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# Diffusion coefficient for random walks on strips with spatially inhomogeneous boundaries 

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#### Abstract

We determine the diffusion constant $K$ for unbiased, discrete-time random walks on infinitely long planar strips of finite width with regularly spaced, stepped edges that model, albeit in a simple and regular manner, some of the features of the corrugated surfaces of diffusion channels in porous media. We derive a formal expression for $K$ and use it to compute $K$ exactly for a range of values of the strip width and the step width, the latter serving as a measure of the roughness of the boundaries. We consider also the role of specific boundary conditions at the edges by determining $K$ for both myopic and blind random walkers in each case. Our results shed some light on the effects of spatially inhomogeneous transverse boundaries on the coefficient of diffusion in the longitudinal direction.


## 1. Introduction

In the diffusion of a fluid through a porous medium [1-4], the fluid flows along channels of various sizes with irregular boundaries. The diffusion constant for flow along any of these channels would depend in general on its structure, and could therefore be used as a probe of the geometry of the medium-in particular, of the transverse size of the channels, the specific shape of the boundary and the boundary conditions. We attempt to find the size and shape dependence of the diffusion constant for a random walk (RW) on a lattice in which the geometry of the 'surface' is modelled in a simple but non-trivial way.

Consider first an unbiased Rw in discrete time $n$, on a square lattice in the form of a strip that is infinitely long in the $x$-direction and of finite width in the $y$-direction. The sites on the strip are labelled $(j, m)$ where $j \in \mathbb{Z}$ and $m=1,2, \ldots, N$. At an interior site (i.e. $2 \leqslant m \leqslant N-1$ ), the walker jumps at the end of a time step to any one of the four nearest-neighbour (nn) sites with a probability equal to $\frac{1}{4}$. Along the edges of the strip, a variety of boundary conditions can be imposed: in general, the walker may be taken to remain at a boundary site with a probability $\Gamma$ at the end of a time step, or to jump with probability $(1-\Gamma) / 3$ (as the Rw is unbiased) to any one of the three nn sites. The stay probability $\Gamma$ serves to parametrize the nature of the boundary. The value $\Gamma=\frac{1}{4}$ corresponds to a blind Rw, i.e. the standard RW with reflecting boundary conditions. Only in this case do the motions along the $x$ and $y$ directions decouple from each other, and the mean square displacement in the unbounded direction, $\left\langle X_{n}^{2}\right\rangle$, is exactly equal to $n / 2$. Thus the diffusion constant, defined as

$$
\begin{equation*}
K=\lim _{n \rightarrow \infty}\left\langle X_{n}^{2}\right\rangle / n \tag{1}
\end{equation*}
$$

is just $\frac{1}{2}$ (the value of $K$ on an infinite two-dimensional lattice), independent of the size of the strip in the $y$-direction. For every other value of $\Gamma$, the boundary condition introduces correlations between the motions along the two directions. This results in a diffusion constant that depends on the lateral size $N$ of the strip (and on $\Gamma$ ) [5]:

$$
\begin{equation*}
K=\frac{N(1-\Gamma)}{2 N(1-\Gamma)+4 \Gamma-1} \tag{2}
\end{equation*}
$$

As stated earlier, the parameter $\Gamma$ is a convenient way of characterizing the nature of the boundaries of the strip. If $\Gamma=0$, we have 'slip' boundary conditions-the walker does not stay at any site after a time step, and he jumps from any site to its nn sites with equal probabilities: $\frac{1}{4}$ from interior sites, $\frac{1}{3}$ from boundary sites. (The RW is a myopic one $[6,7]$.) The boundaries get stickier as $\Gamma \rightarrow 1$, so that $K$ decreases. In the limit $\Gamma=1$, of course, the sites on the edges are perfect traps, and $K$ vanishes because there is no long-range diffusion.

The roughness of the boundary may also be simulated, to some extent, with the help of the parameter $\Gamma$. For instance, suppose there is an identical side branch or cluster of sites of finite size attached to each site on the edges of the strip. If these appendages are connected with each other only through the corresponding base sites $(j, 1)$ or $(j, N)$ on the main strip, then $K$ can be found [5] for such geometries [8,9] from (2), as follows: the mean first passage time [10,11] from a site on the edge to any of its three neighbours on the main strip must be calculated, and substituted for $(1-\Gamma)^{-1}$ in (2).

While this procedure can be used to compute $K$ in several cases, it has a serious limitation that restricts its use in many other situations. Any physical boundary would certainly be corrugated (and also irregular) on various length scales. Moreover, a diffusing particle exploring such a corrugation may simultaneously progress in the direction in which diffusion occurs (here, the $x$-direction). In our Rw model, this means that the walker may leave the strip at some edge site, say ( $j, 1$ ), and re-enter it at another edge site $\left(j^{\prime}, 1\right)$ after diffusing along the sites of a corrugation outside the main strip. We need a simple model that takes this important circumstance (the possibility of such loop-like paths) into account. It must also be sufficiently regular in its geometry to permit an analytic solution to be obtained, so that we may draw reliable conclusions regarding the dependence of $K$ on the degree of roughness of the edges. With these considerations in mind, we set up a suitable model of the boundaries in the next section.

## 2. The model

We consider unbiased RWs on strips with regularly spaced stepped edges as shown in figure 1. The width of the strip is characterized by $N$, as before. The ratio $1 / l$ of the height of each step to its width is a measure of the roughness of the edges of the strip: as $l$ increases, the roughness decreases. We may, of course, consider many other variations of this simple geometry-steps of different heights, shapes, etc. However, the model we consider (and solve exactly for $K$ ) already has the essential features whose effects on $K$ we seek to probe.

The sites on the strip are labelled ( $j, m$ ) as before, but now $m$ runs from 0 to $N+1$. On the main strip ( $1 \leqslant m \leqslant N$ ) we have $j \in \mathbb{Z}$, but on the boundary lines $m=0$ and $m=N+1$, not all sites are present: a row of $l$ sites is followed by a gap of $(l-2)$ sites, and the pattern is repeated. Thus we have sites with 4 nns (these include all the interior


Figure 1. The lattice on which the random walk takes place, in the case $l=4$. The block of sites from the column $j=1$ to the column $j=2 l-2$ is repeated on the left and right to form the infinite strip.
sites and the corner sites on the lines $m=1$ and $m=N$ ), three nns (the edge sites on the lines $m=0, m=1, m=N$ and $m=N+1$ ), and two nns (the corner sites on the lines $m=0$ and $m=N+1$ ). In order to examine simultaneously the effect on $K$ of boundary conditions as well, we consider two basic cases: blind and myopic random walks (BRW and MRw). In the BRW, the walker jumps with a probability $\frac{1}{4}$ from any site $(j, m)$ to each of its $q_{j m}$ available nn sites, and stays at the original site with a probability ( $1-\frac{1}{4} q_{j m}$ ) at the end of a time step. In the MRW, the walker jumps with a probability $1 / q_{j m}$ to each of the available nn sites $[6,7]$, the stay probability at a site being zero.

The diffusion constant $K$ is the coefficient of the leading $(\mathrm{O}(n))$ term in $\left\langle X_{n}^{2}\right\rangle$, and may be extracted without solving the Rw problem exactly. We derive below a compact formula for $K$ in terms of the determinant of a certain matrix, which makes it possible to obtain the exact value of $K$ in quite non-trivial cases.

## 3. Formula for the diffusion constant

One begins with the set of rate equations for the time-dependent probabilities $P_{n}(j, m)$, where $0 \leqslant m \leqslant N+1$ and $1 \leqslant j \leqslant 2 l-2$ (see figure. 1). We need to write equations only for these values of $j$, because of the periodicity in the $x$-direction. Let $R(k, m, \xi)$ denote the discrete double transform of $P_{n}(j, m)$,

$$
\begin{equation*}
R(k, m, \xi)=\sum_{j=-\infty}^{\infty} \sum_{n=0}^{\infty} P_{n}(j, m) \mathrm{e}^{i j k} \xi^{n} . \tag{3}
\end{equation*}
$$

The set of rate equations for $P_{n}(j, m)$ cannot be transformed directly into one for $R(k, m, \xi)$ because the periodicity in $j$ is $(2 l-2)$, rather than 1 . Therefore we break up the summation over $j$ in (3) into ( $2 l-2$ ) parts, such that

$$
\begin{equation*}
R(k, m, \xi)=\sum_{s=1}^{2 l-2} R_{s}(k, m, \xi) \tag{4}
\end{equation*}
$$

where

$$
\begin{equation*}
R_{s}=\sum_{r=-\infty}^{\infty} \sum_{n=0}^{\infty} P_{n}(s+(2 l-2) r, m) \xi^{n} \exp [\mathrm{i} k(s+(2 l-2) r)] . \tag{5}
\end{equation*}
$$

For brevity in writing, we shall henceforth write $R_{s}(k, m, \xi)$ as $R_{s}(m)$, suppressing the $k$ and $\xi$ dependence. Let $\mathbb{R}$ be the column vector with ( $N+2) l+N(l-2)$ elements whose transpose is

$$
\begin{equation*}
\mathbb{R}^{T}=\left(\boldsymbol{R}_{1}^{T}, \ldots, \boldsymbol{R}_{l}^{T}, \boldsymbol{R}_{l+1}^{T}, \ldots, \boldsymbol{R}_{2 l-2}^{T}\right) \tag{6}
\end{equation*}
$$

where $\boldsymbol{R}_{s}$ is itself a column vector with elements $\boldsymbol{R}_{s}(m)$; the index $m$ runs from 0 to $(N+1)$ for $1 \leqslant s \leqslant l$, and from 1 to $N$ for $l+1 \leqslant s \leqslant 2 l-2$. Then $\mathbb{R}$ satisfies a matrix equation of the form $\boldsymbol{M R}=f$, where $\boldsymbol{M}$ is a square matrix of order $(N+2) l+N(l-2)$ which is not tridiagonal, and $f$ depends on the initial distribution $P_{0}(j, m)$. The quantity we seek is $\left\langle X_{n}^{2}\right\rangle$, whose $\xi$-transform is given by

$$
\begin{equation*}
\left\langle X^{2}(\xi)\right\rangle=-\left[\frac{\partial^{2}}{\partial k^{2}}\left\{\sum_{s=1}^{l} \sum_{m=0}^{N+1} R_{s}(m)+\sum_{s=l+1}^{2 l-2} \sum_{m=1}^{N} R_{s}(m)\right\}\right]_{k=0} . \tag{7}
\end{equation*}
$$

(We have not explicitly indicated a further averaging over the initial position of the walker, as $K$ is actually independent of the latter.) The expression in curly brackets is just the sum of all the elements of $\mathbb{R}$. Using the fact that $\mathbb{R}=\boldsymbol{M}^{-1} f$, this is of the form

$$
\begin{equation*}
\sum_{s} \sum_{m} R_{s}(m)=\mathbb{N}(k, \xi) / \Delta(k, \xi) \tag{8}
\end{equation*}
$$

where

$$
\begin{equation*}
\Delta(k, \xi)=\operatorname{det} \boldsymbol{M} \tag{9}
\end{equation*}
$$

and the numerator $\mathbb{N}$ is obtained by operating on $f$ with the matrix formed by the cofactors of $M^{T}$. Both $\mathbb{N}$ and $\Delta$ are polynomials in $\xi$ and entire functions of $k$. The normalization of $P_{n}(j, m)$ implies that $\mathbb{N}(0, \xi) / \Delta(0, \xi)=(1-\xi)^{-1}$. Moreover, it turns out that $\Delta$ depends on $k$ only through $c=\cos k$. (We show this in appendix B.) Using the foregoing, (7) reduces to

$$
\begin{equation*}
\left\langle X^{2}(\xi)\right\rangle=-\left[\Delta^{-1}\left((1-\xi)^{-1} \frac{\partial \Delta}{\partial c}+\frac{\partial^{2} \mathbb{N}}{\partial k^{2}}\right)\right]_{k=0, c=1} \tag{10}
\end{equation*}
$$

As there are no absorbing sites on the lattice, the matrix occurring in the original set of rate equations for $P_{n}(j, m)$ is a stochastic one. This implies that the elements of each column of $\Delta(0, \xi)$ add up to $(1-\xi)$. It is therefore the first term in square brackets in (10) that has a double pole at $\xi=1$, which in turn produces the leading asymptotic behaviour $\left\langle X_{n}^{2}\right\rangle \sim K n$ when the $\xi$-transform is inverted. Writing $\Delta(0, \xi)=$ $(\xi-1)(\partial \Delta(0, \xi) / \partial \xi)_{\xi=1}+\ldots$, the Ieading asymptotic behaviour of $\left\langle X_{n}^{2}\right\rangle$ is therefore contained in

$$
\begin{equation*}
\left\langle X_{n}^{2}\right\rangle \sim(2 \pi \mathrm{i})^{-1} \oint \mathrm{~d} \xi \xi^{-n-1}(\xi-1)^{-2}\left(\frac{\partial \Delta / \partial c}{\partial \Delta / \partial \xi}\right)_{c=1, \xi=1} \tag{11}
\end{equation*}
$$

It is easy to see that this leads to the compact and exact formula

$$
\begin{equation*}
K=\left(\frac{\partial \Delta / \partial c}{\partial \Delta / \partial \xi}\right)_{c=1, \xi=1} \tag{12}
\end{equation*}
$$

on using the definition of $K$ in (1).
The actual computation of $K$ may be simplified further. As $K$ is independent of the initial position of the walker, we may choose $P_{0}(j, m)$ so as to have (for all times $n \geqslant 0)$ the symmetry property $P_{n}(j, m)=P_{n}(j, N+1-m)$. Introduced into the rate equations for $P_{n}(j, m)$, this symmetry essentially halves the number of independent
equations from $2(N l-N+l)$ to $[(N+1) / 2](2 l-2)+l$, where $[\alpha]$ stands for the largest integer $\leqslant \alpha$. The foregoing procedure for finding $K$ essentially goes through, but with a 'reduced' matrix $\boldsymbol{M}^{\prime}$. The determinant of $\boldsymbol{M}$ ' can be shown to be the same as that of $\boldsymbol{M}$, namely, $\Delta$. This makes it easier to evaluate $K$ following (12). In appendix $A$, we have given an explicit illustration of the procedure for a myopic RW in the case $N=2$ and $l=3$, for a general value of the parameter $\Gamma$ (the stay probability at a site on the edge of the strip) introduced in section 1.

## 4. Numerical results and discussion

Using the software package MACSYMA, we have computed $K$ explicitly for a number of values of $N$ and $l$ using (12), for both blind and myopic Rws. The dimensionality $[(N+1) / 2](2 l-2)+l$ of the determinant $\Delta$ increases rapidly with increasing $N$ and $l$ (in particular the latter), making the calculations increasingly complicated. We find that $K$ is always a rational number. Our numerical results are listed in tables 1 and 2. To bring out the considerable variation in $K$ with varying $N$ and $l$, we have plotted $K$ as a function of $1 / N$ for different values of $l$ in figure 2 , for the BRW and the MRW. (B2 denotes a blind walk for $l=2$, etc.) The abscissa has been chosen to be $1 / N$ rather than $N$ so that the entire range of physical values of $N$ can be displayed. The curves shown represent interpolations between points corresponding to integer values of $N$. It is remarkable that these values lie, in each case, on smooth, monotonic curves. The limiting case $N=1$ is actually quasi-one-dimensional; to ensure that this case is part

Table 1. $K$ for lattices with $l=2$.

| $N$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $K($ BRW ) | $\frac{5}{24}$ | $\frac{2}{7}$ | $\frac{79}{240}$ | $\frac{44}{123}$ | $\frac{741}{1960}$ | $\frac{94}{239}$ | $\frac{5951}{14688}$ | $\frac{2888}{6965}$ | $\frac{44197}{104632}$ | $\frac{3482}{8119}$ |
| $K$ (MRW) | $\frac{5}{16}$ | $\frac{8}{21}$ | $\frac{79}{192}$ | $\frac{88}{205}$ | $\frac{247}{560}$ | $\frac{752}{1673}$ | $\frac{5951}{13056}$ | $\frac{5776}{12537}$ | $\frac{44197}{95120}$ | $\frac{41784}{89309}$ |

Table 2. $K$ for lattices with $l=3,4$.

|  | $l=3$ |  |  | $l=4$ |  |  |  |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |  | $K(\mathrm{BRW})$ | $K(\mathrm{MRW})$ |  | $K(\mathrm{BRW})$ | $K(\mathrm{MRW})$ |
| 1 | $\frac{4}{15}$ | $\frac{8}{21}$ | $\frac{207}{700}$ | $\frac{207}{500}$ |  |  |  |  |  |  |  |
| 2 | $\frac{12}{35}$ | $\frac{24}{55}$ | $\frac{63}{170}$ | $\frac{63}{130}$ |  |  |  |  |  |  |  |
| 3 | $\frac{41}{108}$ | $\frac{41}{90}$ | - | - |  |  |  |  |  |  |  |
| 4 | $\frac{84}{209}$ | $\frac{168}{361}$ |  | - | - |  |  |  |  |  |  |



Figure 2. Variation of the diffusion constant $K$ with the inverse strip width $1 / N$. Blind and myopic walks are labelled $B$ and $M$ respectively, while the adjacent numbers denote the value of $l$, the number of sites in the corrugations on the edges of the strip.
of the family of lattices considered here, we have taken the jump probability out of a site on the linear chain part of the structure to either one of its nn sites to be $\frac{1}{2}$ for the MRW and $\frac{1}{4}$ for the BRW.

When the edges of the strip have no corrugations at all (we may consider this to correspond to $l=0$ ), $K=\frac{1}{2}$ for the BRW (for $N \geqslant 2$ ) and $N /(2 N-1)$ for the MRW (obtained [12] by setting $\Gamma=0$ in (2)). It may be noted that the latter value is actually greater than the free two-dimensional value $\frac{1}{2}$. When $l=1$, we have a vertical branch or spike with a single site emanating from each site on the edges of the strip. $K$ may be found analytically [5] as a function of $N$ in this case: we have, respectively, $K=N /(2 N+4)$ for the BRW and $K=N /(2 N+1)$ for the MRW. These expressions (plotted in curves B 1 and M 1 respectively) turn out to be valid for $N=1$ as well.

The cases $l=0$ and $l=1$ do not belong, in some sense, to the family of lattices of primary concern here. The latter commences with $l=2$ : we now have corrugations at the edges in which the walker can get trapped, but in which motion in the $x$-direction is also possible along loop-like paths leaving and re-entering the main strip at different sites. As $l$ increases (for a fixed value of $N$ ), $K$ increases. (For the mrw, we see that $K$ is larger for $l=1$ than it is for $l=2$; but $l=1$ is a different kind of structure, as we have pointed out. For myopic boundary conditions, the enhanced tendency of the walker to be pushed out of the side branch into the main strip overcomes the trapping effect of the branch in the case $l=1$, which is why the curve M1 lies above the curve M2.) Moreover, the value of $K$ for the MRW is always greater than that for the BRW (for a given $N$ and $l$ ), as one would expect: in the BRW, the walker has a non-zero stay probability at the surface sites, which helps reduce the value of $K$.

In order to have a concrete example of the role played by the nature of the boundary in determining the diffusion coefficient, we have also computed $K$ as a function of $\Gamma$, the stay probability at edge sites, for $N=2$ and $l=3$. The details are given in appendix $A$. The final result is

$$
\begin{equation*}
K=\frac{24(2 \Gamma-1)(\Gamma-1)}{5\left(12 \Gamma^{2}-26 \Gamma+11\right)} \tag{13}
\end{equation*}
$$

Now $\Gamma$ is the probability that the walker stays on at the end of a time step at a site on the edges of the strip, while $2 \Gamma$ is the stay probability at a corner site on a corrugation, such as the site $j=1, m=0$ in figure 1 . (We can find $K$ for arbitrary stay probabilities $\Gamma$ and $\gamma$ at edge and corner sites, respectively, but nothing significantly new is learnt from this generalization.) As explained in appendix $A$, the values $\Gamma=0$ and $\frac{1}{4}$ correspond to myopic and blind walks, respectively. The diffusion constant decreases monotonically from the value $\frac{24}{55}$ for the MRW, through $K=\frac{12}{35}$ for the BRW to 0 for $\Gamma=\frac{1}{2}$. We note that this is the maximum possible value of $\Gamma$ in this instance, since the corner sites become perfect traps when $2 \Gamma=1$ : as first passage to any of these sites is a sure event on the lattice concerned, their presence suffices to stop the long-range diffusion of the walker.

Finally, one may ask what happens for very large values of $N$ and $l$. As $N \rightarrow \infty$, the effects of the edges, corrugations and boundary conditions obviously diminish. $K$ approaches $\frac{1}{2}$, the standard value in two dimensions, as expected. On the other hand, the limit $l \rightarrow \infty$ ( $N$ remaining finite) is much more delicate, because the definition of $K$ implies that the $n \rightarrow \infty$ limit of $\left\langle X_{n}^{2}\right\rangle / n$ is to be taken first. Therefore one must compute $K$ analytically as a function of $l$ for a general value of $N$ in order to find its exact limiting value as $l \rightarrow \infty$. In the absence of such an expression, if we assume that the two limits commute, it can be shown that the limiting value of $K$ is given by a certain weighted harmonic mean of the values of $K$ for two uncorrugated strips of widths $N$ and $N+2$, respectively: thus $K$ remains $\frac{1}{2}$ for the BRW, while for the MRW it lies in between the values $N /(2 N-1)$ and $(N+2) /(2 N+3)$. This computation involves the determination of $K$ on a non-periodic lattice, and will be reported elsewhere as part of a general investigation of random walks on inhomogeneous structures.

In conclusion, we have shown by an exact calculation in a simple model that spatially inhomogeneous boundaries in the transverse direction have a significant effect on the coefficient of the leading asymptotic behaviour of the mean square displacement in the longitudinal direction. This conclusion remains valid even in the case of a blind random walk (perfectly reflecting boundary conditions), for which the diffusion constant is actually independent of the transverse size of the strip when the edges have no inhomogeneities. Although we have restricted ourselves to a two-dimensional lattice, the general method used can be applied to higher dimensional lattices to arrive at qualitatively similar conclusions.

## Appendix A. $K$ for the case $N=2, l=3$

In order to illustrate the method outlined in the text for finding the diffusion constant, we calculate $K$ explicitly for a myopic random walk in the relatively simple case $N=2$, $l=3$. In this case, the label $s$ takes on values from 1 to 4 , the last of these corresponding to a column of two sites in the 'regular' $(N=2)$ part of the strip. The sites are labelled by $(s+4 r, m)$ where $r \in \mathbb{Z}$. For $s=1,2$ and 3 , we have $0 \leqslant m \leqslant 3$; while for $s=4, m=1,2$.

We thus have a basic set of (3)(4) $+2=14$ coupled rate equations to deal with. Moreover, we consider a whole family of boundary conditions by introducing the quantity $\Gamma$ that parametrizes the 'stickiness' of the boundaries. The walker stays at the end of a time step with probabilities $0, \Gamma$ and $2 \Gamma$ at sites with 4,3 and 2 nearest neighbours, respectively. The corresponding jump probabilities to any of the nn sites are therefore $\frac{1}{4},(1-\Gamma) / 3$ and $(1-2 \Gamma) / 2$ respectively. Thus $\Gamma=0$ (respectively, $\frac{1}{4}$ ) implies that the walker is myopic (blind) at all sites.

Instead of writing down the full set of 14 coupled equations, let us exploit the symmetry of $P_{n}(j, m)$ to simplify the calculation. As $K$ is independent of the starting point of the walker, we may choose the initial distribution

$$
\begin{equation*}
P_{0}(j, m)=\delta_{j, 0}\left(\delta_{m, 1}+\delta_{m, 2}\right) / 2 \tag{A1}
\end{equation*}
$$

so that the symmetry relation $P_{n}(j, m)=P_{n}(j, 3-m)$ holds good for all $n$. The set of rate equations for $P_{n}(j, m)$ then reduces to a set of seven coupled equations. To save space, we do not write these down here. As in (5), we define the quantities (now symmetry-reduced)

$$
\begin{equation*}
R_{s}(k, m, \xi)=\sum_{r=-\infty}^{\infty} \sum_{n=0}^{\infty} P_{n}(s+4 r, m) \xi^{n} \mathrm{e}^{i k(s+4 r)} \tag{A2}
\end{equation*}
$$

where $0 \leqslant m \leqslant 1$ for $1 \leqslant s \leqslant 3$, and $m=1$ for $s=4$. Recall that we write $R_{s}(k, m, \xi)$ as $R_{s}(m)$ for brevity. The column vector $\mathbb{R}$ (equation (6)) is now given by

$$
\begin{equation*}
\mathbb{R}=\left(R_{1}(0), R_{1}(1), R_{2}(0), R_{2}(1), R_{3}(0), R_{3}(1), R_{4}(1)\right)^{\mathrm{T}} . \tag{A3}
\end{equation*}
$$

The rate equations for $P_{n}(j, m)$ now lead to the matrix equation $M^{\prime} \mathbb{R}=f$ for $\mathbb{R}$, where $\boldsymbol{M}^{\prime}$ is the matrix
$\left[\begin{array}{ccccccc}1-2 \Gamma \xi & -\frac{\xi}{4} & -\frac{\xi}{3} \mu \mathrm{e}^{-\mathrm{i} k} & 0 & 0 & 0 & 0 \\ -\frac{\xi}{2} \nu & 1-\frac{\xi}{4} & 0 & -\frac{\xi}{4} \mathrm{e}^{-i k} & 0 & 0 & -\frac{\xi}{3} \mu \mathrm{e}^{\mathrm{i} k} \\ -\frac{\xi}{2} \nu \mathrm{e}^{\mathrm{i} k} & 0 & 1-\Gamma \xi & -\frac{\xi}{4} & -\frac{\xi}{2} \nu \mathrm{e}^{-\mathrm{i} k} & 0 & 0 \\ 0 & -\frac{\xi}{4} \mathrm{e}^{\mathrm{i} k} & -\frac{\xi}{3} \mu & 1-\frac{\xi}{4} & 0 & -\frac{\xi}{4} \mathrm{e}^{-\mathrm{i} k} & 0 \\ 0 & 0 & -\frac{\xi}{3} \mu \mathrm{e}^{\mathrm{i} k} & 0 & 1-2 \Gamma \xi & -\frac{\xi}{4} & 0 \\ 0 & 0 & 0 & -\frac{\xi}{4} \mathrm{e}^{\mathrm{i} k} & -\frac{\xi}{2} \nu & 1-\frac{\xi}{4} & -\frac{\xi}{3} \mu \mathrm{e}^{-\mathrm{i} k} \\ 0 & -\frac{\xi}{4} \mathrm{e}^{-\mathrm{i} k} & 0 & 0 & 0 & -\frac{\xi}{4} \mathrm{e}^{\mathrm{i} k} & 1-\frac{\xi}{3} \mu-\Gamma \xi\end{array}\right]$

Here we have written $\mu$ for $1-\Gamma$ and $\nu$ for $1-2 \Gamma$, for brevity. We can show that $\Delta=\operatorname{det} \boldsymbol{M}^{\prime}$ is a function of $c=\cos k$ as far as its $k$-dependence is concerned. Using (12), we obtain for $K$ the result quoted in (13).

## Appendix B. Dependence of $\operatorname{det} \boldsymbol{M}$ on $\boldsymbol{k}$

The variable $k$ appears only as $\mathrm{e}^{\mathrm{i} k}$ and $\mathrm{e}^{-\mathrm{i} k}$ in the elements of $\boldsymbol{M}$. Therefore, to prove that $\operatorname{det} \boldsymbol{M}=\Delta$ is a function of $c=\cos k$, we need to show that $\Delta(k, \xi)=\Delta(-k, \xi)$. We recall that the dimensionality of $\boldsymbol{M}$ is $(N+2) l+N(l-2)$. (The index $s$ labels the vertical row of sites on the lattice. When $1 \leqslant s \leqslant l$, the vertical coordinate $m$ runs from 0 to $N+1$; when $l+1 \leqslant s \leqslant 2 l-2, m$ runs from 1 to $N$.) After writing down $\operatorname{det} \boldsymbol{M}=\Delta$, we interchange the block of rows corresponding to $s=i$ with the block corresponding to $s=l+i-1$, for $1 \leqslant s \leqslant l$. Similarly, the corresponding columns are interchanged. For $l+1 \leqslant s \leqslant 2 l-2$, the rows (and columns) corresponding to $s=l+i$ are interchanged with those corresponding to $s=2 l-1-i$. These interchanges take $\Delta(k, \xi)$ into $\Delta(-k, \xi)$. However, the total number of interchanges is $2[l / 2]+2[(l-2) / 2]$, which is even. Therefore $\Delta(k, \xi)=\Delta(-k, \xi)$ in general, and it follows that $\Delta$ is a function of $c=\cos k$

Alternatively, we have the following indirect argument. The counterpart of (10) for the mean displacement itself is

$$
\begin{equation*}
\left\langle X_{n}\right\rangle=-\mathrm{i}\left(\frac{1}{\Delta} \frac{\partial \mathbb{N}}{\partial k}-\frac{\mathbb{N}}{\Delta^{2}} \frac{\partial \Delta}{\partial k}\right)_{k=0} . \tag{B1}
\end{equation*}
$$

The second term on the right has a double pole at $\xi=1$ when $k=0$, and will lead to an $O(n)$ asymptotic behaviour of $\left\langle X_{n}\right\rangle$. But this is impossible, as the walk is unbiased. Hence $(\partial \Delta / \partial k)_{k=0}$ must vanish, which leads to the same conclusion as before.

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