Abstract

The problem of a restricted random walk on graphs which keeps track of the number of immediate reversal steps is considered by using a transfer matrix formulation. A closed-form expression is obtained for the generating function of the number of $n$-step walks with $r$ reversal steps for walks on any graph. In the case of graphs of a uniform valence, we show that our result has a probabilistic meaning, and deduce explicit expressions for the generating function in terms of the eigenvalues of the adjacency matrix. Applications to periodic lattices and the complete graph are given.
1 Introduction

The problem of random walks on lattices has been of pertinent interest in mathematics and physics for decades [1]. Very recently, the study of random walks also arises in the theory of periodic orbits in quantum graphs [2]. In that study one considers random walks on a graph while keeping track of aspects of steps which are immediate reversals of the previous steps, leading to a problem of restricted walks. As is common in analyses of self-avoiding walks [3], the consideration becomes difficult because of the prohibition of returning to previously visited sites. As a result, the walk problem in quantum graphs has remained largely unsolved. Here we introduce and solve a restricted walk problem on graphs which is simpler and more natural in its mathematical formulation. It is hoped that this solution will shed light on self-avoiding walks and the yet unsolved problem of quantum graphs.

Consider a graph $G$ of $q$ sites (vertices) numbered from 1 to $q$. Starting from a site $p_0$, a walker begins a walk by taking “steps” along the edges of $G$. A step from site $p_i$ to site $p_j$ is a reversal if it is taken immediately after a step from $p_j$ to $p_i$, namely, if it reverses the preceding step. We are interested in computing $N_{n,r}(p_0, p_n)$, the number of $n$-step walks starting from a site $p_0$ and ending at site $p_n$, which may or may not coincide with $p_0$, with $r$ ($< n$) reversal steps.

Introduce the generating function

$$Z_n(z|p_0, p_n) = \sum_{r=0}^{n-1} z^r N_{n,r}(p_0, p_n).$$  \hspace{1cm} (1)

Clearly, we have $Z_n(0|p_0, p_n) = N_{n,0}(p_0, p_n)$. It is also clear that $Z_n(1|p_0, p_n)$ is the total number of $n$-step walks from $p_0$ to $p_n$, regardless whether there are reversals. It is also useful to introduce

$$W_n(z|p_0) = \sum_{p_n=1}^{q} Z_n(z|p_0, p_n)$$

$$= \sum_{r=0}^{n-1} z^r M_{n,r}(p_0)$$  \hspace{1cm} (2)

as the generating function of all $n$-step walks which originate from $p_0$. Clearly, $M_{n,r}(p_0)$ is the number of $n$-step walks starting from $p_0$ with $r$ reversals, regardless of the ending site.
Let $A$ be the $q \times q$ adjacency matrix of $G$ with elements

$$A_{ij} = \langle i|A|j \rangle = \begin{cases} 1 & \text{if } i, j \text{ are connected by an edge} \\ 0 & \text{otherwise}. \end{cases}$$

(3)

It is well-known [4, 5] that we have

$$Z_n(1|p_0, p_n) = \sum_{p_1p_2\cdots p_{n-1}} \langle p_0|A|p_1 \rangle \langle p_1|A|p_2 \rangle \cdots \langle p_{n-1}|A|p_n \rangle = \langle p_0|A^n|p_n \rangle.$$

(4)

Here, in (4) and hereafter, all summations are taken from 1 to $q$ unless otherwise stated.

To compute the generating function $Z_n(z|p_0, p_n)$ for general $z$, we introduce a $q \times q$ matrix $W$ with elements

$$W_{ij} = 1 + (z - 1)\delta_{ij},$$

(5)

where $\delta$ is the Kronecker delta, with $z = 0$ corresponding to the case of no reversals. Then, instead of (4), we have the expression

$$Z_n(z|p_0, p_n) = \sum_{p_1p_2\cdots p_{n-1}} A_{p_0p_1}A_{p_1p_2}\cdots A_{p_{n-1}p_n}W_{p_0p_2}W_{p_1p_3}\cdots W_{p_{n-2}p_n}.$$

(6)

A graphical representation of the summand in (6) is depicted in Fig. 1. Note that arrows indicate the sequence of steps taken.

Figure 1: Graphical representation of (6). Arrows denote the sequence of steps as well as the order in which indices of matrix elements appear in (13).
Graphs of uniform valence: If all sites of $G$ have the same valence $v$, such as in a complete graph or a lattice with periodic boundary conditions, then the walker has $v$ choices for the first step, and for each of the remaining $n - 1$ steps, the walker either returns to the previous site with a weight $z$ or walks to any of the $v - 1$ remaining neighboring sites. Then, after summing over all ending sites, we have

$$W_n(z|p_0) = v(z + v - 1)^{n-1}, \quad (7)$$

from which one obtains

$$M_{n,r}(p_0) = v \binom{n-1}{r} (v-1)^{n-1}. \quad (8)$$

Furthermore, the generating function $Z_n$ can be associated with a probabilistic meaning. Consider $n$-step walks for which the walker starts from site $i$ and ends at $j$. At the first step the walker can choose any of the $v$ neighboring sites with an equal probability $\frac{1}{v}$. At step two and thereafter, the walker makes an immediate reversal with a probability $p_1$ and walks to any of the remaining $v - 1$ neighboring sites with a probability $p_2$ subject to

$$p_1 + (v-1)p_2 = 1. \quad (9)$$

Then, the probability that the walker will end at site $j$ after $n$ steps is

$$P_n(i,j) = v^{-1} \sum_{r=0}^{n-1} p_1^r p_2^{n-1-r} N_{n,r}(i,j) = v^{-1} p_2^{n-1} Z_n(p_1/p_2|i,j). \quad (10)$$

Indeed, using (2), (7) and (3), one verifies that

$$\sum_j P_n(i,j) = 1. \quad (11)$$

2 Transfer matrix formulation

Returning now to walks on an arbitrary graph, it is convenient to introduce a $q^2 \times q^2$ transfer matrix $T$ with elements

$$< i|T|jk > = A_{ij} W_{jk} \delta_{i,j}, \quad (12)$$

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or more simply

\[< ij | T | jk > = A_{ij} W_{ik}, \]

(13)

and a \( q \times q \) matrix \( C_0 \) with elements

\[C_0(\alpha \beta | p_n) = A_{\alpha \beta} \delta_{\beta p_n} \]

(14)

as depicted by the heavy line in Fig. 1. One can then rewrite (6) as

\[Z_n(z | p_0, p_n) = \sum_{p_1 \cdots p_{n-1}p} < p_0 p_1 | T | p_1 p_2 > < p_1 p_2 | T | p_2 p_3 > \cdots \times < p_{n-2} p_{n-1} | T | p_{n-1} p | C_0(p_{n-1} p | p_n). \]

(15)

Note that matrix elements in (13) and (15) are indexed in the order along the arrows in Fig. 1. Further introduce the recursion relation

\[C_{m+1}(ij | p) = \sum_k < ij | T | jk > C_m(jk | p), \quad m = 0, 1, 2, \cdots . \]

(16)

and the notation

\[\alpha_m(i | p) = \sum_j C_m(ij | p), \]

(17)

then for walks ending at site \( p \) the recursion relation (16) leads to

\[C_{m+2}(ij | p) = A_{ij} \left[ \alpha_{m+1}(j | p) + (z - 1) C_{m+1}(ji | p) \right] \]

\[= A_{ij} \left[ \alpha_{m+1}(j | p) + (z - 1) \alpha_m(i | p) + (z - 1)^2 C_m(ij | p) \right], \]

\[m = 0, 1, 2, \cdots . \]

(18)

Here, we have iterated the first line once and made use of (5) and (13) and the identity \( A_{ij}^2 = A_{ij} = A_{ji} \). For walks starting at site \( i \) and ending at site \( p \), we have by combining (14) and (16) the boundary condition

\[\alpha_0(i) = A_{ip} \]

\[\alpha_1(i) = [A^2]_{ip} + (z - 1) v_i \delta_{ip} \]

(19)

where

\[v_i = \sum_j A_{ij} \]

(20)
is the valence of the site $i$. In addition, we have the identity

$$Z_n(z|i, p) = \alpha_{n-1}(i|p). \quad (21)$$

Thus, the crux of matter is to analyze the recursion relation (18).

Summing (18) over $j$ and defining $q$-component vectors $\tilde{\alpha}_m(p)$, $m = 1, 2, \cdots, q$, whose components are $\alpha_m(i|p), i = 1, 2, \cdots, q$, we obtain

$$\tilde{\alpha}_{m+2}(p) = A\tilde{\alpha}_{m+1}(p) + B\tilde{\alpha}_m(p), \quad m = 0, 1, 2, \cdots, \quad (22)$$

where $B$ is a $q \times q$ diagonal matrix with elements

$$B_{ij} = (z - 1)(v_i + z - 1)\delta_{ij}. \quad (23)$$

Introducing the generating function

$$\tilde{G}(t) = \sum_{m=0}^{\infty} t^m \tilde{\alpha}_m(p), \quad (24)$$

the summation of (22) from $m = 0$ to $\infty$ after multiplying by $t^m$ then yields

$$\tilde{G}(t) = \left[ I - t^2 B - tA \right]^{-1} \left[ \tilde{\alpha}_0(p) + t\tilde{\alpha}_1(p) - tA\tilde{\alpha}_0(p) \right], \quad (25)$$

where $I$ is the $q \times q$ identity matrix. Introducing (19) and the vector $\tilde{\alpha}_{00}(p)$ with elements

$$a_{00}(i|p) = \delta_{ip}, \quad i = 1, 2, \cdots, q, \quad (26)$$

one obtains

$$\tilde{G}(t) = \left[ I - t^2 B - tA \right]^{-1} \left[ A + (z - 1)tV \right] \tilde{a}_{00}(p), \quad (27)$$

where $V$ is a $q \times q$ diagonal matrix with elements $V_{ij} = v_i \delta_{ij}$.

Finally, after combining (21) and (24), we identify the generating function $Z_n(z|i, p)$ for $n$-step walks from $i$ to $p$ as the coefficient of $t^{n-1}$ in the $i$-th component of (27). This is a very general result which holds for any graph.
3 Graphs of uniform valence

In this section we apply the result of the preceding section to graphs of a uniform valence, such as lattices with periodic boundary conditions and a complete graph. Let $v_i = v$ for all $i$, then $B = bI$, $V = vI$, where

$$b = (z - 1)(v + z - 1),$$

(28)

and the inverse matrix in (27) can be expanded to yield

$$\vec{G}(t) = \sum_{n=0}^{\infty} \sum_{\ell=0}^{\infty} \left( \begin{array}{c} n + \ell \\ \ell \end{array} \right) b^\ell t^{n+2\ell} A^n \left[ A + (z - 1)vtI \right] \vec{\alpha}_{00}(p).$$

(29)

Using $\vec{\alpha}_{00}(p)$ given by (26), we obtain after a little reduction the following explicit expression for the $i$-th component of $\vec{G}(t)$,

$$[\vec{G}(t)]_i = (1 - bt^2)^{-1} A_{ip} + \sum_{n=1}^{\infty} \sum_{\ell=0}^{\infty} b^\ell t^{n+2\ell} \left[ \begin{array}{c} n + \ell \\ \ell \end{array} \right] A^{n+1} + (z - 1)v \left( \begin{array}{c} n + \ell - 1 \\ \ell \end{array} \right) A^{n-1} \right]_{ip}.$$

(30)

Thus, we find

$$Z_2(z|i, p) = [A^2 + (z - 1)vI]_{ip}$$

$$Z_3(z|i, p) = [A^3 + (z - 1)(2v + z - 1)A]_{ip}$$

$$Z_4(z|i, p) = [A^4 + (z - 1)(3v + 2z - 2)A^2 + (z - 1)^2v(v + z - 1)I]_{ip}$$

etc.

(31)

It is now clear that results (29) and (31) can be expressed in terms of the eigenvalues $\lambda_i$ of the adjacency matrix $A$. Note also that, by using (10), the generating function $Z_n(z|i, p)$ gives the probability that a walker will arrive from $i$ to $p$ in $n$ steps with an immediate reversal probability $z/(1 + z)$ at all steps.

For walks returning to the starting point, namely, $i = p$, we use the identities $A_{pp} = 0$, $(A^2)_{pp} = v$ to obtain

$$Z_2(z|p, p) = vz$$

$$Z_3(z|p, p) = [A^3]_{pp}$$

$$Z_4(z|p, p) = [A^4]_{pp} + v(z - 1)(z^2 - 1) + v^2(z - 1)(z + 2).$$

(32)
Furthermore, if all sites are equivalent, such as in a complete graph or a lattice with periodic boundary conditions, we have the simple relation

$$[A^n]_{pp} = q^{-1} \sum_{i=1}^{q} \lambda_i^n.$$ \hspace{1cm} (33)

For walks on an $N_1 \times N_2 \times \cdots \times N_d$ $d$-dimensional hypercubic lattice, for example, this becomes

$$[A^n]_{pp} = (N_1 N_2 \cdots N_d)^{-1} \sum_{n_1=1}^{N_1} \sum_{n_2=1}^{N_2} \cdots \sum_{n_d=1}^{N_d} \left[ \sum_{\alpha=1}^{d} e^{2\pi i n_{\alpha}/N_d} \right]^n,$$ \hspace{1cm} (34)

which reduces to the usual expression of the number of walks returning to the origin on an infinite lattice \cite{footnote} after replacing the sums by integrals in the limit of $N_\alpha \to \infty$, $\alpha = 1, \cdots, d$. For the complete graph it can be shown\cite{footnote} that the solution also assumes the form

$$Z_n(z|i, p) = (q + z - 2)^{n-1} (1 - \delta_{ip}) + (q\delta_{ip} - 1)[B^{n-1}]_{21},$$ \hspace{1cm} (35)

where

$$B = \begin{pmatrix} 0 & q + z - 2 & 0 \\ z & 0 & q - 2 \\ 1 & 0 & q + z - 3 \end{pmatrix},$$ \hspace{1cm} (36)

and the subscript \{21\} denotes the \{21\}-th element. This gives, among other results, the following explicit expressions for walks without reversals at all steps,

$$Z_2(0|p, p) = N_{2,0}(p, p) = 0 \hspace{1cm} Z_3(0|p, p) = N_{3,0}(p, p) = (q - 1)(q - 2) \hspace{1cm} Z_4(0|p, p) = N_{4,0}(p, p) = (q - 1)(q - 2)(q - 3) \hspace{1cm} Z_5(0|p, p) = N_{5,0}(p, p) = (q - 1)(q - 2)(q - 3)^2 \hspace{1cm} Z_6(0|p, p) = N_{6,0}(p, p) = (q - 1)(q - 2)(q^2 - 8q^2 + 23q - 23).$$ \hspace{1cm} (37)

\footnote{For the complete graph the problem can be solved very simply by regarding the walker to be in three “states”: the starting site, just stepping off the starting site, and others. This leads directly to \cite{footnote}. We are indebted to the referee for pointing out this consideration.}
4 Summary and discussions

We have presented a transfer matrix formulation for enumerating $n$-step walks on a graph with $r$ reversal steps, and obtained a closed-form expression for the generating function $Z_n(z|i,p)$ in the form of (27). We have also deduced explicit expressions for the generating function in the case of a uniform valence $v$, with the results given in terms of the eigenvalues of the adjacency matrix, and showed that in this case the generating function possesses a probabilistic meaning.

The transfer matrix approach can be extended to other restricted self-avoiding walks. For walks having a 2-step memory of not stepping into the two immediate preceding sites, for example, the generating function (8) can be similarly written down, and one needs to consider a $q^3 \times q^3$ transfer matrix, where $q$ is the number of sites in the graph. It is hoped that such considerations can shed light to the problem of self-avoid walks and the yet unsolved walk problems in quantum chaos.

5 Acknowledgement

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References

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