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LETTER TO THE EDITOR

Matrix method for random walks on lattices

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Abstract. By defining a structure factor matrix we propose a generating function matrix method for studying random walks on a class of lattices, such as superlattices or crystals with finite k atoms per cell. As an illustration of this method, the problem of random walks on a one-dimensional dimerization chain is solved exactly.

It is well known that random walk theory has been applied to many fields of science and technology ranging from astronomy and solid state physics to polymer chemistry and biology. Many problems such as diffusion, Brownian motion, lattice vibrations, spin waves, polymer in solution, chemistry kinetics and so on can be related to random walks [1–4]. A simple model of random walk is the lattice walk proposed by Polya [5]. A systematic generating function scheme for dealing with lattice walks has been established [6–8]. However, one is only able to use this generating function method to study random walks on some simple regular networks. Analytic methods applied to the problem of random walks on irregular networks are obviously needed and have been considered by Goldhirsch and Gefen [9, 10]. In this letter we will define a structure factor matrix and generalize the generating function method to study random walks on a class of complex networks, namely those consisting of a finite number k of translated copies of a given lattice. In more elementary words, such a network may be a superlattice or a lattice with k atoms per cell.

The elementary quantity of lattice walks is the probability $P_n(J, I)$ that the walker starts from point(vector) I and is at J after n steps. For simple regular networks, the probability distribution $f(J, I)$ depends only on the difference of its arguments

$$f(J, I) = f(J - I) \tag{1}$$

and one can define a function by an identical distribution $f(I)$:

$$S(\Omega) = \sum_I f(I) e^{i\Omega \cdot I} \tag{2}$$

which is called the structure factor of the walk [1]. With $S(\Omega)$ the generating function technique can be used conveniently. For complex networks, however, equation (1) is untenable and one cannot define the structure factor by equation (2). The generating function scheme seems to be powerless.

Consider an infinitely d-dimensional complex network. In general, the probability distribution $f(J, I)$ is a function of both I and J and it does not satisfy equation (1). However, if we can divide all lattice points into k categories provided that the lattice points belonging to the same category are translationally invariant. Then, given $i (i = 1, 2, ..., k)$, for all I_i one has

$$f(I, I_i) = f^i(I - I_i) \tag{3}$$

where $f^i(I - I_i)$ denotes the probability distribution of category i. Furthermore, equation (3) satisfies

$$\sum_{I'} f(I, I') = \sum_{i=1} \sum_{I'_i} f^i(I - I'_i). \tag{4}$$

To use the generating function technique, we introduce a structure factor matrix $\hat{S}(\Omega)$ with its elements defined by

$$S_{ij}(\Omega) = \sum_{I_j} f^i(I_j - I_i) e^{i\Omega \cdot (I_j - I_i)} \qquad (i, j = 1, 2, \ldots, k) \tag{5}$$

where the summation are over all the lattice vectors of category j. Given i and j, one can see from equation (5) that $S_{ij}(\Omega)$ can be determined solely.

We now turn to the derivation of the probability $P_n(J, I)$ that the walker starts from I and is at J after n steps. Note that $P_n(J, I)$ satisfies the difference equation

$$P_{n+1}(J, I) = \sum_{I'} f(J, I') P_n(I', I). \tag{6}$$

In order to solve equation (6) we define the generating function

$$P(J, I, Z) = \sum_{n=0}^{\infty} P_n(J, I) Z^n \tag{7}$$

and the transformed generating function

$$G(\Omega, I, Z) = \sum_{J} P(J, I, Z) e^{i\Omega \cdot J} \tag{8}$$

respectively. For convenience, we write the transformed generating function in another form

$$G(\Omega, I, Z) = \sum_{n=0}^{\infty} P_n(\Omega, I) Z^n \tag{9}$$

where

$$P_n(\Omega, I) = \sum_{J} P_n(J, I) e^{i\Omega \cdot I} \tag{10}$$

is the characteristic function of $P_n(J, I)$. To derive $P_n(J, I)$, consider first the probability $P_n(J_j, I)$ that the walker starts from I and is at J_j of category j after n steps. $P_n(J_j, I)$ also satisfies the difference equation

$$P_{n+1}(J_j, I) = \sum_{I'} f(J_j, I') P_n(I', I). \tag{11}$$

Using equation (4) we have

$$P_{n+1}(J_j, I) = \sum_{i=1}^{k} \sum_{I'_i} f^i(J_j - I'_i) P_n(I'_i, I). \tag{12}$$

Multiplying equation (12) by $e^{i\Omega\cdot J_j}$ and summing over all the lattice points of category j, one obtains

$$\begin{aligned} P_{n+1}^j(\Omega, I) &= \sum_{J_j}\sum_{i=1}^{k}\sum_{I_i'} f^i(J_j - I_i')P_n(I_i', I)e^{i\Omega\cdot J_j} \\ &= \sum_{i=1}^{k}\sum_{I_i'}\{\sum_{J_j} f^i(J_j - I_i')e^{i\Omega\cdot(J_j - I_i')}\}P_n(I_i', I)e^{i\Omega\cdot I_i'} \\ &= \sum_{i=1}^{k}\sum_{I_i'} S_{ij}(\Omega)P_n(I_i', I)e^{i\Omega\cdot I_i'} \\ &= \sum_{i=1}^{k} S_{ij}(\Omega)P_n^i(\Omega, I) \end{aligned} \tag{13}$$

where

$$P_n^i(\Omega, I) = \sum_{J_i} P_n(J_i, I)e^{i\Omega\cdot J_i} \tag{14}$$

and

$$P_n(\Omega, I) = \sum_{i=1}^{k} P_n^i(\Omega, I). \tag{15}$$

Multiplying equation (13) by Z^{n+1} and summing over n, we have

$$G^j(\Omega, I, Z) - P_0^j(\Omega, I) = \sum_{i=1}^{k} S_{ij}(\Omega)G^i(\Omega, I, Z)Z \tag{16}$$

where

$$G^i(\Omega, I, Z) = \sum_{J_i} P(J_i, I, Z)e^{i\Omega\cdot J_i} = \sum_{n=0}^{\infty} P_n^i(\Omega, I)Z^n \tag{17}$$

and

$$G(\Omega, I, Z) = \sum_{i=1}^{k} G^i(\Omega, I, Z). \tag{18}$$

Obviously the set of equations (16) can be rewritten in a matrix form:

$$[\hat{1} - Z\hat{S}(\Omega)]\hat{G}(\Omega, I, Z) = \hat{P}_0(\Omega, I) \tag{19}$$

with $\hat{1}$ being a $k \times k$ unit matrix. Let $k = 1$ and $I = 0$, matrix equation (19) will reduce to an algebraic equation:

$$[1 - ZS(\Omega)]G(\Omega, 0, Z) = 1 \tag{20}$$

which is well known for simple lattices [1]. So far, it can be seen that as long as the matrix elements of the structure factor can be found, the transformed generating functions $G^i(\Omega, I, Z)$ $(i = 1, 2, \ldots, k)$ can be determined by matrix equation (19) or the set of equations (16). Then the characteristic function $P_n(\Omega, I)$ can be obtained from equation (9) by Cauchy's theorem which yields

$$P_n(\Omega, I) = (2\pi i)^{-1} \oint dZ\, G(\Omega, I, Z)/Z^{n+1} \tag{21}$$

where the transformed generating function $G(\Omega, I, Z)$ may be obtained from equation (18). The probability $P_n(J, I)$ will be given by the inverse Fourier transform of equation (10) as

$$P_n(J, I) = (2\pi)^{-d} \int e^{-i\Omega \cdot I} P_n(\Omega, I)\, d\Omega. \tag{22}$$

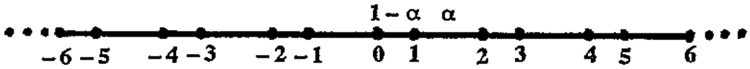

Figure 1. Random walks on an infinitely one-dimensional dimerization chain.

Finally, as an illustration of the above method, we consider a random walk on an infinitely one-dimensional dimerization chain as shown in figure 1. The coordinates of the lattice points are denoted by $I = 0, \pm1, \pm2, \ldots$. For simplicity we consider only a Polya walk in which steps to nearest-neighbour lattice sites only are allowed. All the lattice points on the chain can be divided into two categories denoted by $I_1 = \pm1, \pm3, \ldots$, and $I_2 = 0, \pm2, \pm4, \ldots$, respectively. Let α be the probability of a step from I_1 to $I_1 - 1$ or from I_2 to $I_2 + 1$ and $1 - \alpha$ that from I_1 to $I_1 + 1$ or from I_2 to $I_2 - 1$, respectively. Using equation (5) it is easy to obtain the matrix elements of the structure factor of the walk

$$S_{11}(\Omega) = S_{22}(\Omega) = 0 \tag{23}$$

$$\begin{aligned} S_{12}(\Omega) &= \sum_{I_2} f^1(I_2 - I_1) e^{i\Omega(I_2 - I_1)} \\ &= \alpha e^{-i\Omega} + (1-\alpha) e^{i\Omega} \end{aligned} \tag{24}$$

$$\begin{aligned} S_{21}(\Omega) &= \sum_{I_1} f^2(I_1 - I_2) e^{i\Omega(I_1 - I_2)} \\ &= (1-\alpha) e^{-i\Omega} + \alpha e^{i\Omega} \end{aligned} \tag{25}$$

where we have used

$$f^1(I_1' - I_1) = f^2(I_2' - I_2) = 0 \tag{26}$$

for a Polya walk. Suppose the walker starts from 0, then using equation (14) one has

$$P_0^i(\Omega, 0) = \sum_{I_i} \delta_{I_i,0} e^{i\Omega I_i} \qquad (i = 1, 2) \tag{27}$$

and then

$$P_0^1(\Omega, 0) = 0 \qquad P_0^2(\Omega, 0) = 1. \tag{28}$$

Substituting equations (23) and (28) in matrix equation (19) or the set of equations (16), it is easy to obtain that

$$G^1(\Omega, 0, Z) = Z S_{21}(\Omega)/[1 - Z^2 S_{12}(\Omega) S_{21}(\Omega)] \tag{29}$$

$$G^2(\Omega, 0, Z) = 1/[1 - Z^2 S_{12}(\Omega) S_{21}(\Omega)]. \tag{30}$$

And, further, using equation (18) yields

$$G(\Omega, 0, Z) = [1 + Z S_{21}(\Omega)] \sum_{m=0}^{\infty} Z^{2m} S_{12}^m(\Omega) S_{21}^m(\Omega). \tag{31}$$

Substituting equation (31) in equation (21), it can easily be shown that

$$P_n(\Omega, 0) = \begin{cases} S_{12}^{n/2}(\Omega) S_{21}^{n/2}(\Omega) & n = 0, 2, 4, \ldots \\ S_{12}^{(n-1)/2}(\Omega) S_{21}^{(n+1)/2}(\Omega) & n = 1, 3, 5, \ldots. \end{cases} \tag{32}$$

The probability $P_n(I, 0)$ can be obtained by substituting equation (32) in equation (22) and using equation (24) and equation (25) which yields

$$P_n(I,0) = \begin{cases} \alpha^{n/2}(1-\alpha)\sum_{m=0}^{\infty}\frac{[(\frac{1}{2}n)!]^2[\alpha/(1-\alpha)]^{(1+n-4m)/2}}{m![\frac{1}{2}(I+n)-m]!(\frac{1}{2}n-m)!(m-\frac{1}{2}I)!} \\ \qquad n=0,2,4,\ldots \\ \alpha^{(n-1)/2}(1-\alpha)^{(n+1)/2}\sum_{m=0}^{\infty}\frac{[(\frac{1}{2}n)!]^2[\alpha/(1-\alpha)]^{(1+n-4m)/2}}{m![\frac{1}{2}(I+n)-m]![\frac{1}{2}(n-1)-m]![m-\frac{1}{2}(I-1)]!} \\ \qquad n=1,3,5,\ldots. \end{cases} \tag{33}$$

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