orientations, namely $O_{R_k}a(1) = a(k)$, $k = 1, 2, \ldots, g$. Defining a projection operator by Eq. (5), and denoting $P_i^{(\mu)}/n_\mu$ by P_i and $D_{ii}^{(\mu)}$ by D_{ii} for convenience of notation, we write

$$\begin{aligned} P_i a(1) &= D_{ii}(R_1^{-1})O_{R_1}a(1) + D_{ii}(R_2^{-1})O_{R_2}a(1) + \cdots + D_{ii}(R_g^{-1})O_{R_g}a(1) \\ P_i a(2) &= D_{ii}(R_1^{-1})O_{R_1}a(2) + D_{ii}(R_2^{-1})O_{R_2}a(2) + \cdots + D_{ii}(R_g^{-1})O_{R_g}a(2) \\ &\cdots \\ P_i a(g) &= D_{ii}(R_1^{-1})O_{R_1}a(g) + D_{ii}(R_2^{-1})O_{R_2}a(g) + \cdots + D_{ii}(R_g^{-1})O_{R_g}a(g) \end{aligned} \tag{9}$$

If in $P_i a(p)$ and $P_i a(q)$, say, we find

$$O_{R_u}a(p) = O_{R_v}a(q)$$

then

$$O_{R_u}O_{R_p} = O_{R_v}O_{R_q} \tag{10}$$

Suppose that the matrix representation $D(R_i)$, $i = 1, 2, \ldots, g$, has the property that every row and column of the matrix has only one nonzero element; then if $D_{ii}(R_u^{-1}) \neq 0$ and $D_{ii}(R_v^{-1}) \neq 0$, we have

$$\frac{D_{ii}(R_u^{-1})}{D_{ii}(R_v^{-1})} = \frac{D_{ii}(R_p R_q^{-1} R_v^{-1})}{D_{ii}(R_v^{-1})} = D_{ii}(R_p R_q^{-1}) \tag{11}$$

which is independent of u and v. We then find that $P_i a(p)$ is simply related to $P_i a(q)$ by

$$\frac{P_i a(p)}{P_i a(q)} = D_{ii}(R_p R_q^{-1}) \tag{12}$$

The general procedure for finding the appropriate substitutions for our matrix reduction is therefore as follows.

We start with $a(1)$ and "relate" all those $a(m)$ for which $D_{ii}(R_m) \neq 0$ by the relation

$$P_i a(m) = D_{ii}(R_m) P_i a(1) \tag{13}$$

Suppose $D_{ii}(R^{-1}) = 0$ for $R = R_{i_1}, R_{i_2}, \ldots, R_{i_h}$; then we start again with $a(i_1)$ and consider

$$P_i a(i_1) = \sum_{k=1}^{g} D_{ii}(R_k^{-1}) O_{R_k} a(i_1) \tag{14}$$

It is easy to show that $P_i a(i_1)$ has no nonzero term in common with any of the nonzero terms of $P_i a(1)$, for if in (14) we have $O_{R_p}a(i_1) \equiv O_{R_p}O_{R_{i_1}}a(1) =$ one of the nonzero terms appearing in $P_i a(1)$, $a(s)$ say, with $D_{ii}(R_s^{-1}) \neq 0$, then $O_{R_p}O_{R_{i_1}} = O_{R_s}$ and $O_{R_p} = O_{R_s}O_{R_{i_1}}^{-1}$. But since $D_{ii}(R_{R_{i_1}}^{-1}) = 0$ by assumption, and $D(R_i)$, $i = 1, 2, \ldots, g$, has the property that every row and column of the matrix has only one nonzero element, then $D_{ii}(R_{i_1}) = 0$; hence $D_{ii}(R_p) = 0$ and $D_{ii}(R_p^{-1}) = 0$ and the term containing $a(s)$ does not appear in Eq. (14). Continuing in this way, the set of $P_i a(m)$, $m = 1, 2, \ldots, g$, will be subsequently divided into one or more classes whereby the members in each of the classes are simply related to each other.

It becomes clear that the possibility of the existence of a simple substitution such as Eq. (4) depends on whether for the given representation of the group a matrix representation can be found such that for every element of the group the matrix has the property that every row and column has only one nonzero element. If this is the case, we say that the given representation of the group can be truthfully represented. It is known that every representation of the crystal point groups can be truthfully represented. The situation, however, is less clear regarding a general symmetric group (every one-dimensional representation of a group is, of course, a truthful representation).

3. CORRELATIONS AMONG THE STEPS

Consider a walk of n steps and let us denote the individual step vectors (of unit length) by $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n$. If the vector from the origin to the endpoint of the walk is denoted by $\mathbf{R}_n$ say, then

$$\mathbf{R}_n = \mathbf{u}_1 + \mathbf{u}_2 + \cdots + \mathbf{u}_n \tag{15}$$

The correlation $\langle \mathbf{u}_i \mathbf{u}_j \rangle$ between the ith and jth steps is defined by

$$\langle \mathbf{u}_i \mathbf{u}_j \rangle_n = \left(\sum \mathbf{u}_i \cdot \mathbf{u}_j\right) / c_n \tag{16}$$

where the summation of the scalar product of the vectors $\mathbf{u}_i$ and $\mathbf{u}_j$ is taken over all possible n-step walks of the given order, and c_n is the total number of n-step walks of the given order. For an unrestricted random walk all $\langle \mathbf{u}_i \mathbf{u}_j \rangle_n = 0$ for $i \neq j$. For walks excluding reversals it is easy to show that $\langle \mathbf{u}_s \mathbf{u}_{s+t} \rangle_n = 1/(q-1)^t$, $t \geqslant 1$, where q denotes the lattice coordination number. For a restricted walk of order r ($\geqslant 3$) the correlation can be expressed in terms of the eigenvalues and eigenvectors of the full transition matrix corresponding to the walk, which we now wish to show.

Our problem is to find the number of n-step walks the sth step of which ends in type l, say, and the $(s + t)$th step of which ends in type m, say. If this number is $c_n(s, s + t)$, and if the sth step vector ending in type l is expressed in Cartesian coordinates by $(x_s(l), y_s(l), z_s(l))$ and the $(s + t)$th step vector ending in type m is expressed by $(x_{s+t}(m), y_{s+t}(m), z_{s+t}(m))$, then the correlation between the sth step and the $(s + t)$th step is defined by

$$\langle \mathbf{u}_s \mathbf{u}_{s+t} \rangle_n = c_n^{-1} \sum_l \sum_m c_n(s, s+t)\{x_s(l)x_{s+t}(m) + y_s(l)y_{s+t}(m) + z_s(l)z_{s+t}(m)\} \tag{17}$$

where c_n is the total number of n-step walks.

Let us first consider the case when $s \geqslant r - 1$ and $s + t > r - 1$, where r is the order of the finite walk. We bear in mind that when a walk of order r is considered we start by considering all possible $(r - 1)$-step walks.

Let $\mathbf{w}_s$ be the number of walks at the sth step. $\mathbf{w}_s$ can be expressed in terms of the eigenvalues λ_i and the right-hand eigenvectors $\boldsymbol{\phi}_i$ and the left-hand eigenvectors $\boldsymbol{\psi}_i$ of A by

$$\mathbf{w}_s = \sum_i C_i \lambda_i^s \boldsymbol{\phi}_i \tag{18}$$

where

$$C_i = \mathbf{w}_{r-1} \cdot \boldsymbol{\psi}_i / \lambda_i^{r-1}$$

Let $\mathbf{w}_s^{(l)}$ denote the vector obtained from $\mathbf{w}_s$ by putting all its components zero except the lth. Then if we express $\mathbf{w}_s^{(l)}$ in terms of λ_k and $\boldsymbol{\phi}_k$, we have

$$\mathbf{w}_s^{(l)} = \sum_{k=1}^{N} d_k \lambda_k^s \boldsymbol{\phi}_k \tag{19}$$

where

$$d_k = \psi_k(l) \mathbf{w}_s(l) / \lambda_k^s = [\psi_k(l)/\lambda_k^s] \sum_i C_i \lambda_i^s \phi_i(l)$$

[we have denoted the lth component of a vector $\mathbf{V}$, say, by $\mathbf{V}(l)$]. Starting with walks the sth step of which ends in type l, the numbers of walks at the $(s + t)$th step ending in various types are given by the components of the vector $\mathsf{A}^t \mathbf{w}_s^{(l)}$. Thus

$$\mathsf{A}^t \mathbf{w}_s^{(l)} = \sum_{k=1}^{N} d_k \lambda_k^{s+t} \boldsymbol{\phi}_k = \sum_{k=1}^{N} \psi_k(l) \left[\sum_i C_i \lambda_i^s \phi_i(l) \right] \lambda_k^t \boldsymbol{\phi}_k \tag{20}$$

If we pick out the walks ending in type m, then

$$(\mathsf{A}^t \mathbf{w}_s^{(l)})^{(m)} = \sum_{k=1}^{N} f_k \lambda_k^{s+t} \boldsymbol{\phi}_k \tag{21}$$

where

$$f_k = \frac{\psi_k(m)}{\lambda_k^{s+t}} (\mathsf{A}^t \mathbf{w}_s^{(l)})(m) = \frac{\psi_k(m)}{\lambda_k^{s+t}} \sum_{p=1}^{N} \psi_p(l) \left[\sum_i C_i \lambda_i^s \phi_i(l) \right] \lambda_p^t \phi_p(m)$$

We now start with walks the $(s + t)$th step of which ends in type m (the sth step of which ends in type l) and obtain the numbers of walks after $n =$

$s + t + q$ steps ending in various types by multiplying $(\mathsf{A}^t\mathbf{w}_s^{(l)})^{(m)}$ by A^q, that is

$$\begin{aligned}\mathsf{A}^q(\mathsf{A}^t\mathbf{w}_s^{(l)})^{(m)} &= \sum_{k=1}^{N} f_k\lambda_k^{s+t+q}\boldsymbol{\phi}_k \\ &= \sum_{k=1}^{N} \psi_k(m)\lambda_k^{q}\boldsymbol{\phi}_k \sum_{p=1}^{N} \psi_p(l)\Big[\sum_i C_i\lambda_i^{s}\boldsymbol{\phi}_i(l)\Big]\lambda_p^{t}\boldsymbol{\phi}_p(m) \qquad (22)\end{aligned}$$

This gives the numbers of walks after n steps ending in various types, the sth step being of type l and the $(s + t)$th step being of type m. The sum of all its components is then the number $c_n(s, s + t)$ we require.

For $s \geqslant r - 1$ and $s + t > r - 1$ the step vectors are $x_s(l) = x_{s+t}(l) = x_{r-1}(l)$, and similarly for y and z, i.e., the step vectors are defined by the last steps of all the $(r - 1)$-step walks which specify the various endings of the walks. The correlation between the sth step and the $(s + t)$th step when the total number of steps is n is therefore given by

$$\begin{aligned}\langle \mathbf{u}_s\mathbf{u}_{s+t}\rangle_{n=s+t+q} = &\Big\{\sum_l\sum_m\Big[\sum_i \psi_i(m)\lambda_i^{q}(\mathbf{1}\cdot\boldsymbol{\phi})\Big]\Big[\sum_j \psi_j(l)\lambda_j^{t}\boldsymbol{\phi}_j(m)\Big] \\ &\times\Big[\sum_i C_i\lambda_i^{s}\boldsymbol{\phi}_i(l)\Big][x(l)x(m) + y(l)y(m) + z(l)z(m)]\Big\} \\ &\times\Big(\sum_i C_i\lambda_i^{n}\Big)^{-1} \qquad \text{for} \quad s \geqslant r-1, \quad s+t > r-1\end{aligned} \qquad (23)$$

where for simplicity we have denoted the components of the $(r - 1)$th step vector of the walk of type l by $x(l), y(l), z(l)$.

If $s < r - 1$, the formula giving the distribution of walks $\sum_i C_i\lambda_i^s\boldsymbol{\phi}_i(l)$ is no longer valid. But if $s + t > r - 1$, we may very well start off with the $(r - 1)$-step walks and simply replace formula (23) by the following one:

$$\begin{aligned}&\langle \mathbf{u}_s\mathbf{u}_{s+t}\rangle_{n=s+t+q} \\ &\quad= \Big\{\sum_l\sum_m\Big[\sum_i \psi_i(m)\lambda_i^{q}(\mathbf{1}\cdot\boldsymbol{\phi}_i)\Big]\Big[\sum_j \psi_j(l)\lambda_j^{s+t-(r-1)}\boldsymbol{\phi}_j(m)\Big] \\ &\quad\times\Big[\sum_i C_i\lambda_i^{r-1}\boldsymbol{\phi}_i(l)\Big][x_s(l)x(m) + y_s(l)y(m) + z_s(l)z(m)]\Big\} \\ &\quad\times (C_i\lambda_i^{n})^{-1} \qquad \text{for} \quad s < r-1, \quad s+t > r-1 \qquad (24)\end{aligned}$$

where $x_s(l)$, $y_s(l)$, and $z_s(l)$ are now defined by the sth step vectors of the walk. Since $s + t > r - 1$, then $z(m)$ are defined as before by the last steps of all the $(r - 1)$-step walks.

If $s < r - 1$ and $s + t \leqslant r - 1$, we may again begin by considering all $(r - 1)$-step walks and then obtain the number of walks after n steps the $(r - 1)$th step of which ends in type l, say. Since $s < r - 1$ and $s + t \leqslant r - 1$, this is equivalent to saying that we want to obtain the number of walks after n steps, the sth step of which ends in type l, the $(s + t)$th step of which also ends in type l. Thus we have

$$\mathbf{w}_{r-1} = \sum_i C_i \lambda_i^{r-1} \boldsymbol{\phi}_i \tag{25}$$

$$\mathbf{w}_{r-1}^{(l)} = \sum_{k=1}^{N} d_k \lambda_k^{r-1} \boldsymbol{\phi}_k,$$

$$d_k = \frac{\boldsymbol{\psi}_k(l)\mathbf{w}_{r-1}(l)}{\lambda_k^{r-1}} = \frac{\boldsymbol{\psi}_k(l)}{\lambda_k^{r-1}} \sum_i C_i \lambda_i^{r-1} \boldsymbol{\phi}_i(l) \tag{26}$$

Therefore

$$\mathsf{A}^{n-(r-1)} \mathbf{w}_{r-1}^{(l)} = \sum_{k=1}^{N} d_k \lambda_k^{n} \boldsymbol{\phi}_k = \sum_{k=1}^{N} \boldsymbol{\psi}_k(l) \left[\sum_i C_i \lambda_i^{r-1} \boldsymbol{\phi}_i(l) \right] \lambda_k^{n-(r-1)} \boldsymbol{\phi}_k \tag{27}$$

The correlation is therefore given by

$$\begin{aligned} \langle \mathbf{u}_s \mathbf{u}_{s+t} \rangle_{n=s+t+q} = & \left\{ \sum_l \left[\sum_i \boldsymbol{\psi}_i(l) \lambda_i^{n-(r-1)} (\mathbf{1} \cdot \boldsymbol{\phi}_i) \right] \left[\sum_i C_i \lambda_i^{r-1} \boldsymbol{\phi}_i(l) \right] \right. \\ & \left. \times \left[x_s(l) x_{s+t}(l) + y_s(l) y_{s+t}(l) + z_s(l)\, z_{s+t}(l) \right] \right\} \\ & \times \left(\sum_i C_i \lambda_i^{n} \right)^{-1} \qquad \text{for} \quad s < r - 1, \quad s + t \leqslant r - 1 \end{aligned} \tag{28}$$

where $x_s(l)$, $y_s(l)$, $z_s(l)$ and $x_{s+t}(l)$, $y_{s+t}(l)$, $z_{s+t}(l)$ are defined respectively by the sth and $(s + t)$th steps of the walk.

We have thus derived the exact expressions for the correlation between any two steps in a restricted walk of order r [Eqs. (23), (24), and (28)] in terms of the eigenvalues and eigenvectors of the full transition matrix A corresponding to the walk. We now wish to show that not all eigenvalues of A contribute to the correlations. In fact we have deliberately labeled the summations over the eigenvalues by two different indices i and j in Eqs. (23), (24), and (28) and we wish to show that (a) the summation $\sum_i$ need only be taken over the eigenvalues corresponding to the identity representation, and (b) the summation $\sum_j$ need only be taken over the eigenvalues corresponding to the "maximal" representation, which is the E representation for group C_{4v}, the E_1 representation for group C_{6v}, the F_1 representation for group O, and the $F_1^{(-)}$ representation for group O_h. The eigenvalues and eigenvectors corresponding to other representations of the group are, as far as the correlations among the steps of the walks are concerned, completely irrelevant. To show this, let us first consider a two-dimensional case such as the plane triangular lattice. The components of the eigenvectors are of the form $(a, \omega_s a, \omega_s^2 a, \omega_s^3 a, \omega_s^4 a, \omega_s^5 a;\ b, \omega_s b, \omega_s^2 b, \omega_s^3 b, \omega_s^4 b, \omega_s^5 b; \ldots)$, where $\omega_s = e^{2\pi i s/6}$. The first and the third brackets of (23) involve the sum over all components $(\mathbf{1}\cdot\boldsymbol{\phi}_i)$ and $C_i = (\mathbf{1}\cdot\boldsymbol{\psi}_i)$ and it immediately follows that only those eigenvalues corresponding to the identity representation ($\omega_0 = 1$) contribute, because

$$\sum_{t=0}^{5} \omega_s^{\,t} = \sum_{t=0}^{5} e^{2\pi i t s/6} = 0 \qquad \text{if} \quad s \neq 0 \tag{29}$$

To show that the second bracket $[\sum_j \boldsymbol{\psi}_j(l)\lambda_j^{\,t}\boldsymbol{\phi}_j(m)]$ need only be summed over the eigenvalues corresponding to the E_1 representation, let us rearrange the sum in (23) and consider the sum

$$\sum_m \boldsymbol{\psi}_i(m)x(m)\boldsymbol{\phi}_j(m) \tag{30}$$

where i, as we have just shown, refers to the eigenvector corresponding to the identity representation which is of the form $(a, a, a, a, a, a;\ b, b, b, b, b, b; \ldots)$. From the relation

$$\sum_{t=0}^{5} e^{2\pi i t s/6} \cos(2\pi t/6) = 0 \qquad \text{unless} \quad s = 1 \quad \text{or} \quad -1 \tag{31}$$

it readily follows that the summation over j need only be taken over the eigenvalues corresponding to the E_1 representation ($\omega_1 = e^{2\pi i/6}$, $\omega_5 = e^{-2\pi i/6}$).

It is clear that the relations (29) and (31) are connected with the orthogonality of different representations of a group. In Eq. (30), for example, one sees that only those $\boldsymbol{\phi}_j(m)$ whose components "transform" in the same way as the components of $x(m)$ give a nonzero contribution. The meaning of the maximal representation of a group also becomes apparent: It is the representation that "generates" all the possible orientations of a particular type of walk.

Generally, let us consider a particular type of walk $a(1)$, and let a set of symmetry operators $O_{R_1}, O_{R_2}, \ldots, O_{R_g}$ of a group G of g elements generate all its possible orientations, namely $O_{R_k}a(1) = a(k)$, $k = 1, 2, \ldots, g$. If we consider

$$\sum_m \boldsymbol{\psi}_i(m)x(m)\boldsymbol{\phi}_j(m) \tag{32}$$

where the sum is taken over all possible orientations of a particular component, then since $\boldsymbol{\psi}_i(1) = \boldsymbol{\psi}_i(2) = \cdots = \boldsymbol{\psi}_i(g)$, (32) becomes

$$\boldsymbol{\psi}_i(1) \sum_{m=1}^{g} x(m)\boldsymbol{\phi}_j(m) \tag{33}$$

If ϕ_j belongs to the lth row of the μ representation, say, then

$$\phi_j(m) = (n_\mu/g) \sum_{k=1}^{g} D_{il}^{(\mu)}(R_k^{-1}) O_{R_k} a(m) \tag{34}$$

(33) becomes

$$(n_\mu/g)\psi_i(1) \sum_{m=1}^{g} x(m) \left[\sum_{k=1}^{g} D_{il}^{(\mu)}(R_k^{-1}) O_{R_k} a(m) \right] \tag{35}$$

Let us first collect the term containing $a(1)$, say, in Eq. (35). The coefficient of $a(1)$ is readily seen to be given by

$$[n_\mu \psi_i(1)/g] \sum_{m=1}^{g} x(m) D_{il}^{(\mu)}(R_m) \tag{36}$$

It follows from the orthogonality relation

$$(n_\mu/g) \sum_R D_{il}^{(\mu)}(R) D_{jm}^{(\nu)}(R^{-1}) = \delta_{\mu\nu}\delta_{ij}\delta_{lm}$$

that (36) is zero unless μ corresponds to the maximal representation of the group [which is the representation that generates all the possible orientations $a(1), a(2),..., a(g)$]. Similarly, by collecting the terms containing $a(2), a(3), ..., a(g)$ and noting that $D^{(\mu)}(R_i)$, $i = 1, 2,..., g$, are truthful matrices, it can be readily shown that only those eigenvalues corresponding to the maximal representation of the group contribute to (32). That only the eigenvalues corresponding to the identity representation contribute to $(\mathbf{1}\cdot\phi_i)$ and $C_i = (\mathbf{1}\cdot\psi_i)$ can be readily proved in a similar fashion.

4. DISTRIBUTION OF EIGENVALUES

The various results and formulas derived in the preceding sections are exact. To proceed further, we must consider the eigenvalues corresponding to the identity and the maximal representations. The distributions of eigenvalues corresponding to the identity representation have been studied in Ref. 7 for walks of various orders on the plane triangular and fcc lattices, and the remarkable features of these distributions were already summarized in the introduction of this paper. The largest eigenvalue, as was pointed out, is not only well separated from the others, but also predominates over the rest of the eigenvalues since these are distributed symmetrically about the origin. If we replace the summation $\sum_i$ in Eq. (23) by the largest term alone, the expressions for the correlations simplify considerably and $\langle \mathbf{u}_s \mathbf{u}_{s+t} \rangle_n$ becomes

$$\langle \mathbf{u}_s \mathbf{u}_{s+t} \rangle_n \approx \sum_j b_j (\lambda_j/\lambda_1)^t \qquad \text{for} \quad s \geq r-1, \quad s+t > r-1 \tag{37}$$

where λ_1 is the largest eigenvalue corresponding to the identity representation (which is also the largest eigenvalue of the full transition matrix corresponding to the walk) and

$$b_j = \sum_{x,y,z} \left[\sum_m \psi_1(m)x(m)\phi_j(m)\right]\left[\sum_l \psi_j(l)x(l)\phi_1(l)\right] \tag{38}$$

The summation $\sum_j$ is taken over the eigenvalues corresponding to the maximal representation. Remembering the dependence on r, the order of the walk, we write

$$\langle \mathbf{u}_s\mathbf{u}_{s+t}\rangle_{n(r)} \approx \sum_j b_{jr}(\lambda_{jr}/\lambda_{1r})^t, \qquad s \geqslant r-1, \quad s+t > r-1 \tag{39}$$

It should be remembered that the eigenvalues corresponding to the maximal representation are doubly degenerate in two dimensions and triply degenerate in three dimensions. If the two steps are separated by a large number of steps, the correlation $\langle \mathbf{u}_s\mathbf{u}_{s+t}\rangle_{n(r)}$ is clearly given by

$$\langle \mathbf{u}_s\mathbf{u}_{s+t}\rangle_{n(r)} \approx b_{j_1r}(\lambda_{j_1r}/\lambda_{1r})^t \tag{40}$$

where λ_{j_1r} is the largest eigenvalue corresponding to the maximal representation. The question naturally arises as to how the largest term in (39) accounts for the total contribution to the correlation when t is small. The distribution of eigenvalues corresponding to the maximal representation, plotted in a complex plane, is found to show a certain pattern common to all the lattices and to all r we have studied. The eigenvalues corresponding to the E_1 representation for walks of order $r = 5$ on the plane triangular lattice and the eigenvalues corresponding to the $F_1^{(-)}$ representation for walks of order $r = 4$ are given in Tables III and IV, and they are plotted in Figs. 1 and 2.

Table III. Eigenvalues Corresponding to the E_1 Representation for Walks of Order $r = 5$ on the Plane Triangular Lattice

2.668007	0.401820 + 0.576490i
0.500000 + 0.866025i	0.401820 − 0.576490i
0.500000 − 0.866025i	−0.652150 + 1.039107i
0.393602 + 0.706476i	−0.652150 − 1.039107i
0.393602 − 0.706476i	−0.724073 + 0.705563i
0.837042 + 1.180631i	−0.724073 − 0.705563i
0.837042 − 1.180631i	−0.870251
0.884545 + 0.421829i	−1.084904
0.884545 − 0.421829i	−1
0.002788 + 0.891345i	−1
0.002788 − 0.891345i	
and four small complex eigenvalues close to the origin	

Table IV. Eigenvalues Corresponding to the F_1^- Representation for Walks of Order $r = 4$ on the fcc Lattice

3.527318	0.835595 + 0.399451i
0.410592 + 1.792721i	0.835595 − 0.399451i
0.419592 − 1.792721i	0.887667 + 0.166149i
−1.498032 + 0.404895i	0.887667 − 0.166149i
−1.498032 − 0.404895i	0.007733 + 0.948202i
−1.114717 + 0.681990i	0.007733 − 0.948202i
−1.114717 − 0.681990i	0.093972 + 0.746236i
0.937353 + 0.803726i	0.093972 − 0.746236i
0.937353 − 0.803726i	−1
1.385121	−0.067426 + 0.461243i
−1.209516 + 0.210059i	−0.067426 − 0.461243i
−1.209516 − 0.210059i	0.373989
	−0.426435 + 0.199072i
	−0.426435 − 0.199072i

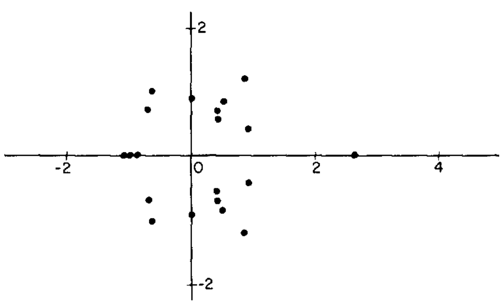


Fig. 1. Distribution of eigenvalues corresponding to the E_1 representation for walks of order $r = 5$ on the plane triangular lattice.

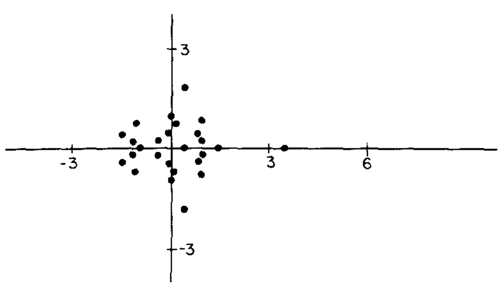


Fig. 2. Distribution of eigenvalues corresponding to the $F_1^{(-)}$ representation for walks of order $r = 4$ on the fcc lattice.

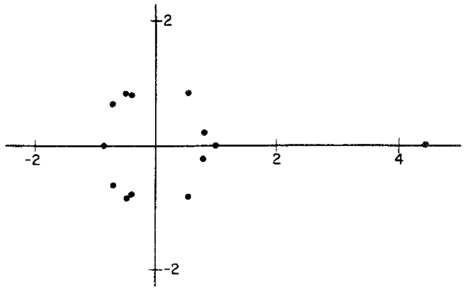


Fig. 3. Distribution of eigenvalues corresponding to the A_1 representation for walks of order $r = 5$ on the plane triangular lattice.

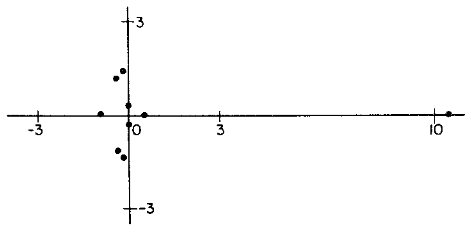


Fig. 4. Distribution of eigenvalues corresponding to the A_1 representation for walks of order $r = 4$ on the fcc lattice.

These distribution diagrams are seen to be strikingly similar to the distributions of eigenvalues corresponding to the identity representation, which are shown on the same scale in Figs. 3 and 4. They show the remarkable features characterized by (a) the largest eigenvalue is real, distinct, and well separated from the others, and (b) the rest of the eigenvalues are rather symmetrically distributed about the origin. This suggests that the contribution to the correlation $\langle \mathbf{u}_s \mathbf{u}_{s+t} \rangle_{n(r)}$ in Eq. (39) comes predominantly from the largest eigenvalue in j even for small t. This is indeed supported by our available numerical data. The correlations among the steps of a restricted walk of order r are thus characterized by the ratio $\lambda_{j_1 r}/\lambda_{1r}$. At this point one naturally suspects that $\lambda_{j_1 r}$ is the second largest eigenvalue of the full transition matrix. While the proof that λ_{1r} is real and is the largest eigenvalue of our nonnegative full transition matrix follows immediately from the Peron–Frobenius theorem (see, e.g., Ref. 10), a rigorous proof that $\lambda_{j_1 r}$ is real and is the second largest eigenvalue of our full transition matrix is lacking, although our numerical data do suggest that this is the case. The distribution of eigenvalues corresponding to every representation of the full transition matrix for walks of orders $r = 4$ and 5 on the plane triangular lattice is presented on the same scale in Fig. 5. It is interesting to note that none of the distribution of eigenvalues

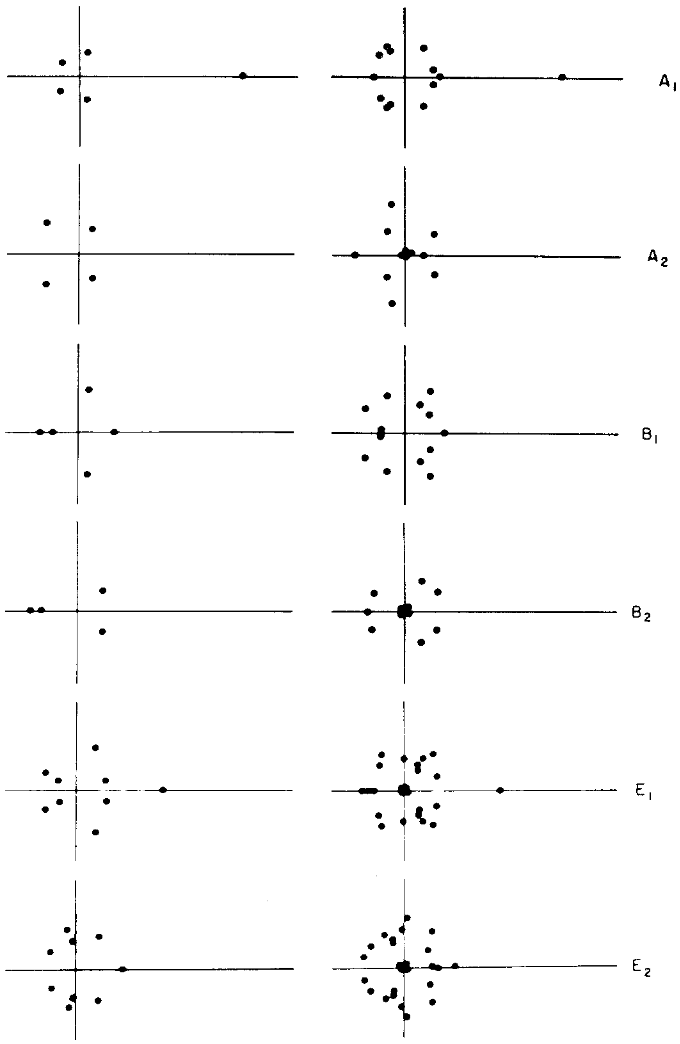


Fig. 5. Distributions of eigenvalues corresponding to all representations (A_1, A_2, B_1, B_2, E_1, and E_2) of the full transition matrix for walks of orders r = 4 and 5 on the plane triangular lattice.

corresponding to representations other than the A_1 (identity) and E_1 (maximal) representations has a distinct eigenvalue well separated from the others.

Let us now consider the ratio $\lambda_{j_1r}/\lambda_{1r}$, which characterizes the correlations, and consider its dependence on r. The values of $\lambda_{j_1r}/\lambda_{1r}$ as well as the values of λ_{1r} and λ_{j_1r} up to $r = 7$ for walks on the plane triangular lattice

Table V. Values of λ_{1r}, λ_{j_1r}, and $\lambda_{j_1r}/\lambda_{1r}$ for Plane Triangular Lattice

r	λ_{1r}	λ_{j_1r}	$\lambda_{j_1r}/\lambda_{1r}$
1	6.000000	0.000000	0.000000
2	5.000000	1.000000	0.200000
3	4.645751	2.000000	0.430501
4	4.506407	2.426253	0.538401
5	4.433593	2.668007	0.601771
6	4.386422	2.843906	0.648343
7	4.353059	2.982805	0.685220

Table VI. Values of λ_{1r}, λ_{j_1r}, and $\lambda_{j_1r}/\lambda_{1r}$ for the fcc Lattice

r	λ_{1r}	λ_{j_1r}	$\lambda_{j_1r}/\lambda_{1r}$
1	12.000000	0.000000	0.000000
2	11.000000	1.000000	0.090909
3	10.656854	2.485584	0.233238
4	10.489137	3.527318	0.336283
5	10.392318	$\sim$ 4.36	$\sim$ 0.42

(for which the reduced transition matrix corresponding to the E_1 representation is of order 260) and up to $r = 5$ for walks on the fcc lattice (for which the reduced matrix corresponding to the $F_1^{(-)}$ representation is of order 170) are presented in Tables V and VI, and they are plotted against $1/r$ in Fig. 6. It will be observed that the values of $\lambda_{j_1r}/\lambda_{1r}$ increase rather rapidly as r increases. Using the procedure developed by Domb and Sykes,[(11)] let us consider the increasing sequence of $\lambda_{j_1r}/\lambda_{1r}$ against $1/r$ and take the successive linear extrapolations and examine the points where these extrapolations cut the $\lambda_{j_1r}/\lambda_{1r}$ axis (corresponding to $r = \infty$). For the plane triangular lattice the intercepts are found to be 0.400000, 0.891503, 0.862101, 0.855251, 0.881203, 0.906482,..., and for the fcc lattice the intercepts are 0.181818, 0.517896, 0.645418, 0.75...,.... These values appear to us to be approaching one as $r \to \infty$, which, as is well known, would signify the onset of long-range order. Since it is of considerable importance to know whether the limit of $\lambda_{j_1r}/\lambda_{1r}$ as $r \to \infty$ is really equal to one or less than one, we believe that more data would be helpful in deciding this point.

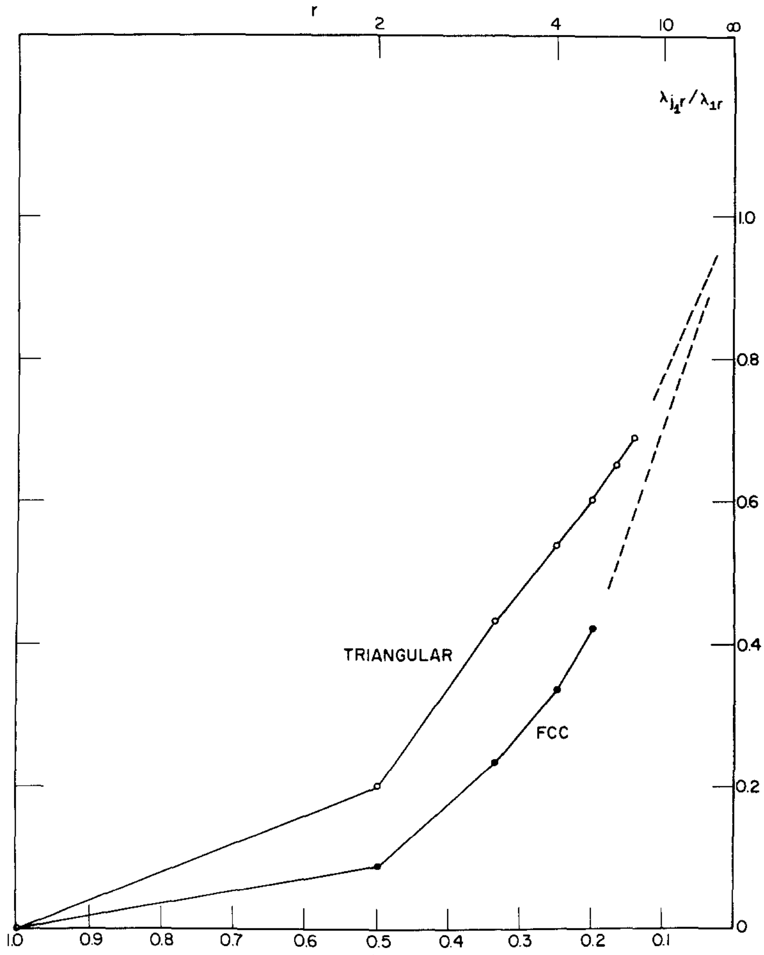


Fig. 6. Plots of $\lambda_{j_1r}/\lambda_{1r}$ vs. $1/r$ for the plane triangular lattice and the fcc lattice.

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