J. Phys. A: Math. Theor. **43** (2010) 035001 (21pp) doi:10.1088/1751-8113/43/3/035001

Diffusion coefficients for multi-step persistent random walks on lattices

Thomas Gilbert[1] **and David P Sanders**[2]

[1] Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles, C. P. 231, Campus Plaine, B-1050 Brussels, Belgium
[2] Departamento de Física, Facultad de Ciencias, Universidad Nacional Autónoma de México, 04510 México D.F., Mexico

E-mail: thomas.gilbert@ulb.ac.be and dps@fciencias.unam.mx

Received 10 August 2009, in final form 28 October 2009
Published 17 December 2009
Online at stacks.iop.org/JPhysA/43/035001

Abstract
We calculate the diffusion coefficients of persistent random walks on lattices, where the direction of a walker at a given step depends on the memory of a certain number of previous steps. In particular, we describe a simple method which enables us to obtain explicit expressions for the diffusion coefficients of walks with a two-step memory on different classes of one-, two- and higher dimensional lattices.

PACS numbers: 05.60.Cd, 05.10.−a, 02.50.−r

1. Introduction

Random walks are widely used throughout physics as a model for systems in which the state of the system can be viewed as evolving in a stochastic way from one time step to the next. Their properties have been extensively explored and the techniques to study them are well developed [1]. In particular, at a large scale, random walks behave diffusively.

The most-studied case is that of random walkers which have no memory of their past history. Many physical applications, however, call for a model in which the choice of possible directions for the walker's next step are given by probabilities which are influenced by the path it took prior to making that choice, so that its jumps are correlated; this is often called a *persistent* or *correlated* random walk [2].

A walk with zero memory corresponds to the Bernoulli process of the usual uncorrelated random walk. Walks with single-step memories are the most commonly studied cases of persistent random walks, where the random walker determines the direction it takes at a given step in terms of the direction taken on the immediately preceding step [1]. Such walks—not necessarily restricted to lattices, as will be the case here—were first discussed in the context of Brownian motion [3] and fluid dynamics [4], and have since found many applications in the physics literature, most prominently in polymer conformation theory [5] and tracer diffusion in metals [6], but also in relation to the telegrapher's equation in the context of thermodynamics [7]. Previous works dealing with random walks on lattices with higher order memory effects include that of Montroll [8], with applications to models of polymers, and Bender and Richmond [9].

The state of the walker is thus specified by two variables, its location and the direction it took at the preceding step. The statistical properties of such persistent walks can be described by simple Markov chains and have already been thoroughly investigated in the literature; see in particular [10]. We will only provide a short review of results relevant to our purposes, with specific emphasis on the diffusive properties.

The statistics of random walks with multi-step memory can in principle be analysed in terms of Markov chains, in a similar way to their single-step memory counterpart. However, the number of states of these chains grows exponentially with the number of steps accounted for. This is the source of great technical difficulties, which are present already at the level of two-step processes.

Of specific interest to us are random walks with a two-step memory. Among the class of persistent walks under consideration, these are the simplest case beyond those with a single-step memory, and are therefore relevant to problems dealing with the persistence of motion of tracer particles where the single-step-memory approximation breaks down. An example where this occurs is given in recent work by the present authors, on diffusion in a class of periodic billiard tables [11].

The paper is organized as follows. The general framework of walks on lattices is briefly reviewed in section 2, where we provide the expression of the diffusion coefficient of such walks in terms of the velocity autocorrelations. Successive approximation schemes for the computation of these autocorrelation functions are presented in sections 3, 4 and 5, pertaining to the number of steps of memory of the walkers, respectively 0, 1 and 2. Specific examples are discussed, namely the one-dimensional lattice and the two-dimensional square, honeycomb and triangular lattices, and their diffusion coefficients are computed. Section 6 provides an alternative derivation of the diffusion coefficients of two-step memory persistent walks with special left–right symmetries. Conclusions are drawn in section 7.

2. Diffusion on a lattice

We consider the motion of independent tracer particles undergoing random walks on a regular lattice $\mathscr{L}$. Their trajectories are specified by their initial position $\boldsymbol{r}_0$ at time $t = 0$, and the sequence $\{\boldsymbol{v}_0, \dots, \boldsymbol{v}_n\}$ of the successive values $\boldsymbol{v}_i \in \mathscr{V}_{\boldsymbol{r}_i}$ of their direction vectors at positions $\boldsymbol{r}_i$, where $\mathscr{V}_{\boldsymbol{r}_i}$ denotes the space of direction vectors allowed at site $\boldsymbol{r}_i$, which point to the lattice sites adjacent to $\boldsymbol{r}_i$. Here we consider dynamics in discrete time, so that the time sequences are simply assumed to be incremented by identical time steps τ as the tracers move from site to site. In what follows we will loosely refer to the direction vectors as velocity vectors; they are in fact dimensionless unit vectors.

Examples of such motions are random walks on one- and two-dimensional lattices such as honeycomb, square and triangular lattices, but also include persistent random walks where memory effects must be accounted for, i.e. when the probability of occurrence of $\boldsymbol{v}_n$ depends on the past history $\boldsymbol{v}_{n-1}, \boldsymbol{v}_{n-2}, \dots$.

The quantity we will be concerned with is the diffusion coefficient D of such persistent processes, which measures the linear growth in time of the mean-squared displacement of walkers. This can be written in terms of velocity autocorrelations using the Taylor–Green–Kubo expression:

$$D = \frac{\ell^2}{2d\tau}\left[1 + 2\lim_{K\to\infty}\sum_{n=1}^{K}\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n\rangle\right], \tag{2.1}$$

where d denotes the dimensionality of the lattice $\mathscr{L}$, and ℓ is the lattice spacing. The (dimensionless) velocity autocorrelations are computed as averages $\langle\cdot\rangle$ over the equilibrium distribution μ, so that the problem reduces to computing

$$\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n\rangle = \sum_{\boldsymbol{v}_0,\ldots,\boldsymbol{v}_n} \boldsymbol{v}_0 \cdot \boldsymbol{v}_n\, \mu(\{\boldsymbol{v}_0,\ldots,\boldsymbol{v}_n\}). \tag{2.2}$$

As reviewed below, this can be easily carried out in the simple examples of random walks with zero- and single-step memories. The main achievement of this paper is to describe the computation of the velocity autocorrelations of random walks with two-step memory. All these cases involve factorizations of the measure $\mu(\{\boldsymbol{v}_0,\ldots,\boldsymbol{v}_n\})$ by products of probability measures which depend on a number of velocity vectors, equal to the number of steps of memory of the walkers. These measures will be denoted by p throughout the paper.

The next three sections, sections 3, 4 and 5, are devoted to the computation of the diffusion coefficient (2.1) for random walks with zero-, one- and two-step memories, respectively.

3. No-memory approximation (NMA)

In the simplest case, the walkers have no memory of their history as they proceed to their next position. This gives a Bernoulli process for the velocity trials, for which the probability measure factorizes:

$$\mu(\{\boldsymbol{v}_0,\ldots,\boldsymbol{v}_n\}) = \prod_{i=0}^{n} p(\boldsymbol{v}_i). \tag{3.1}$$

Given that the lattice is isotropic and that p is uniform, the velocity autocorrelation (2.2) vanishes:

$$\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n\rangle = \delta_{n,0}. \tag{3.2}$$

The diffusion coefficient of the random walk without memory is then given by

$$D_{\mathrm{NMA}} = \frac{\ell^2}{2d\tau}. \tag{3.3}$$

4. One-step memory approximation (1-SMA)

We now assume that the velocity vectors obey a Markov process for which $\boldsymbol{v}_n$ takes on different values according to the velocity at the previous step $\boldsymbol{v}_{n-1}$. We may then write

$$\mu(\{\boldsymbol{v}_0,\ldots,\boldsymbol{v}_n\}) = \prod_{i=1}^{n} P(\boldsymbol{v}_i|\boldsymbol{v}_{i-1})p(\boldsymbol{v}_0). \tag{4.1}$$

Here, $P(\mathbf{b}|\mathbf{a})$ denotes the one-step conditional probability that the walker moves in a direction $\mathbf{b}$, given that it had direction $\mathbf{a}$ at the previous step.

We denote by z the coordination number of the lattice, i.e. the number of neighbouring sites accessible from each site, and we denote by R the rotation operation which takes a vector $\boldsymbol{v}$ through all the lattice directions $\boldsymbol{v}, \mathsf{R}\boldsymbol{v}, \ldots, \mathsf{R}^{z-1}\boldsymbol{v}$. In general, the set of allowed orientations of $\boldsymbol{v}$ depends on the lattice site, such as in the two-dimensional honeycomb lattice. We denote by T the symmetry operator that maps a cell to its neighbours, which corresponds simply to the identity for square lattices and to a reflection for the honeycomb lattice.

The idea of our calculation is to express each velocity vector $\boldsymbol{v}_k$ in terms of the first one, $\boldsymbol{v}_0$, as $\boldsymbol{v}_k = \mathsf{R}^{i_k}\mathsf{T}^k\boldsymbol{v}_0$, where i_k lies between 0 and $z-1$. Substituting this into the expression for the velocity autocorrelation $\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n\rangle$, equation (2.2), we obtain

$$\sum_{\boldsymbol{v}_0,\ldots,\boldsymbol{v}_n} \boldsymbol{v}_0 \cdot \boldsymbol{v}_n \prod_{i=1}^{n} P(\boldsymbol{v}_i|\boldsymbol{v}_{i-1})p(\boldsymbol{v}_0) = \sum_{i_0,\ldots,i_n=1}^{z} \boldsymbol{v}_0 \cdot \mathsf{R}^{i_n}\mathsf{T}^n\boldsymbol{v}_0\, \mathsf{m}_{i_n,i_{n-1}} \cdots \mathsf{m}_{i_1,i_0}\mathsf{p}_{i_0}, \tag{4.2}$$

where

$$\mathsf{m}_{i_n,i_{n-1}} \equiv P(\mathsf{R}^{i_n}\mathsf{T}^n\boldsymbol{v}_0|\mathsf{R}^{i_{n-1}}\mathsf{T}^{n-1}\boldsymbol{v}_0) \tag{4.3}$$

are the elements of the stochastic matrix M of the Markov chain associated with the persistent random walk, and $\mathsf{p}_i \equiv p(\mathbf{i})$ are the elements of its invariant (equilibrium) distribution, denoted P, evaluated with a velocity in the ith lattice direction. The invariance of P is expressed as $\sum_j \mathsf{m}_{i,j}\mathsf{p}_j = \mathsf{p}_i$. These notations will be used throughout this paper.

The terms involving M in (4.2) constitute the matrix product of n copies of M. Furthermore, since the invariant distribution is uniform over the z possible lattice directions, we can choose an arbitrary direction for $\boldsymbol{v}_0$, and hence write

$$\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n\rangle = \boldsymbol{v}_0 \cdot \mathsf{T}^n\boldsymbol{v}_0\, \mathsf{m}^{(n)}_{1,1} + \boldsymbol{v}_0 \cdot \mathsf{R}\mathsf{T}^n\boldsymbol{v}_0\, \mathsf{m}^{(n)}_{2,1} + \cdots + \boldsymbol{v}_0 \cdot \mathsf{R}^{z-1}\mathsf{T}^n\boldsymbol{v}_0\, \mathsf{m}^{(n)}_{z,1}, \tag{4.4}$$

where $\mathsf{m}^{(n)}_{i,j}$ denote the elements of M^n.

Under special symmetry assumptions to be discussed in the examples below, one has

$$\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n\rangle = \langle \cos\theta\rangle^n, \tag{4.5}$$

where $\langle \cos\theta\rangle$ denotes the average angle between two successive velocity vectors. It is then a general, well-known, result for such symmetric persistent random walks with single-step memory [2] that their diffusion coefficients have the form

$$D_{\mathrm{1SMA}} = D_{\mathrm{NMA}}\frac{1+\langle\cos\theta\rangle}{1-\langle\cos\theta\rangle} \quad \text{(symmetric walks)}. \tag{4.6}$$

The actual value of the diffusion coefficient depends on the probabilities $P(\mathsf{R}^j\mathsf{T}\boldsymbol{v}|\boldsymbol{v})$, which are parameters of the model. Specific applications of equation (4.6) are given in the examples below, such as shown in figure 1. To simplify the notation, we denote the conditional probabilities of these walks by P_j, where $j = 0, \ldots, z-1$ corresponds to the relative angle $2\pi j/z$ of the direction that the walker takes with respect to its previous step (up to a reflection in the case of the honeycomb lattice). These conventions are shown in figure 2.

4.1. One-dimensional lattice

The simplest case is that of a regular one-dimensional lattice. In this case, each site is equivalent, and so T is the identity. Each velocity vector $\boldsymbol{v}_k$ has only two possible values, v and $-v$, so that R is a reflection. We denote by $P_0 \equiv P(v|v)$ the probability that the random walker continues in the same direction at the next step, and by $P_1 \equiv P(-v|v)$ the probability that it reverses direction.

It is easy to check that the velocity autocorrelation (4.4) yields (4.5):

$$\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n\rangle = (P_0 - P_1)^n = \langle\cos\theta\rangle^n, \tag{4.7}$$

and so the diffusion coefficient is given by

$$D_{\mathrm{1SMA}} = D_{\mathrm{NMA}}\frac{P_0}{P_1}. \tag{4.8}$$

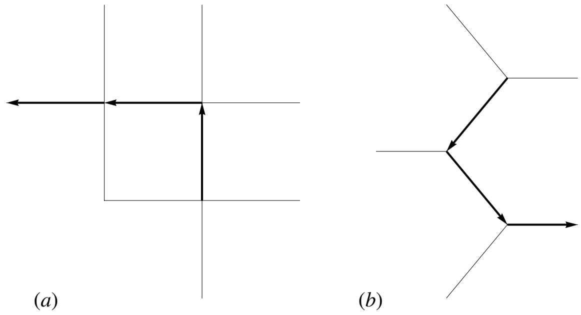

Figure 1. Examples of walks on (*a*) square and (*b*) honeycomb lattices. Note the inversion of the allowed directions at neighbouring sites on the honeycomb lattice.

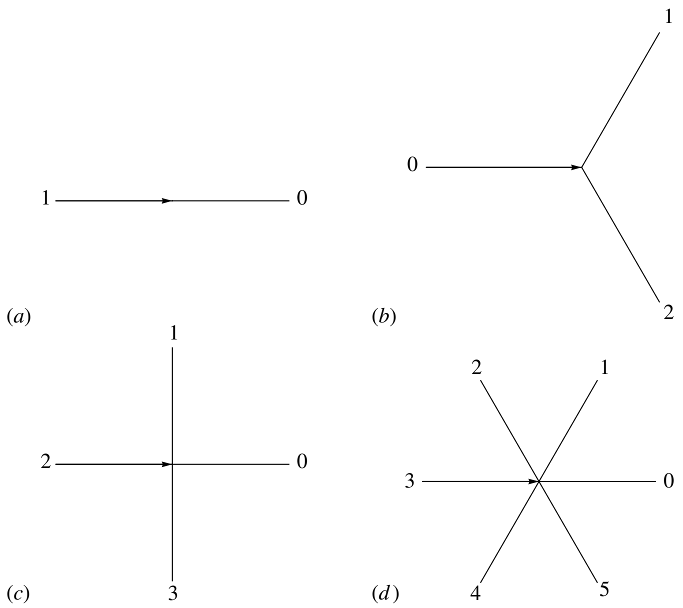

Figure 2. The possible directions of motion at a given step for different lattices, *relative* to the incoming direction which is shown by the arrow, are labelled from 0 to $z-1$, corresponding to the angle $2\pi j/z$ that the lattice direction j makes with respect to the reference direction, up to a reflection inversion in the case of the honeycomb lattice. (*a*) One-dimensional lattice ($z=2$); (*b*) honeycomb lattice ($z=3$); (*c*) square lattice ($z=4$); (*d*) triangular lattice ($z=6$).

4.2. Two-dimensional square lattice

On a two-dimensional square lattice, $\boldsymbol{v}_k$ can take four possible values, and each lattice site is again equivalent. Thus, T is the identity and R can be taken as an anticlockwise rotation by angle $\pi/2$. We denote by $P_0 \equiv P(\boldsymbol{v}|\boldsymbol{v})$ the probability that the particle proceeds in the same direction as on its previous step, by $P_1 \equiv P(\mathsf{R}\boldsymbol{v}|\boldsymbol{v})$ the probability that the particle turns to the left relative to its previous direction, by $P_2 \equiv P(\mathsf{R}^2\boldsymbol{v}|\boldsymbol{v})$ the probability that it turns around and by $P_3 \equiv P(\mathsf{R}^3\boldsymbol{v}|\boldsymbol{v})$ the probability that it turns right.

From (4.4), the velocity autocorrelation $\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n \rangle$ is given by

$$\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n \rangle = \mathsf{m}_{1,1}^{(n)} - \mathsf{m}_{1,3}^{(n)}. \tag{4.9}$$

The transition matrix M given by (4.3) is thus the following cyclic matrix:

$$\mathsf{M} = \begin{pmatrix} P_0 & P_1 & P_2 & P_3 \\ P_3 & P_0 & P_1 & P_2 \\ P_2 & P_3 & P_0 & P_1 \\ P_1 & P_2 & P_3 & P_0 \end{pmatrix}. \tag{4.10}$$

To calculate the elements $\mathsf{m}_{i,j}^{(n)}$ of the powers M^n, it is possible to compute the eigenvalues and eigenvectors of M and then decompose it as $\mathsf{M} = \mathsf{Q}\cdot\mathsf{L}\cdot\mathsf{Q}^{-1}$, where L is the diagonal matrix of the eigenvalues of M and Q is the matrix of its eigenvectors. This procedure is, however, not necessary here, since we only require the combination of $\mathsf{m}_{i,j}^{(n)}$ which appears in (4.9). To proceed, we label the *distinct* entries of M^n as $\mathsf{a}_i^{(n)}$, using the fact that M^n is also cyclic if M is:

$$\mathsf{M}^n \equiv \begin{pmatrix} \mathsf{a}_1^{(n)} & \mathsf{a}_2^{(n)} & \mathsf{a}_3^{(n)} & \mathsf{a}_4^{(n)} \\ \mathsf{a}_4^{(n)} & \mathsf{a}_1^{(n)} & \mathsf{a}_2^{(n)} & \mathsf{a}_3^{(n)} \\ \mathsf{a}_3^{(n)} & \mathsf{a}_4^{(n)} & \mathsf{a}_1^{(n)} & \mathsf{a}_2^{(n)} \\ \mathsf{a}_2^{(n)} & \mathsf{a}_3^{(n)} & \mathsf{a}_4^{(n)} & \mathsf{a}_1^{(n)} \end{pmatrix}. \tag{4.11}$$

Writing $\mathsf{M}^n = \mathsf{M}\mathsf{M}^{n-1}$, we can exploit the particular structure of the matrix to reduce it from a (4×4) matrix to a (2×2) matrix, by considering the following differences:

$$\begin{aligned} \begin{pmatrix} \mathsf{a}_1^{(n)} - \mathsf{a}_3^{(n)} \\ \mathsf{a}_2^{(n)} - \mathsf{a}_4^{(n)} \end{pmatrix} &= \begin{pmatrix} P_0 - P_2 & P_3 - P_1 \\ P_1 - P_3 & P_0 - P_2 \end{pmatrix} \begin{pmatrix} \mathsf{a}_1^{(n-1)} - \mathsf{a}_3^{(n-1)} \\ \mathsf{a}_2^{(n-1)} - \mathsf{a}_4^{(n-1)} \end{pmatrix} \\ &= \begin{pmatrix} P_0 - P_2 & P_3 - P_1 \\ P_1 - P_3 & P_0 - P_2 \end{pmatrix}^{n-1} \begin{pmatrix} P_0 - P_2 \\ P_1 - P_3 \end{pmatrix}. \end{aligned} \tag{4.12}$$

The velocity autocorrelation (4.9) is thus given by

$$\begin{aligned} \langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n \rangle &= \mathsf{a}_1^{(n)} - \mathsf{a}_3^{(n)} \\ &= (1 \quad 0) \begin{pmatrix} P_0 - P_2 & P_3 - P_1 \\ P_1 - P_3 & P_0 - P_2 \end{pmatrix}^{n-1} \begin{pmatrix} P_0 - P_2 \\ P_1 - P_3 \end{pmatrix}. \end{aligned} \tag{4.13}$$

Summing the previous expression over all n, and using the fact that $\sum_{n=0}^{\infty} \mathsf{A}^n = (\mathsf{I} - \mathsf{A})^{-1}$ for a matrix A, where I is the identity matrix, we obtain the diffusion coefficient (2.1) as

$$D_{1\mathrm{SMA}} = D_{\mathrm{NMA}} \left[1 + 2(1 \quad 0) \begin{pmatrix} 1 - P_0 + P_2 & P_1 - P_3 \\ P_3 - P_1 & 1 - P_0 + P_2 \end{pmatrix}^{-1} \begin{pmatrix} P_0 - P_2 \\ P_1 - P_3 \end{pmatrix} \right]. \tag{4.14}$$

For a symmetric process in which $P_1 = P_3$, which is often imposed by a symmetry of the physical system, equation (4.5) holds, and the diffusion coefficient takes the form (4.6), namely

$$D_{1\mathrm{SMA}} = D_{\mathrm{NMA}} \frac{1 + P_0 - P_2}{1 - P_0 + P_2}. \tag{4.15}$$

If, however, $P_1 \neq P_3$, then equation (4.6) is no longer valid. Instead, we have the more complicated expression

$$D_{1\mathrm{SMA}} = D_{\mathrm{NMA}} \frac{1 - (P_0 - P_2)^2 - (P_1 - P_3)^2}{(1 - P_0 + P_2)^2 + (P_1 - P_3)^2}. \tag{4.16}$$

Such asymmetric walks are the lattice equivalent of the continuous-space models of persistent random walks with chirality considered in [12].

4.3. Two-dimensional honeycomb lattice

On the two-dimensional honeycomb lattice, shown in figure 1(*b*), each site has $z = 3$ neighbours. Here, R is taken to be a clockwise rotation[3] by angle $2\pi/3$ and the arrangement of neighbours differs by a reflection T. We denote by $P_0 \equiv P(-\boldsymbol{v}|\boldsymbol{v})$ the probability that the particle turns around, $P_1 \equiv P(-\mathsf{R}^2\boldsymbol{v}|\boldsymbol{v})$ that it turns left relative to its previous direction and $P_2 \equiv P(-\mathsf{R}\boldsymbol{v}|\boldsymbol{v})$ that it turns right. The transition matrix M is thus

$$\mathsf{M} = \begin{pmatrix} P_0 & P_1 & P_2 \\ P_2 & P_0 & P_1 \\ P_1 & P_2 & P_0 \end{pmatrix}. \tag{4.17}$$

Proceeding as with the square lattice, we let

$$\mathsf{M}^n \equiv \begin{pmatrix} \mathsf{a}_1^{(n)} & \mathsf{a}_2^{(n)} & \mathsf{a}_3^{(n)} \\ \mathsf{a}_3^{(n)} & \mathsf{a}_1^{(n)} & \mathsf{a}_2^{(n)} \\ \mathsf{a}_2^{(n)} & \mathsf{a}_3^{(n)} & \mathsf{a}_1^{(n)} \end{pmatrix}, \tag{4.18}$$

and obtain the matrix equation

$$\begin{aligned} \begin{pmatrix} -\mathsf{a}_1^{(n)} + \frac{1}{2}\big[\mathsf{a}_2^{(n)} + \mathsf{a}_3^{(n)}\big] \\ -\mathsf{a}_2^{(n)} + \frac{1}{2}\big[\mathsf{a}_1^{(n)} + \mathsf{a}_3^{(n)}\big] \\ -\mathsf{a}_3^{(n)} + \frac{1}{2}\big[\mathsf{a}_1^{(n)} + \mathsf{a}_2^{(n)}\big] \end{pmatrix} &= \begin{pmatrix} P_0 & P_1 & P_2 \\ P_2 & P_0 & P_1 \\ P_1 & P_2 & P_0 \end{pmatrix} \begin{pmatrix} -\mathsf{a}_1^{(n-1)} + \frac{1}{2}\big[\mathsf{a}_2^{(n-1)} + \mathsf{a}_3^{(n-1)}\big] \\ -\mathsf{a}_2^{(n-1)} + \frac{1}{2}\big[\mathsf{a}_1^{(n-1)} + \mathsf{a}_3^{(n-1)}\big] \\ -\mathsf{a}_3^{(n-1)} + \frac{1}{2}\big[\mathsf{a}_1^{(n-1)} + \mathsf{a}_2^{(n-1)}\big] \end{pmatrix}, \\ &= \frac{1}{2} \begin{pmatrix} P_0 & P_1 & P_2 \\ P_2 & P_0 & P_1 \\ P_1 & P_2 & P_0 \end{pmatrix}^{n-1} \begin{pmatrix} 1 - 3P_0 \\ 1 - 3P_2 \\ 1 - 3P_1 \end{pmatrix}. \end{aligned} \tag{4.19}$$

The velocity autocorrelation (4.4) is thus

$$\begin{aligned} \langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n \rangle &= -\mathsf{a}_1^{(n)} + \frac{1}{2}\big[\mathsf{a}_2^{(n)} + \mathsf{a}_3^{(n)}\big], \\ &= \frac{1}{2}(1 \quad 0 \quad 0) \begin{pmatrix} P_0 & P_1 & P_2 \\ P_2 & P_0 & P_1 \\ P_1 & P_2 & P_0 \end{pmatrix}^{n-1} \begin{pmatrix} 1 - 3P_0 \\ 1 - 3P_2 \\ 1 - 3P_1 \end{pmatrix}. \end{aligned} \tag{4.20}$$

Hence, the diffusion coefficient (2.1) is

$$D_{\mathrm{1SMA}} = D_{\mathrm{NMA}} \left[1 + (1 \quad 0 \quad 0) \begin{pmatrix} 1 - P_0 & -P_1 & -P_2 \\ -P_2 & 1 - P_0 & -P_1 \\ -P_1 & -P_2 & 1 - P_0 \end{pmatrix}^{-1} \begin{pmatrix} 1 - 3P_0 \\ 1 - 3P_2 \\ 1 - 3P_1 \end{pmatrix} \right]. \tag{4.21}$$

Again, in the case of an isotropic process for which $P_2 = P_1 \equiv P_{\mathrm{s}}$ ('symmetric'), equation (4.5) holds, and substituting $P_{\mathrm{s}} = (1 - P_0)/2$ gives the following expression for the diffusion coefficient:

$$D_{\mathrm{1SMA}} = D_{\mathrm{NMA}} \frac{1 - P_0 + P_{\mathrm{s}}}{1 + P_0 - P_{\mathrm{s}}} = D_{\mathrm{NMA}} \frac{3(1 - P_0)}{1 + 3P_0}. \tag{4.22}$$

For an asymmetric process for which $P_1 \neq P_2$, defining the symmetric and antisymmetric parts $P_{\mathrm{s}} \equiv (P_1 + P_2)/2$ and $P_{\mathrm{a}} \equiv (P_1 - P_2)/2$, we instead obtain

[3] We take a clockwise rotation as opposed to an anticlockwise one in the other examples so that the lattice directions are still labelled anticlockwise.

$$\begin{aligned} D_{1\mathrm{SMA}} &= D_{\mathrm{NMA}} \frac{1 - 3P_{\mathrm{a}}^2 - (P_0 - P_{\mathrm{s}})^2}{3P_{\mathrm{a}}^2 + (1 + P_0 - P_{\mathrm{s}})^2}, \\ &= D_{\mathrm{NMA}} \frac{3(1 - P_0)(1 + 3P_0) - 12P_{\mathrm{a}}^2}{(1 + 3P_0)^2 + 12P_{\mathrm{a}}^2}. \end{aligned} \tag{4.23}$$

4.4. Two-dimensional triangular lattice

Persistent walks on a triangular lattice were made popular by Fink and Mao [13] in connection with tie knots. Here, each site has $z = 6$ neighbours, so that R is an anticlockwise rotation by angle $\pi/3$. Following our convention (see figure 2(*d*)), we denote by $P_0 \equiv P(\boldsymbol{v}|\boldsymbol{v})$ the probability that the particle moves forward, $P_1 \equiv P(\mathsf{R}\boldsymbol{v}|\boldsymbol{v})$ that it moves in the forward left direction relative to its previous direction and similarly for P_2, P_3, P_4 and P_5.

Proceeding along the lines of the previous subsection, we let

$$\mathsf{M}^n \equiv \begin{pmatrix} \mathsf{a}_1^{(n)} & \mathsf{a}_2^{(n)} & \cdots & \mathsf{a}_6^{(n)} \\ \mathsf{a}_6^{(n)} & \mathsf{a}_1^{(n)} & \cdots & \mathsf{a}_5^{(n)} \\ \vdots & \vdots & \ddots & \vdots \\ \mathsf{a}_2^{(n)} & \mathsf{a}_3^{(n)} & \cdots & \mathsf{a}_1^{(n)} \end{pmatrix}, \tag{4.24}$$

in terms of which the velocity autocorrelation (4.4) is given by

$$\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n \rangle = \mathsf{a}_1^{(n)} + \tfrac{1}{2}\big[\mathsf{a}_2^{(n)} + \mathsf{a}_6^{(n)} - \mathsf{a}_3^{(n)} - \mathsf{a}_5^{(n)}\big] - \mathsf{a}_4^{(n)}. \tag{4.25}$$

A computation similar to that of equation (4.19) yields

$$\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n \rangle = (1 \quad 0 \quad \cdots \quad 0) \begin{pmatrix} P_0 & P_1 & \cdots & P_5 \\ P_5 & P_0 & \cdots & P_4 \\ \vdots & \vdots & \ddots & \vdots \\ P_1 & P_2 & \cdots & P_0 \end{pmatrix}^{n-1} \begin{pmatrix} P_0 - P_3 + \frac{1}{2}(P_1 - P_2 - P_4 + P_5) \\ P_1 - P_4 + \frac{1}{2}(P_2 - P_3 - P_5 + P_0) \\ \vdots \\ P_5 - P_2 + \frac{1}{2}(P_0 - P_1 - P_3 + P_4) \end{pmatrix}. \tag{4.26}$$

The diffusion coefficient (2.1) is then

$$\begin{aligned} D_{1\mathrm{SMA}} = D_{\mathrm{NMA}} \Bigg[& 1 + (1 \quad 0 \quad \cdots \quad 0) \begin{pmatrix} 1 - P_0 & -P_1 & \cdots & -P_5 \\ -P_5 & 1 - P_0 & \cdots & -P_4 \\ \vdots & \vdots & \ddots & \vdots \\ -P_1 & -P_2 & \cdots & 1 - P_0 \end{pmatrix}^{-1} \\ & \times \begin{pmatrix} P_0 - P_3 + \frac{1}{2}(P_1 - P_2 - P_4 + P_5) \\ P_1 - P_4 + \frac{1}{2}(P_2 - P_3 - P_5 + P_0) \\ \vdots \\ P_5 - P_2 + \frac{1}{2}(P_0 - P_1 - P_3 + P_4) \end{pmatrix} \Bigg]. \end{aligned} \tag{4.27}$$

4.5. d-dimensional hypercubic lattice

The case of a hypercubic lattice in arbitrary dimension d with coordination number $z = 2d$ can also be treated, provided that the same probability P_{s} is assigned to scattering along all new directions which are perpendicular to the previous direction of motion. We then have

$P_0 + P_{z/2} + 2(d-1)P_{\mathrm{s}} = 1$, and the invariant distribution of velocities $p(\boldsymbol{v}) = 1/(2d)$ is uniform. We then recover an expression similar to (4.15) for the diffusion coefficient in this case.

5. Two-step memory approximation (2-SMA)

We now turn to the main contribution of this paper, namely the development of a technique for the calculation of the diffusion coefficient for persistent random walks with a 2-step memory on lattices.

We thus assume that the velocity vectors obey a random process for which the probability of $\boldsymbol{v}_n$ takes on different values according to the velocities at the two previous steps, $\boldsymbol{v}_{n-1}$ and $\boldsymbol{v}_{n-2}$, so that we may write

$$\mu(\{\boldsymbol{v}_0, \ldots, \boldsymbol{v}_n\}) = \prod_{i=2}^{n} P(\boldsymbol{v}_i|\boldsymbol{v}_{i-1}, \boldsymbol{v}_{i-2})\, p(\boldsymbol{v}_0, \boldsymbol{v}_1). \tag{5.1}$$

The velocity autocorrelation function (2.2) is then

$$\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n\rangle = \sum_{\{\boldsymbol{v}_n,\ldots,\boldsymbol{v}_0\}} \boldsymbol{v}_0 \cdot \boldsymbol{v}_n \prod_{i=2}^{n} P(\boldsymbol{v}_i|\boldsymbol{v}_{i-1}, \boldsymbol{v}_{i-2})\, p(\boldsymbol{v}_0, \boldsymbol{v}_1). \tag{5.2}$$

The calculation of these correlations proceeds in the most straightforward way by transposing the calculation leading to equation (2.2) to the two-step probability transitions as characterizing the probability transitions of a two-dimensional Markov chain. Considering a lattice with coordination number z, the state of the Markov chain is a normalized vector of dimension z^2. The time evolution is specified by the $(z^2 \times z^2)$ stochastic matrix M with entries

$$\mathsf{m}_{i=(i_1-1)z+i_2,\, j=(j_1-1)z+j_2} \equiv \delta_{i_2,j_1} P(\mathsf{R}^{i_1}\mathsf{T}^2\boldsymbol{v}|\mathsf{R}^{j_1}\mathsf{T}\boldsymbol{v}, \mathsf{R}^{j_2}\boldsymbol{v}), \tag{5.3}$$

where i_1, i_2, j_1 and j_2 take values between 1 and z. Denoting by P the invariant distribution of this Markov chain, i.e. the z^2-dimensional vector with components p_i such that $\sum_{j=1}^{z^2} \mathsf{m}_{i,j}\mathsf{p}_j = \mathsf{p}_i$, equation (5.2) becomes

$$\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n\rangle = \sum_{i_0,i_n=1}^{z^2} \mathsf{J}^{(n)}_{i_n,i_0}\, \mathsf{m}^{(n-1)}_{i_n,i_0}\, \mathsf{p}_{i_0}, \tag{5.4}$$

where $\mathsf{J}^{(n)}$ is the $(z^2 \times z^2)$ matrix with elements

$$\mathsf{J}^{(n)}_{i=(i_1-1)z+i_2,\, j=(j_1-1)z+j_2} \equiv \boldsymbol{e}_{i_1} \cdot \mathsf{T}^n \boldsymbol{e}_{j_2}, \tag{5.5}$$

and $\boldsymbol{e}_k$ denotes the unit vector along the kth lattice direction.

Using the symmetries of the problem and writing $P_{jk} = P(\mathsf{R}^k\mathsf{T}\mathsf{R}^j\mathsf{T}\boldsymbol{v}|\mathsf{R}^j\mathsf{T}\boldsymbol{v}, \boldsymbol{v})$ for the conditional probability of turning successively by angles $2\pi j/z$ and $2\pi k/z$ with respect to the current direction (with reflection by T where needed), we define $\phi \equiv \exp(2\mathrm{i}\pi/z)$, where i denotes the imaginary unit, $\mathrm{i} = \sqrt{-1}$, and show, through the examples below, that equation (5.4) reduces to the general expression

$$\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n\rangle = \sigma^n \frac{z}{2}(1 \quad \cdots \quad 1) \left[\begin{pmatrix} P_{0\,0} & P_{1\,0} & \cdots & P_{z-1,0} \\ \phi P_{0\,1} & \phi P_{1\,1} & \cdots & \phi P_{z-1,1} \\ \vdots & \vdots & \ddots & \vdots \\ \phi^{z-1}P_{0,z-1} & \phi^{z-1}P_{1,z-1} & \cdots & \phi^{z-1}P_{z-1,1} \end{pmatrix}^{n-1} \right.$$
$$\times\, \mathrm{diag}(1, \phi, \ldots, \phi^{z-1})$$

$$
+ \begin{pmatrix} P_{00} & P_{10} & \cdots & P_{z-1,0} \\ \phi^{-1} P_{01} & \phi^{-1} P_{11} & \cdots & \phi^{-1} P_{z-1,1} \\ \vdots & \vdots & \ddots & \vdots \\ \phi^{1-z} P_{0,z-1} & \phi^{1-z} P_{1,z-1} & \cdots & \phi^{1-z} P_{z-1,1} \end{pmatrix}^{n-1}
$$

$$
\left. \times \operatorname{diag}(1, \phi^{-1}, \ldots, \phi^{1-z}) \right] \begin{pmatrix} \mathsf{p}_1 \\ \vdots \\ \mathsf{p}_z \end{pmatrix}, \tag{5.6}
$$

where $\operatorname{diag}(1, \phi, \ldots, \phi^{z-1})$ denotes the matrix with elements listed on the main diagonal and 0 elsewhere. Here, σ is a sign factor which is -1 for the honeycomb lattice and $+1$ for the other lattices, and reflects the action of T. Note that the second term in the summation is the complex conjugate of the first, so that the result is real. The main result of our paper follows, which is the expression of the diffusion coefficient for persistent random walks with 2-step memory:

$$
\frac{D_{\mathrm{2SMA}}}{D_{\mathrm{NMA}}} = 1 + \sigma z (1 \cdots 1) \left[\begin{pmatrix} 1 - P_{00} & -P_{10} & \cdots & -P_{z-1,0} \\ -\phi P_{01} & 1 - \phi P_{11} & \cdots & -\phi P_{z-1,1} \\ \vdots & \vdots & \ddots & \vdots \\ -\phi^{z-1} P_{0,z-1} & -\phi^{z-1} P_{1,z-1} & \cdots & 1 - \phi^{z-1} P_{z-1,1} \end{pmatrix}^{-1} \right.
$$

$$
\times \operatorname{diag}(1, \phi, \ldots, \phi^{z-1})
$$

$$
+ \begin{pmatrix} 1 - P_{00} & -P_{10} & \cdots & -P_{z-1,0} \\ -\phi^{-1} P_{01} & -\phi^{-1} P_{11} & \cdots & -\phi^{-1} P_{z-1,1} \\ \vdots & \vdots & \ddots & \vdots \\ -\phi^{1-z} P_{0,z-1} & -\phi^{1-z} P_{1,z-1} & \cdots & 1 - \phi^{1-z} P_{z-1,1} \end{pmatrix}^{-1}
$$

$$
\left. \times \operatorname{diag}(1, \phi^{-1}, \ldots, \phi^{1-z}) \right] \begin{pmatrix} \mathsf{p}_1 \\ \vdots \\ \mathsf{p}_z \end{pmatrix}. \tag{5.7}
$$

The remainder of this section serves to illustrate the derivation of this formula in the specific examples of a walk on a one-dimensional lattice, and on a two-dimensional honeycomb lattice. Similar arguments can be used to establish the validity of equation (5.7) in the case of square and triangular lattices.

5.1. One-dimensional lattice

We first consider the simplest case, namely the one-dimensional lattice. The stochastic matrix M from equation (5.3) is the (4×4) matrix

$$\mathsf{M} = \begin{pmatrix} P(v|v,v) & P(v|v,-v) & 0 & 0 \\ 0 & 0 & P(-v|v,-v) & P(-v|v,v) \\ P(-v|v,v) & P(-v|v,-v) & 0 & 0 \\ 0 & 0 & P(v|v,-v) & P(v|v,v) \end{pmatrix},$$
$$= \begin{pmatrix} P_{00} & P_{10} & 0 & 0 \\ 0 & 0 & P_{11} & P_{01} \\ P_{01} & P_{11} & 0 & 0 \\ 0 & 0 & P_{10} & P_{00} \end{pmatrix}, \tag{5.8}$$

where $P_{00} + P_{01} = 1$ and $P_{10} + P_{11} = 1$.

Considering equation (5.4), we compute the invariant distribution of M, which is the vector P whose components correspond to the four states $p(v, v)$, $p(-v, v)$, $p(v, -v)$ and $p(-v, -v)$. Given that we must have $p(-v, -v) = p(v, v)$ and $p(v, -v) = p(-v, v)$, the equilibrium distribution is obtained as the solution of the system of equations

$$\begin{aligned} p(v, v) &= P_{00}\, p(v, v) + P_{10}\, p(-v, v), \\ p(v, v) &+ p(-v, v) = \tfrac{1}{2}, \end{aligned} \tag{5.9}$$

giving

$$\begin{aligned} \mathsf{p}_1 = \mathsf{p}_4 = p(v, v) &= \frac{P_{10}}{2[1 - P_{00} + P_{10}]}, \\ \mathsf{p}_2 = \mathsf{p}_3 = p(-v, v) &= \frac{1 - P_{00}}{2[1 - P_{00} + P_{10}]}. \end{aligned} \tag{5.10}$$

The matrix $\mathsf{J}^{(n)}$, equation (5.5), is here the same for all n, and has the expression

$$\mathsf{J} = \begin{pmatrix} 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ -1 & 1 & -1 & 1 \end{pmatrix}. \tag{5.11}$$

The velocity autocorrelation (5.4) is thus

$$\begin{aligned} \langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n \rangle = 2\big[&\big(\mathsf{m}_{1,1}^{(n-1)} - \mathsf{m}_{1,4}^{(n-1)} + \mathsf{m}_{3,4}^{(n-1)} - \mathsf{m}_{3,1}^{(n-1)}\big)\mathsf{p}_1 \\ &+ \big(\mathsf{m}_{1,3}^{(n-1)} - \mathsf{m}_{1,2}^{(n-1)} + \mathsf{m}_{3,2}^{(n-1)} - \mathsf{m}_{3,3}^{(n-1)}\big)\mathsf{p}_2\big], \\ = 2\,(1 \quad 1) &\begin{pmatrix} \mathsf{m}_{1,1}^{(n-1)} - \mathsf{m}_{1,4}^{(n-1)} & \mathsf{m}_{1,3}^{(n-1)} - \mathsf{m}_{1,2}^{(n-1)} \\ \mathsf{m}_{3,4}^{(n-1)} - \mathsf{m}_{3,1}^{(n-1)} & \mathsf{m}_{3,2}^{(n-1)} - \mathsf{m}_{3,3}^{(n-1)} \end{pmatrix} \begin{pmatrix} \mathsf{p}_1 \\ \mathsf{p}_2 \end{pmatrix}. \end{aligned} \tag{5.12}$$

Since M^n, the nth power of M, has the symmetries of M, its entries $\mathsf{m}_{i,j}^{(n)}$ are such that

$$\begin{aligned} \mathsf{m}_{1,1}^{(n)} &= \mathsf{m}_{4,4}^{(n)} \equiv \mathsf{a}_1^{(n)}, & \mathsf{m}_{2,1}^{(n)} &= \mathsf{m}_{3,4}^{(n)} \equiv \mathsf{b}_4^{(n)}, \\ \mathsf{m}_{1,2}^{(n)} &= \mathsf{m}_{4,3}^{(n)} \equiv \mathsf{a}_2^{(n)}, & \mathsf{m}_{2,2}^{(n)} &= \mathsf{m}_{3,3}^{(n)} \equiv \mathsf{b}_3^{(n)}, \\ \mathsf{m}_{1,3}^{(n)} &= \mathsf{m}_{4,2}^{(n)} \equiv \mathsf{a}_3^{(n)}, & \mathsf{m}_{2,3}^{(n)} &= \mathsf{m}_{3,2}^{(n)} \equiv \mathsf{b}_2^{(n)}, \\ \mathsf{m}_{1,4}^{(n)} &= \mathsf{m}_{4,1}^{(n)} \equiv \mathsf{a}_4^{(n)}, & \mathsf{m}_{2,4}^{(n)} &= \mathsf{m}_{3,1}^{(n)} \equiv \mathsf{b}_1^{(n)}. \end{aligned} \tag{5.13}$$

Writing $\mathsf{M}^n = \mathsf{M}\mathsf{M}^{n-1}$, we obtain two separate sets of equations for (2×2) matrices, one involving $\mathsf{a}_1^{(n)}, \mathsf{a}_4^{(n)}$ and $\mathsf{b}_1^{(n)}, \mathsf{b}_4^{(n)}$, and the other involving $\mathsf{a}_2^{(n)}, \mathsf{a}_3^{(n)}$ and $\mathsf{b}_2^{(n)}, \mathsf{b}_3^{(n)}$:

$$\begin{aligned} \begin{pmatrix} \mathsf{a}_1^{(n)} & \mathsf{a}_4^{(n)} \\ \mathsf{b}_1^{(n)} & \mathsf{b}_4^{(n)} \end{pmatrix} &= \begin{pmatrix} P_{00} & P_{10} \\ P_{01} & P_{11} \end{pmatrix} \begin{pmatrix} \mathsf{a}_1^{(n-1)} & \mathsf{a}_4^{(n-1)} \\ \mathsf{b}_4^{(n-1)} & \mathsf{b}_1^{(n-1)} \end{pmatrix}, \\ \begin{pmatrix} \mathsf{a}_2^{(n)} & \mathsf{a}_3^{(n)} \\ \mathsf{b}_2^{(n)} & \mathsf{b}_3^{(n)} \end{pmatrix} &= \begin{pmatrix} P_{00} & P_{10} \\ P_{01} & P_{11} \end{pmatrix} \begin{pmatrix} \mathsf{a}_2^{(n-1)} & \mathsf{a}_3^{(n-1)} \\ \mathsf{b}_3^{(n-1)} & \mathsf{b}_2^{(n-1)} \end{pmatrix}. \end{aligned} \tag{5.14}$$

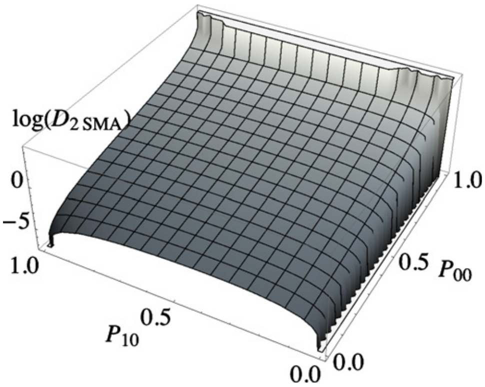

Figure 3. Diffusion coefficient of the two-step memory walk on a one-dimensional lattice, equation (5.17), as a function of its two parameters, $P_{0\,0}$ and $P_{1\,0}$.

Note that these equations do not have a simple recursive form, since the elements of the matrices on the two sides do not appear in the same places. However, taking the differences $\mathsf{a}_1^{(n)} - \mathsf{a}_4^{(n)}$, $\mathsf{a}_3^{(n)} - \mathsf{a}_2^{(n)}$, $\mathsf{b}_4^{(n)} - \mathsf{b}_1^{(n)}$ and $\mathsf{b}_2^{(n)} - \mathsf{b}_3^{(n)}$, we obtain the recursive system

$$\begin{aligned}
\begin{pmatrix} \mathsf{a}_1^{(n)} - \mathsf{a}_4^{(n)} & \mathsf{a}_3^{(n)} - \mathsf{a}_2^{(n)} \\ \mathsf{b}_4^{(n)} - \mathsf{b}_1^{(n)} & \mathsf{b}_2^{(n)} - \mathsf{b}_3^{(n)} \end{pmatrix} &= \begin{pmatrix} P_{0\,0} & P_{1\,0} \\ -P_{0\,1} & -P_{1\,1} \end{pmatrix} \begin{pmatrix} \mathsf{a}_1^{(n-1)} - \mathsf{a}_4^{(n-1)} & \mathsf{a}_3^{(n-1)} - \mathsf{a}_2^{(n-1)} \\ \mathsf{b}_4^{(n-1)} - \mathsf{b}_1^{(n-1)} & \mathsf{b}_2^{(n-1)} - \mathsf{b}_3^{(n-1)} \end{pmatrix}, \\
&= \begin{pmatrix} P_{0\,0} & P_{1\,0} \\ -P_{0\,1} & -P_{1\,1} \end{pmatrix}^{n-1} \begin{pmatrix} \mathsf{a}_1^{(1)} - \mathsf{a}_4^{(1)} & \mathsf{a}_3^{(1)} - \mathsf{a}_2^{(1)} \\ \mathsf{b}_4^{(1)} - \mathsf{b}_1^{(1)} & \mathsf{b}_2^{(1)} - \mathsf{b}_3^{(1)} \end{pmatrix}, \\
&= \begin{pmatrix} P_{0\,0} & P_{1\,0} \\ -P_{0\,1} & -P_{1\,1} \end{pmatrix}^{n-1} \begin{pmatrix} P_{0\,0} & -P_{1\,0} \\ -P_{0\,1} & P_{1\,1} \end{pmatrix}, \\
&= \begin{pmatrix} P_{0\,0} & P_{1\,0} \\ -P_{0\,1} & -P_{1\,1} \end{pmatrix}^{n} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \qquad (5.15)
\end{aligned}$$

Plugging this equation into equation (5.12), we obtain

$$\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n \rangle = 2\,(1 \quad 1) \begin{pmatrix} P_{0\,0} & P_{1\,0} \\ -P_{0\,1} & -P_{1\,1} \end{pmatrix}^{n-1} \begin{pmatrix} \mathsf{p}_1 \\ -\mathsf{p}_2 \end{pmatrix}. \qquad (5.16)$$

This is equation (5.6), where $\phi = \exp(2\mathrm{i}\pi/2) = -1$. The diffusion coefficient is therefore given by equation (5.7):

$$\begin{aligned}
D_{2\mathrm{SMA}} &= D_{\mathrm{NMA}} \left[1 + 4(1 \quad 1) \begin{pmatrix} 1 - P_{0\,0} & -P_{1\,0} \\ P_{0\,1} & 1 + P_{1\,1} \end{pmatrix}^{-1} \begin{pmatrix} \mathsf{p}_1 \\ -\mathsf{p}_2 \end{pmatrix} \right], \\
&= D_{\mathrm{NMA}} \frac{P_{1\,0}}{[1 - P_{0\,0}]} \frac{[1 + P_{0\,0} - P_{1\,0}]}{[1 - P_{0\,0} + P_{1\,0}]}. \qquad (5.17)
\end{aligned}$$

It is a function of the two parameters $P_{0\,0}$ and $P_{1\,0}$, with graph shown in figure 3; when these are equal, the process reduces to a walk with single-step memory, and the diffusion coefficient to that of the single-step memory approximation (4.8), as it should.

5.2. Two-dimensional honeycomb lattice

For the two-dimensional honeycomb lattice, the stochastic matrix M of equation (5.3) is a (9×9) matrix with the following non-zero entries:

$$
\begin{aligned}
\mathsf{m}_{1,1} &= \mathsf{m}_{5,5} = \mathsf{m}_{9,9} = P(\boldsymbol{v}| - \boldsymbol{v}, \boldsymbol{v}) = P_{0\,0},\\
\mathsf{m}_{1,2} &= \mathsf{m}_{5,6} = \mathsf{m}_{9,7} = P(\mathsf{R}^2\boldsymbol{v}| - \mathsf{R}^2\boldsymbol{v}, \boldsymbol{v}) = P_{1\,0},\\
\mathsf{m}_{1,3} &= \mathsf{m}_{5,4} = \mathsf{m}_{9,8} = P(\mathsf{R}\boldsymbol{v}| - \mathsf{R}\boldsymbol{v}, \boldsymbol{v}) = P_{2\,0},\\
\mathsf{m}_{4,1} &= \mathsf{m}_{8,5} = \mathsf{m}_{3,9} = P(\mathsf{R}\boldsymbol{v}| - \boldsymbol{v}, \boldsymbol{v}) = P_{0\,2},\\
\mathsf{m}_{4,2} &= \mathsf{m}_{8,6} = \mathsf{m}_{3,7} = P(\boldsymbol{v}| - \mathsf{R}^2\boldsymbol{v}, \boldsymbol{v}) = P_{1\,2},\\
\mathsf{m}_{4,3} &= \mathsf{m}_{8,4} = \mathsf{m}_{3,8} = P(\mathsf{R}^2\boldsymbol{v}| - \mathsf{R}\boldsymbol{v}, \boldsymbol{v}) = P_{2\,2},\\
\mathsf{m}_{7,1} &= \mathsf{m}_{2,5} = \mathsf{m}_{6,9} = P(\mathsf{R}^2\boldsymbol{v}| - \boldsymbol{v}, \boldsymbol{v}) = P_{0\,1},\\
\mathsf{m}_{7,2} &= \mathsf{m}_{2,6} = \mathsf{m}_{6,7} = P(\mathsf{R}\boldsymbol{v}| - \mathsf{R}^2\boldsymbol{v}, \boldsymbol{v}) = P_{1\,1},\\
\mathsf{m}_{7,3} &= \mathsf{m}_{2,4} = \mathsf{m}_{6,8} = P(\boldsymbol{v}| - \mathsf{R}\boldsymbol{v}, \boldsymbol{v}) = P_{2\,1}.
\end{aligned}
\tag{5.18}
$$

Given the three constraints

$$
\begin{aligned}
P_{0\,0} + P_{0\,1} + P_{0\,2} &= 1,\\
P_{1\,0} + P_{1\,1} + P_{1\,2} &= 1,\\
P_{2\,0} + P_{2\,1} + P_{2\,2} &= 1,
\end{aligned}
\tag{5.19}
$$

the actual number of independent parameters is 6. Note that the matrix M, as in the one-dimensional case of the previous subsection, can be thought of as a cyclic matrix of 3×3 blocks, where the blocks themselves are however also cyclically permuted.

The invariant distribution P with components p_i can be written in terms of the three probabilities $p(\boldsymbol{v}, -\boldsymbol{v})$, $p(\boldsymbol{v}, -\mathsf{R}\boldsymbol{v})$, $p(\boldsymbol{v}, -\mathsf{R}^2\boldsymbol{v})$,

$$
\begin{aligned}
\mathsf{p}_1 &= \mathsf{p}_5 = \mathsf{p}_9 = p(\boldsymbol{v}, -\boldsymbol{v}),\\
\mathsf{p}_2 &= \mathsf{p}_6 = \mathsf{p}_7 = p(\boldsymbol{v}, -\mathsf{R}\boldsymbol{v}),\\
\mathsf{p}_3 &= \mathsf{p}_4 = \mathsf{p}_8 = p(\boldsymbol{v}, -\mathsf{R}^2\boldsymbol{v}),
\end{aligned}
\tag{5.20}
$$

which are solutions of the system of equations

$$
p(\boldsymbol{v}, -\boldsymbol{v}) = P_{0\,0}\, p(\boldsymbol{v}, -\boldsymbol{v}) + P_{1\,0}\, p(\boldsymbol{v}, -\mathsf{R}^2\boldsymbol{v}) + P_{2\,0}\, p(\boldsymbol{v}, -\mathsf{R}\boldsymbol{v}), \tag{5.21}
$$

$$
p(\boldsymbol{v}, -\mathsf{R}^2\boldsymbol{v}) = P_{0\,1}\, p(\boldsymbol{v}, -\boldsymbol{v}) + P_{1\,1}\, p(\boldsymbol{v}, -\mathsf{R}^2\boldsymbol{v}) + P_{2\,1}\, p(\boldsymbol{v}, -\mathsf{R}\boldsymbol{v}), \tag{5.22}
$$

$$
p(\boldsymbol{v}, -\boldsymbol{v}) + p(\boldsymbol{v}, -\mathsf{R}\boldsymbol{v}) + p(\boldsymbol{v}, -\mathsf{R}^2\boldsymbol{v}) = \tfrac{1}{3}. \tag{5.23}
$$

The matrix (5.5) has the block structure

$$
\mathsf{J}^{(n)} = (-1)^n \begin{pmatrix} \mathsf{B}_1 & \mathsf{B}_1 & \mathsf{B}_1 \\ \mathsf{B}_2 & \mathsf{B}_2 & \mathsf{B}_2 \\ \mathsf{B}_3 & \mathsf{B}_3 & \mathsf{B}_3 \end{pmatrix}, \tag{5.24}
$$

where

$$
\mathsf{B}_1 = \begin{pmatrix} -1 & 1/2 & 1/2 \\ -1 & 1/2 & 1/2 \\ -1 & 1/2 & 1/2 \end{pmatrix}, \quad
\mathsf{B}_2 = \begin{pmatrix} 1/2 & -1 & 1/2 \\ 1/2 & -1 & 1/2 \\ 1/2 & -1 & 1/2 \end{pmatrix}, \quad
\mathsf{B}_3 = \begin{pmatrix} 1/2 & 1/2 & -1 \\ 1/2 & 1/2 & -1 \\ 1/2 & 1/2 & -1 \end{pmatrix}. \tag{5.25}
$$

Substituting these expressions into equation (5.4), we find

$$\begin{aligned}\langle \boldsymbol{v}_{n+1}\cdot\boldsymbol{v}_0\rangle &= 3(-1)^{n+1}\Bigg\{\Bigg[\mathsf{m}^{(n)}_{1,1} - \frac{1}{2}\mathsf{m}^{(n)}_{1,5} - \frac{1}{2}\mathsf{m}^{(n)}_{1,9} - \frac{1}{2}\mathsf{m}^{(n)}_{4,1} + \mathsf{m}^{(n)}_{4,5} - \frac{1}{2}\mathsf{m}^{(n)}_{4,9} - \frac{1}{2}\mathsf{m}^{(n)}_{7,1}\\ &\quad - \frac{1}{2}\mathsf{m}^{(n)}_{7,5} + \mathsf{m}^{(n)}_{7,9}\Bigg]\mathsf{p}_1 + \Bigg[-\frac{1}{2}\mathsf{m}^{(n)}_{1,2} - \frac{1}{2}\mathsf{m}^{(n)}_{1,6} + \mathsf{m}^{(n)}_{1,7} + \mathsf{m}^{(m,n)}_{4,2} - \frac{1}{2}\mathsf{m}^{(n)}_{4,6}\\ &\quad - \frac{1}{2}\mathsf{m}^{(n)}_{4,7} - \frac{1}{2}\mathsf{m}^{(n)}_{7,2} + \mathsf{m}^{(n)}_{7,6} - \frac{1}{2}\mathsf{m}^{(n)}_{7,7}\Bigg]\mathsf{p}_2 + \Bigg[-\frac{1}{2}\mathsf{m}^{(n)}_{1,3} + \mathsf{m}^{(n)}_{1,4} - \frac{1}{2}\mathsf{m}^{(n)}_{1,8}\\ &\quad - \frac{1}{2}\mathsf{m}^{(n)}_{4,3} - \frac{1}{2}\mathsf{m}^{(n)}_{4,4} + \mathsf{m}^{(n)}_{4,8} + \mathsf{m}^{(n)}_{7,3} - \frac{1}{2}\mathsf{m}^{(n)}_{7,4} - \frac{1}{2}\mathsf{m}^{(n)}_{7,8}\Bigg]\mathsf{p}_3\Bigg\},\\ &= 3(-1)^{n+1}(1\quad 1\quad 1)\\ &\quad\times\begin{pmatrix} \mathsf{m}^{(n)}_{1,1} - \frac{1}{2}\mathsf{m}^{(n)}_{1,5} - \frac{1}{2}\mathsf{m}^{(n)}_{1,9} & -\frac{1}{2}\mathsf{m}^{(n)}_{1,2} - \frac{1}{2}\mathsf{m}^{(n)}_{1,6} + \mathsf{m}^{(n)}_{1,7} & -\frac{1}{2}\mathsf{m}^{(n)}_{1,3} + \mathsf{m}^{(n)}_{1,4} - \frac{1}{2}\mathsf{m}^{(n)}_{1,8}\\ -\frac{1}{2}\mathsf{m}^{(n)}_{7,1} - \frac{1}{2}\mathsf{m}^{(n)}_{7,5} + \mathsf{m}^{(n)}_{7,9} & -\frac{1}{2}\mathsf{m}^{(n)}_{7,2} + \mathsf{m}^{(n)}_{7,6} - \frac{1}{2}\mathsf{m}^{(n)}_{7,7} & \mathsf{m}^{(n)}_{7,3} - \frac{1}{2}\mathsf{m}^{(n)}_{7,4} - \frac{1}{2}\mathsf{m}^{(n)}_{7,8}\\ -\frac{1}{2}\mathsf{m}^{(n)}_{4,1} + \mathsf{m}^{(n)}_{4,5} - \frac{1}{2}\mathsf{m}^{(n)}_{4,9} & \mathsf{m}^{(n)}_{4,2} - \frac{1}{2}\mathsf{m}^{(n)}_{4,6} - \frac{1}{2}\mathsf{m}^{(n)}_{4,7} & -\frac{1}{2}\mathsf{m}^{(n)}_{4,3} - \frac{1}{2}\mathsf{m}^{(n)}_{4,4} + \mathsf{m}^{(n)}_{4,8}\end{pmatrix}\\ &\quad\times\begin{pmatrix}\mathsf{p}_1\\ \mathsf{p}_2\\ \mathsf{p}_3\end{pmatrix}.\end{aligned}\tag{5.26}$$

Proceeding along the lines of the computation presented in subsection 5.1, we obtain a set of recursive matrix equations (A.9) involving the coefficients of M^n. We refer the reader to appendix A for the details of this derivation.

We note that the coefficients which appear in equation (5.26) satisfy identities such as, for instance,

$$\begin{aligned}\mathsf{m}^{(n)}_{1,1} - \tfrac{1}{2}\mathsf{m}^{(n)}_{1,5} - \tfrac{1}{2}\mathsf{m}^{(n)}_{1,9} &= \tfrac{1}{2}\big[\mathsf{m}^{(n)}_{1,1} + \mathrm{e}^{2\mathrm{i}\pi/3}\mathsf{m}^{(n)}_{1,5} + \mathrm{e}^{-2\mathrm{i}\pi/3}\mathsf{m}^{(n)}_{1,9}\big]\\ &\quad + \tfrac{1}{2}\big[\mathsf{m}^{(n)}_{1,1} + \mathrm{e}^{-2\mathrm{i}\pi/3}\mathsf{m}^{(n)}_{1,5} + \mathrm{e}^{2\mathrm{i}\pi/3}\mathsf{m}^{(n)}_{1,9}\big].\end{aligned}\tag{5.27}$$

Thus, letting $\phi = \exp(2\mathrm{i}\pi/3)$, we can combine the results of equation (A.9) with equation (5.26) to find

$$\begin{aligned}\langle \boldsymbol{v}_n\cdot\boldsymbol{v}_0\rangle = (-1)^n\frac{3}{2}(1\quad 1\quad 1)&\left[\begin{pmatrix}P_{00} & P_{10} & P_{20}\\ \phi P_{01} & \phi P_{11} & \phi P_{21}\\ \phi^2 P_{02} & \phi^2 P_{12} & \phi^2 P_{22}\end{pmatrix}^{n-1}\begin{pmatrix}1 & 0 & 0\\ 0 & \phi & 0\\ 0 & 0 & \phi^2\end{pmatrix}\right.\\ &\left. + \begin{pmatrix}P_{00} & P_{10} & P_{20}\\ \phi^2 P_{01} & \phi^2 P_{11} & \phi^2 P_{21}\\ \phi P_{02} & \phi P_{12} & \phi P_{22}\end{pmatrix}^{n-1}\begin{pmatrix}1 & 0 & 0\\ 0 & \phi^2 & 0\\ 0 & 0 & \phi\end{pmatrix}\right]\begin{pmatrix}\mathsf{p}_1\\ \mathsf{p}_2\\ \mathsf{p}_3\end{pmatrix}.\end{aligned}\tag{5.28}$$

This is equation (5.6). The diffusion coefficient (2.1) is therefore given by (5.7), which is here

$$\begin{aligned}\frac{D_{\mathrm{2SMA}}}{D_{\mathrm{NMA}}} = 1 - 3(1\quad 1\quad 1)&\left[\begin{pmatrix}1+P_{00} & P_{10} & P_{20}\\ \phi P_{01} & 1+\phi P_{11} & \phi P_{21}\\ \phi^2 P_{02} & \phi^2 P_{12} & 1+\phi^2 P_{22}\end{pmatrix}^{-1}\begin{pmatrix}1 & 0 & 0\\ 0 & \phi & 0\\ 0 & 0 & \phi^2\end{pmatrix}\right.\\ &\left. + \begin{pmatrix}1+P_{00} & P_{10} & P_{20}\\ \phi^2 P_{01} & 1+\phi^2 P_{11} & \phi^2 P_{21}\\ \phi P_{02} & \phi P_{12} & 1+\phi P_{22}\end{pmatrix}^{-1}\begin{pmatrix}1 & 0 & 0\\ 0 & \phi^2 & 0\\ 0 & 0 & \phi\end{pmatrix}\right]\begin{pmatrix}\mathsf{p}_1\\ \mathsf{p}_2\\ \mathsf{p}_3\end{pmatrix}.\end{aligned}\tag{5.29}$$

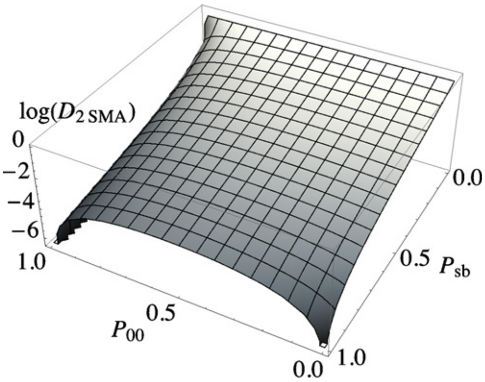

Figure 4. Diffusion coefficient of the two-step memory completely symmetric walk on a two-dimensional honeycomb lattice, equation (5.33), as a function of its two parameters, P_{00} and P_{sb}.

Given a symmetric process for which left and right probabilities are equal, but the probability of a left–left turn is different than that of a right–left turn, we let

$$\begin{aligned} &P_{02} = P_{01} \equiv P_{\mathrm{bs}} = \frac{1 - P_{00}}{2}, \\ &P_{10} = P_{20} \equiv P_{\mathrm{sb}}, \qquad P_{11} = P_{22} \equiv P_{\mathrm{ss}}, \qquad P_{12} = P_{21} = 1 - P_{\mathrm{sb}} - P_{\mathrm{ss}}. \end{aligned} \tag{5.30}$$

Carrying out the matrix inversions in (5.29), we find the diffusion coefficient

$$D_{2\mathrm{SMA}} = D_{\mathrm{NMA}} \frac{3(1 - P_{00})(1 + P_{00} - P_{\mathrm{sb}})(2 - P_{\mathrm{sb}} - 2P_{\mathrm{ss}})}{(1 - P_{00} + P_{\mathrm{sb}})[P_{\mathrm{sb}}(7 + P_{00} - 8P_{\mathrm{ss}}) + 2(1 + P_{00})P_{\mathrm{ss}} - 4P_{\mathrm{sb}}^2]}. \tag{5.31}$$

If we further assume complete left–right symmetry and identify the probabilities of left–left turns and left–right turns, thus letting

$$P_{12} = P_{21} = P_{11} = P_{22} = \frac{1 - P_{\mathrm{sb}}}{2}, \tag{5.32}$$

equation (5.31) simplifies to

$$D_{2\mathrm{SMA}} = D_{\mathrm{NMA}} \frac{3(1 - P_{00})(1 + P_{00} - P_{\mathrm{sb}})}{(1 - P_{00} + P_{\mathrm{sb}})(1 + P_{00} + 2P_{\mathrm{sb}})}. \tag{5.33}$$

A graphical representation is displayed in figure 4.

6. Two-step memory approximation revisited

As seen in the previous section, the symbolic computation of (5.4) quickly becomes tricky. However, an alternative to the above scheme can be found, provided that the walk has special symmetries. Returning to (5.2), we write

$$\begin{aligned} \langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n \rangle = \sum_{\boldsymbol{v}_0} \sum_{i_1,\ldots,i_n} &\boldsymbol{v}_0 \cdot \mathsf{S}^{i_1,\ldots,i_n} \boldsymbol{v}_0 P(\mathsf{S}^{i_1,\ldots,i_n} \boldsymbol{v}_0 | \mathsf{S}^{i_1,\ldots,i_{n-1}} \boldsymbol{v}_0, \mathsf{S}^{i_1,\ldots,i_{n-2}} \boldsymbol{v}_0) \\ &\times \cdots \times P(\mathsf{S}^{i_1,i_2} \boldsymbol{v}_0 | \mathsf{S}^{i_1} \boldsymbol{v}_0, \boldsymbol{v}_0) p(\boldsymbol{v}_0, \mathsf{S}^{i_1} \boldsymbol{v}_0), \end{aligned} \tag{6.1}$$

where we introduce the compact notation $\mathsf{S}^i \equiv \mathsf{R}^i \mathsf{T}$, and sequences in the exponent denote multiple composition: $\mathsf{S}^{i_1,\ldots,i_n} \equiv \mathsf{S}^{i_n} \circ \mathsf{S}^{i_{n-1}} \circ \cdots \circ \mathsf{S}^{i_1}$, where each i_k takes values between 1 and z. Note that in general $\mathsf{S}^j \circ \mathsf{S}^i \neq \mathsf{S}^{i+j}$ when T is non-trivial. The transition probabilities

$P(\mathsf{S}^{j_2}\boldsymbol{v}_0|\mathsf{S}^{j_1}\boldsymbol{v}_0, S^{j_0}\boldsymbol{v}_0)$ can be seen as matrix elements $\tilde{\mathsf{Q}}_{j_2-j_1,j_1-j_0}$, so that (6.1) may be rewritten as

$$\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n \rangle = \sum_{\boldsymbol{v}_0} \sum_{i_1,\dots,i_n} \boldsymbol{v}_0 \cdot \mathsf{S}^{i_1,\dots,i_n} \boldsymbol{v}_0 \tilde{\mathsf{Q}}_{i_n,i_{n-1}} \cdots \tilde{\mathsf{Q}}_{i_2,i_1} p(\boldsymbol{v}_0, \mathsf{S}^{i_1}\boldsymbol{v}_0). \tag{6.2}$$

We would like to rewrite this expression as a matrix product. However, this is in general not possible, and further approximations are needed. Thus, assuming that the scalar product $\boldsymbol{v}_n \cdot \boldsymbol{v}_0$ factorizes as

$$\mathsf{S}^{i_1,\dots,i_n} \boldsymbol{v}_0 \cdot \boldsymbol{v}_0 = \prod_{k=1}^{n} \mathsf{S}^{i_k} \boldsymbol{v}_0 \cdot \boldsymbol{v}_0, \tag{6.3}$$

and defining

$$\mathsf{Q}_{i,j} \equiv \tilde{\mathsf{Q}}_{i,j} \mathsf{S}^j \boldsymbol{v}_0 \cdot \boldsymbol{v}_0 = P(\mathsf{S}^{j,i}\boldsymbol{v}_0|\mathsf{S}^j\boldsymbol{v}_0, \boldsymbol{v}_0)\mathsf{S}^j\boldsymbol{v}_0 \cdot \boldsymbol{v}_0, \tag{6.4}$$

equation (6.2) becomes

$$\begin{aligned}\langle \boldsymbol{v}_0 \cdot \boldsymbol{v}_n \rangle &= \sum_{\boldsymbol{v}_0} \sum_{i_1,\dots,i_n} \boldsymbol{v}_0 \cdot \mathsf{S}^{i_n} \boldsymbol{v}_0 \mathsf{Q}_{i_n,i_{n-1}} \cdots \mathsf{Q}_{i_2,i_1}\, p(\boldsymbol{v}_0, \mathsf{S}^{i_1}\boldsymbol{v}_0),\\ &= z \sum_{i_1,i_n} \mathsf{V}^\dagger_{i_n} \mathsf{Q}^{n-1}_{i_n,i_1} \mathsf{p}_{i_1},\end{aligned} \tag{6.5}$$

where we have introduced the vectors $\mathsf{V}_{i_n} \equiv \boldsymbol{v}_0 \cdot \mathsf{S}^{i_n}\boldsymbol{v}_0$ and $\mathsf{p}_{i_1} \equiv p(\boldsymbol{v}_0, \mathsf{S}^{i_1}\boldsymbol{v}_0)$. As can be seen, equation (6.5) has an appropriate matrix form and can easily be resummed over n to compute the diffusion coefficient (2.1).

Since Q is a $(z \times z)$ matrix, equation (6.5) is much easier to evaluate than (5.4). The trouble is that equation (6.3) is in general incorrect, and turns out to be strictly valid only for one-dimensional walks. Nonetheless, it may also be applied to higher dimensional walks satisfying special symmetry conditions. We consider the different geometries separately in the following and discuss the conditions under which equation (6.5) can be applied. For higher dimensional lattices, we recover by this simpler method the results obtained earlier under the relevant symmetry assumptions.

6.1. One-dimensional lattice

The result (5.17) follows from equation (6.5). Indeed, $\mathsf{R}^{i_n,\dots,i_1}\boldsymbol{v}_0 \cdot \boldsymbol{v}_0 = \mathsf{R}^{i_n+\cdots+i_1}\boldsymbol{v}_0 \cdot \boldsymbol{v}_0 = \pm 1$ according to the parity of $i_n + \cdots + i_1$, and since this is also a property of the product $\prod_{k=1}^{n} \mathsf{R}^{i_k}\boldsymbol{v}_0 \cdot \boldsymbol{v}_0$, we see that equation (6.3) is valid.

The vector p_i on the right-hand side of equation (6.5) is

$$\begin{aligned}\mathsf{p}_1 &= p(-v, v) = \frac{1 - P_{00}}{2(1 - P_{00} + P_{10})},\\ \mathsf{p}_2 &= p(v, v) = \frac{P_{10}}{2(1 - P_{00} + P_{10})}.\end{aligned} \tag{6.6}$$

The vector V_i, on the other hand, has components

$$\begin{aligned}\mathsf{V}_1 &= -1,\\ \mathsf{V}_2 &= 1.\end{aligned} \tag{6.7}$$

The matrix elements $\mathsf{Q}_{i,j}$ are defined according to equation (6.4):

$$\begin{aligned}\mathsf{Q} &= \begin{pmatrix} -P_{11} & P_{01} \\ -P_{10} & P_{00} \end{pmatrix}\\ &= \begin{pmatrix} P_{10} - 1 & 1 - P_{00} \\ -P_{10} & P_{00} \end{pmatrix}.\end{aligned} \tag{6.8}$$

Considering equation (2.1) and plugging the above expressions into equation (6.5), we have

$$D_{2SMA} = D_{NMA}\{1 + 4\mathsf{V}^{\dagger}[\mathsf{I}_2 - \mathsf{Q}]^{-1}\mathsf{P}\}, \tag{6.9}$$

and we recover equation (5.17).

6.2. *Two-dimensional honeycomb lattice*

Consider equation (6.3) in the case of a honeycomb lattice. The operation $\mathsf{S}^i\boldsymbol{v}$ is a clockwise rotation of $\boldsymbol{v}$ by angle $-\pi/3$ if $i = 1$, $\pi/3$ if $i = 2$, or π if $i = 3$. The operation $\mathsf{S}^{i_1,\dots,i_n}\boldsymbol{v}$ is thus a rotation by angle $[2(i_1 + \cdots + i_n) - 3n]\pi/3$, and the scalar product

$$\mathsf{S}^{i_1,\dots,i_n}\boldsymbol{v}\cdot\boldsymbol{v} = \cos[2(i_1 + \cdots + i_n) - 3n]\pi/3. \tag{6.10}$$

This expression is in general different from the product

$$\mathsf{S}^{i_n}\boldsymbol{v}\cdot\boldsymbol{v}\cdots\mathsf{S}^{i_1}\boldsymbol{v}\cdot\boldsymbol{v} = \prod_{k=1}^{n}\cos[2(i_k) - 3]\pi/3. \tag{6.11}$$

This is so, for instance, when $n = 2$ and $i_1 = i_2 = 1$, for which (6.10) yields $-1/2$, whereas (6.11) yields $1/4$.

There is however a special case under which the product structure that we seek can be retrieved, as follows. There are *a priori* nine transition probabilities $P(\mathsf{S}^{j,i}\boldsymbol{v}|\mathsf{S}^j\boldsymbol{v},\boldsymbol{v})$. There are, however, a number of left–right symmetries in the system which reduce the number of independent transition probabilities to 3:

$$P(\mathsf{S}^{1,1}\boldsymbol{v}|\mathsf{S}^1\boldsymbol{v},\boldsymbol{v}),\ P(\mathsf{S}^{3,3}\boldsymbol{v}|\mathsf{S}^3\boldsymbol{v},\boldsymbol{v}),\ P(\mathsf{S}^{1,2}\boldsymbol{v}|\mathsf{S}^1\boldsymbol{v},\boldsymbol{v}). \tag{6.12}$$

In the event that the two probabilities $P(\mathsf{S}^{1,2}\boldsymbol{v}|\mathsf{S}^1\boldsymbol{v},\boldsymbol{v})$ and $P(\mathsf{S}^{1,1}\boldsymbol{v}|\mathsf{S}^1\boldsymbol{v},\boldsymbol{v})$ are equal

$$P(\mathsf{S}^{1,2}\boldsymbol{v}|\mathsf{S}^1\boldsymbol{v},\boldsymbol{v}) = P(\mathsf{S}^{1,1}\boldsymbol{v}|\mathsf{S}^1\boldsymbol{v},\boldsymbol{v}) \equiv P_{ss}, \tag{6.13}$$

which is to say that forward–left and right scatterings are treated as identical events, then the number of independent parameters reduces to 2, which we take to be P_{00} and P_{ss}.

In this case, the expression of the diffusion coefficient can be obtained in a way similar to equation (5.17) for the one-dimensional lattice. This is so because

$$\begin{aligned}\mathsf{S}^{i_1\dots,i_{n-1},1}\boldsymbol{v}\cdot\boldsymbol{v} &= \cos\left\{[2(i_1 + \cdots + i_{n-1} + 1) - 3n]\frac{\pi}{3}\right\}\\ &= \cos\frac{\pi}{3}\cos\left\{[2(i_1 + \cdots + i_{n-1}) - 3(n-1)]\frac{\pi}{3}\right\}\\ &\quad + \sin\frac{\pi}{3}\sin\left\{[2(i_1 + \cdots + i_{n-1}) - 3(n-1)]\frac{\pi}{3}\right\},\end{aligned} \tag{6.14}$$

$$\begin{aligned}\mathsf{S}^{i_1\dots,i_{n-1},2}\boldsymbol{v}\cdot\boldsymbol{v} &= \cos\left\{[2(i_1 + \cdots + i_{n-1} + 2) - 3n]\frac{\pi}{3}\right\}\\ &= \cos\frac{\pi}{3}\cos\left\{[2(i_1 + \cdots + i_{n-1}) - 3(n-1)]\frac{\pi}{3}\right\}\\ &\quad - \sin\frac{\pi}{3}\sin\left\{[2(i_1 + \cdots + i_{n-1}) - 3(n-1)]\frac{\pi}{3}\right\},\end{aligned} \tag{6.15}$$

$$\begin{aligned}\mathsf{S}^{i_1\dots,i_{n-1},3}\boldsymbol{v}\cdot\boldsymbol{v} &= \cos\left\{[2(i_1 + \cdots + i_{n-1} + 3) - 3n]\frac{\pi}{3}\right\}\\ &= -\cos\left\{[2(i_1 + \cdots + i_{n-1}) - 3(n-1)]\frac{\pi}{3}\right\}.\end{aligned} \tag{6.16}$$

Thus, given the symmetry between forward–left and right scatterings, the two sine contributions in equations (6.14) and (6.15) cancel, whereas the cosines add up to 1:

$$\begin{aligned}\mathsf{S}^{i_1\ldots,i_{n-1},1}\boldsymbol{v}\cdot\boldsymbol{v} + \mathsf{S}^{i_1\ldots,i_{n-1},2}\boldsymbol{v}\cdot\boldsymbol{v} &= \mathsf{S}^{i_1\ldots,i_{n-1}}\boldsymbol{v}\cdot\boldsymbol{v},\\ &= \mathsf{S}^{i_1\ldots,i_{n-1}}\boldsymbol{v}\cdot\boldsymbol{v}(\mathsf{S}^1\boldsymbol{v}\cdot\boldsymbol{v} + \mathsf{S}^2\boldsymbol{v}\cdot\boldsymbol{v}),\end{aligned}\tag{6.17}$$

$$\mathsf{S}^{i_1\ldots,i_{n-1},3}\boldsymbol{v}\cdot\boldsymbol{v} = -\mathsf{S}^{i_1\ldots,i_{n-1}}\boldsymbol{v}\cdot\boldsymbol{v} = \mathsf{S}^{i_1\ldots,i_{n-1}}\boldsymbol{v}\cdot\boldsymbol{v}\,\mathsf{S}^3\boldsymbol{v}\cdot\boldsymbol{v}.\tag{6.18}$$

We therefore retrieve an effective product structure, as in equation (6.3), and can compute the diffusion coefficient using equation (6.5), with

$$\mathsf{P} = \frac{1}{3(2-2P_{\mathrm{ss}}-P_{00})}\begin{pmatrix}\frac{1}{2}(1-P_{00})\\ 1-2P_{\mathrm{ss}}\end{pmatrix},\tag{6.19}$$

$$\mathsf{V} = \begin{pmatrix}1\\-1\end{pmatrix},\tag{6.20}$$

and

$$\mathsf{Q} = \begin{pmatrix}P_{\mathrm{ss}} & 1/2P_{00}-1/2\\ 1-2P_{\mathrm{ss}} & -P_{00}\end{pmatrix}.\tag{6.21}$$

We obtain the expression of the diffusion coefficient for the symmetric (in the sense of equation (6.13)) two-step memory approximation on the honeycomb lattice:

$$D^{\mathrm{s}}_{\mathrm{2SMA}} = D_{\mathrm{NMA}}\frac{3(1-P_{00})}{(3-4P_{\mathrm{ss}}+P_{00})}\frac{(2P_{\mathrm{ss}}+P_{00})}{(2-2P_{\mathrm{ss}}-P_{00})}.\tag{6.22}$$

This is equation (5.33).

6.3. Two-dimensional square lattice

For the two-dimensional square lattice, recall that T is the identity and the operation $\mathsf{S}^i\boldsymbol{v} = \mathsf{R}^i\boldsymbol{v}$ is a anticlockwise rotation of $\boldsymbol{v}$ by angle $i\pi/2$, with $i = 0,\ldots,3$. The operation $\mathsf{S}^{i_1,\ldots,i_n}\boldsymbol{v}$ is thus a rotation by angle $(i_1+\cdots+i_n)\pi/2$. Equations similar to (6.14)–(6.16) hold[4]:

$$\begin{aligned}\mathsf{R}^{i_1\ldots,i_n}\boldsymbol{v}\cdot\boldsymbol{v} &= \cos\left[(i_1+\cdots+i_n)\frac{\pi}{2}\right],\\ &= \cos\frac{i_n\pi}{2}\cos\left[(i_1+\cdots+i_{n-1})\frac{\pi}{2}\right]\\ &\quad -\sin\frac{i_n\pi}{2}\sin\left[(i_1+\cdots+i_{n-1})\frac{\pi}{2}\right],\\ &= \mathsf{R}^{i_1\ldots,i_{n-1}}\boldsymbol{v}\cdot\boldsymbol{v}\,\mathsf{R}^{i_n}\boldsymbol{v}\cdot\boldsymbol{v}\\ &\quad -\left(\delta_{i_n,1}-\delta_{i_n,3}\right)\sin\left[(i_1+\cdots+i_{n-1})\frac{\pi}{2}\right].\end{aligned}\tag{6.23}$$

[4] Note that, in general, we have the decomposition

$$\mathsf{R}^{i_1\ldots,i_n}\boldsymbol{v}\cdot\boldsymbol{v} = \sum_{\omega_1,\ldots,\omega_n\in\{0,1\}}\mathrm{sgn}(\omega_1,\ldots,\omega_n)\mathsf{R}^{i_1}\boldsymbol{v}\cdot\boldsymbol{v}_{\omega_1}\cdots\mathsf{R}^{i_n}\boldsymbol{v}\cdot\boldsymbol{v}_{\omega_n},$$

where we introduced the notation $\boldsymbol{v}_\omega = \boldsymbol{v}$ if $\omega = 0$ and $\boldsymbol{v}_\omega = \boldsymbol{v}_\perp$ if $\omega = 1$, and the function $\mathrm{sgn}(\omega_1,\ldots,\omega_n) = \pm 1$, depending on the sequence $\omega_1,\ldots,\omega_n$. Equation (6.5) would then be replaced by a more complicated expression involving the mixed products of two matrices $P(\mathsf{R}^{j+i}\boldsymbol{v}|\mathsf{R}^j\boldsymbol{v},\boldsymbol{v})\mathsf{R}^j\boldsymbol{v}\cdot\boldsymbol{v}$ and $P(\mathsf{R}^{j+i}\boldsymbol{v}|\mathsf{R}^j\boldsymbol{v},\boldsymbol{v})\mathsf{R}^j\boldsymbol{v}\cdot\boldsymbol{v}_\perp$.

The last term drops out provided

$$P(\mathsf{R}^{i+1}\boldsymbol{v}|\mathsf{R}^{i}\boldsymbol{v},\boldsymbol{v}) = P(\mathsf{R}^{i+3}\boldsymbol{v}|\mathsf{R}^{i}\boldsymbol{v},\boldsymbol{v}). \tag{6.24}$$

Under the additional assumption that

$$P(\mathsf{R}^{1+i}\boldsymbol{v}|\mathsf{R}^{1}\boldsymbol{v},\boldsymbol{v}) = P(\mathsf{R}^{3+i}\boldsymbol{v}|\mathsf{R}^{3}\boldsymbol{v},\boldsymbol{v}), \tag{6.25}$$

we retrieve an effective factorization similar to that postulated in (6.3), and we can then use (6.5) to obtain the corresponding diffusion coefficient. We refer to equations (6.24) and (6.25) as defining a complete left–right symmetry. In this case, the invariant distribution is the solution of

$$p(\boldsymbol{v},\mathsf{R}^{i}\boldsymbol{v}) = \sum_{j} P(\mathsf{R}^{i+j}\boldsymbol{v}|\mathsf{R}^{j}\boldsymbol{v},\boldsymbol{v})\,p(\mathsf{R}^{i}\boldsymbol{v},\mathsf{R}^{j}\boldsymbol{v}), \tag{6.26}$$

$$\sum_{i} p(\boldsymbol{v},\mathsf{R}^{i}\boldsymbol{v}) = \frac{1}{4}. \tag{6.27}$$

We solve these equations for $p(\boldsymbol{v},\boldsymbol{v})$ and $p(\boldsymbol{v},-\boldsymbol{v})$, identifying $p(\boldsymbol{v},\mathsf{R}^{1}\boldsymbol{v})$ and $p(\boldsymbol{v},\mathsf{R}^{3}\boldsymbol{v})$, and define

$$\mathsf{V} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \qquad \mathsf{P} = \begin{pmatrix} p(\boldsymbol{v},-\boldsymbol{v}) \\ p(\boldsymbol{v},\boldsymbol{v}) \end{pmatrix}, \tag{6.28}$$

with the transition matrix

$$\mathsf{Q} = \begin{pmatrix} -P(\boldsymbol{v}|-\boldsymbol{v},\boldsymbol{v}) & P(-\boldsymbol{v}|\boldsymbol{v},\boldsymbol{v}) \\ -P(-\boldsymbol{v}|-\boldsymbol{v},\boldsymbol{v}) & P(\boldsymbol{v}|\boldsymbol{v},\boldsymbol{v}) \end{pmatrix} = \begin{pmatrix} -P_{22} & P_{02} \\ -P_{20} & P_{00} \end{pmatrix}. \tag{6.29}$$

The expression of the diffusion coefficient follows, but will not be written down explicitly as it is rather lengthy and not very transparent. The validity of this expression extends to d-dimensional orthogonal lattices under the symmetry assumptions (6.24) and (6.25).

7. Conclusions

We have shown that it is possible to find exact results for the diffusion coefficient of persistent random walks with a two-step memory on one- and two-dimensional regular lattices, by finding the matrix elements which give the velocity autocorrelation function and then resumming them.

We have applied the results obtained here to approximate the diffusion coefficients of certain periodic billiard tables in [11].

The extension to lattice random walks with longer memory is possible, albeit difficult for obvious technical reasons. Finally, we remark that the extension to lattices in three dimensions is not direct, since in that case, additional information must be specified in order to uniquely define relative directions [12].

Acknowledgments

The authors thank Hernán Larralde for helpful discussions. This research benefitted from the joint support of FNRS (Belgium) and CONACYT (Mexico) through a bilateral collaboration project. The work of TG is financially supported by the Belgian Federal Government under the Inter-university Attraction Pole project NOSY P06/02. TG is financially supported by the Fonds de la Recherche Scientifique F.R.S.-FNRS. DPS acknowledges financial support from DGAPA-UNAM project PAPIIT IN105209, and the hospitality of the Université Libre de Bruxelles, where most of this work was carried out. TG acknowledges the hospitality of the Weizmann Institute of Science, where part of this work was completed.

Appendix A. 2-SMA on a honeycomb lattice

In analogy to equation (5.13), we may write

$$\mathsf{M}^n \equiv \begin{pmatrix} \mathsf{a}_1^{(n)} & \mathsf{a}_2^{(n)} & \mathsf{a}_3^{(n)} & \mathsf{a}_4^{(n)} & \mathsf{a}_5^{(n)} & \mathsf{a}_6^{(n)} & \mathsf{a}_7^{(n)} & \mathsf{a}_8^{(n)} & \mathsf{a}_9^{(n)} \\ \mathsf{c}_9^{(n)} & \mathsf{c}_7^{(n)} & \mathsf{c}_8^{(n)} & \mathsf{c}_3^{(n)} & \mathsf{c}_1^{(n)} & \mathsf{c}_2^{(n)} & \mathsf{c}_6^{(n)} & \mathsf{c}_4^{(n)} & \mathsf{c}_5^{(n)} \\ \mathsf{b}_5^{(n)} & \mathsf{b}_6^{(n)} & \mathsf{b}_4^{(n)} & \mathsf{b}_8^{(n)} & \mathsf{b}_9^{(n)} & \mathsf{b}_7^{(n)} & \mathsf{b}_2^{(n)} & \mathsf{b}_3^{(n)} & \mathsf{b}_1^{(n)} \\ \mathsf{b}_1^{(n)} & \mathsf{b}_2^{(n)} & \mathsf{b}_3^{(n)} & \mathsf{b}_4^{(n)} & \mathsf{b}_5^{(n)} & \mathsf{b}_6^{(n)} & \mathsf{b}_7^{(n)} & \mathsf{b}_8^{(n)} & \mathsf{b}_9^{(n)} \\ \mathsf{a}_9^{(n)} & \mathsf{a}_7^{(n)} & \mathsf{a}_8^{(n)} & \mathsf{a}_3^{(n)} & \mathsf{a}_1^{(n)} & \mathsf{a}_2^{(n)} & \mathsf{a}_6^{(n)} & \mathsf{a}_4^{(n)} & \mathsf{a}_5^{(n)} \\ \mathsf{c}_5^{(n)} & \mathsf{c}_6^{(n)} & \mathsf{c}_4^{(n)} & \mathsf{c}_8^{(n)} & \mathsf{c}_9^{(n)} & \mathsf{c}_7^{(n)} & \mathsf{c}_2^{(n)} & \mathsf{c}_3^{(n)} & \mathsf{c}_1^{(n)} \\ \mathsf{c}_1^{(n)} & \mathsf{c}_2^{(n)} & \mathsf{c}_3^{(n)} & \mathsf{c}_4^{(n)} & \mathsf{c}_5^{(n)} & \mathsf{c}_6^{(n)} & \mathsf{c}_7^{(n)} & \mathsf{c}_8^{(n)} & \mathsf{c}_9^{(n)} \\ \mathsf{b}_9^{(n)} & \mathsf{b}_7^{(n)} & \mathsf{b}_8^{(n)} & \mathsf{b}_3^{(n)} & \mathsf{b}_1^{(n)} & \mathsf{b}_2^{(n)} & \mathsf{b}_6^{(n)} & \mathsf{b}_4^{(n)} & \mathsf{b}_5^{(n)} \\ \mathsf{a}_5^{(n)} & \mathsf{a}_6^{(n)} & \mathsf{a}_4^{(n)} & \mathsf{a}_8^{(n)} & \mathsf{a}_9^{(n)} & \mathsf{a}_7^{(n)} & \mathsf{a}_2^{(n)} & \mathsf{a}_3^{(n)} & \mathsf{a}_1^{(n)} \end{pmatrix}. \tag{A.1}$$

We have the three sets of equations

$$\begin{pmatrix} \mathsf{a}_1^{(n)} & \mathsf{a}_5^{(n)} & \mathsf{a}_9^{(n)} \\ \mathsf{c}_1^{(n)} & \mathsf{c}_5^{(n)} & \mathsf{c}_9^{(n)} \\ \mathsf{b}_1^{(n)} & \mathsf{b}_5^{(n)} & \mathsf{b}_9^{(n)} \end{pmatrix} = \begin{pmatrix} P_{00} & P_{10} & P_{20} \\ P_{01} & P_{11} & P_{21} \\ P_{02} & P_{12} & P_{22} \end{pmatrix} \begin{pmatrix} \mathsf{a}_1^{(n-1)} & \mathsf{a}_5^{(n-1)} & \mathsf{a}_9^{(n-1)} \\ \mathsf{c}_9^{(n-1)} & \mathsf{c}_1^{(n-1)} & \mathsf{c}_5^{(n-1)} \\ \mathsf{b}_5^{(n-1)} & \mathsf{b}_9^{(n-1)} & \mathsf{b}_1^{(n-1)} \end{pmatrix}, \tag{A.2}$$

$$\begin{pmatrix} \mathsf{a}_2^{(n)} & \mathsf{a}_6^{(n)} & \mathsf{a}_7^{(n)} \\ \mathsf{c}_2^{(n)} & \mathsf{c}_6^{(n)} & \mathsf{c}_7^{(n)} \\ \mathsf{b}_2^{(n)} & \mathsf{b}_6^{(n)} & \mathsf{b}_7^{(n)} \end{pmatrix} = \begin{pmatrix} P_{00} & P_{10} & P_{20} \\ P_{01} & P_{11} & P_{21} \\ P_{02} & P_{12} & P_{22} \end{pmatrix} \begin{pmatrix} \mathsf{a}_2^{(n-1)} & \mathsf{a}_6^{(n-1)} & \mathsf{a}_7^{(n-1)} \\ \mathsf{c}_7^{(n-1)} & \mathsf{c}_2^{(n-1)} & \mathsf{c}_6^{(n-1)} \\ \mathsf{b}_6^{(n-1)} & \mathsf{b}_7^{(n-1)} & \mathsf{b}_2^{(n-1)} \end{pmatrix}, \tag{A.3}$$

$$\begin{pmatrix} \mathsf{a}_3^{(n)} & \mathsf{a}_4^{(n)} & \mathsf{a}_8^{(n)} \\ \mathsf{c}_3^{(n)} & \mathsf{c}_4^{(n)} & \mathsf{c}_8^{(n)} \\ \mathsf{b}_3^{(n)} & \mathsf{b}_4^{(n)} & \mathsf{b}_8^{(n)} \end{pmatrix} = \begin{pmatrix} P_{00} & P_{10} & P_{20} \\ P_{01} & P_{11} & P_{21} \\ P_{02} & P_{12} & P_{22} \end{pmatrix} \begin{pmatrix} \mathsf{a}_3^{(n-1)} & \mathsf{a}_4^{(n-1)} & \mathsf{a}_8^{(n-1)} \\ \mathsf{c}_8^{(n-1)} & \mathsf{c}_3^{(n-1)} & \mathsf{c}_4^{(n-1)} \\ \mathsf{b}_4^{(n-1)} & \mathsf{b}_8^{(n-1)} & \mathsf{b}_3^{(n-1)} \end{pmatrix}. \tag{A.4}$$

Proceeding with our analogy, we seek linear combinations of the elements in the rows of the matrices on the left-hand side of the above equations, so as to obtain a single matrix equation similar to equation (5.15). Considering the elements in equation (A.2), we write

$$\begin{pmatrix} \mathsf{a}_1^{(n)} + \phi \mathsf{a}_5^{(n)} + \phi^2 \mathsf{a}_9^{(n)} \\ \phi \mathsf{c}_1^{(n)} + \phi^2 \mathsf{c}_5^{(n)} + \mathsf{c}_9^{(n)} \\ \phi^2 \mathsf{b}_1^{(n)} + \mathsf{b}_5^{(n)} + \phi \mathsf{b}_9^{(n)} \end{pmatrix} = \begin{pmatrix} P_{00} & P_{10} & P_{20} \\ \phi P_{01} & \phi P_{11} & \phi P_{21} \\ \phi^2 P_{02} & \phi^2 P_{12} & \phi^2 P_{22} \end{pmatrix} \begin{pmatrix} \mathsf{a}_1^{(n-1)} + \phi \mathsf{a}_5^{(n-1)} + \phi^2 \mathsf{a}_9^{(n-1)} \\ \phi \mathsf{c}_1^{(n-1)} + \phi^2 \mathsf{c}_5^{(n-1)} + \mathsf{c}_9^{(n-1)} \\ \phi^2 \mathsf{b}_1^{(n-1)} + \mathsf{b}_5^{(n-1)} + \phi \mathsf{b}_9^{(n-1)} \end{pmatrix}. \tag{A.5}$$

Comparing with equation (A.2), we infer

$$\phi^3 = 1 \quad \Leftrightarrow \quad \begin{cases} \phi = 1, \\ \phi = \exp(2\mathrm{i}\pi/3) = -\dfrac{1 - \mathrm{i}\sqrt{3}}{2}, \\ \phi = \exp(-2\mathrm{i}\pi/3) = -\dfrac{1 + \mathrm{i}\sqrt{3}}{2}. \end{cases} \tag{A.6}$$

Applying the same procedure to equations (A.3) and (A.4), we obtain

$$\begin{pmatrix} \phi \mathsf{a}_2^{(n)} + \phi^2 \mathsf{a}_6^{(n)} + \mathsf{a}_7^{(n)} \\ \phi^2 \mathsf{c}_2^{(n)} + \mathsf{c}_6^{(n)} + \phi \mathsf{c}_7^{(n)} \\ \mathsf{b}_2^{(n)} + \phi \mathsf{b}_6^{(n)} + \phi^2 \mathsf{b}_7^{(n)} \end{pmatrix} = \begin{pmatrix} P_{00} & P_{10} & P_{20} \\ \phi P_{01} & \phi P_{11} & \phi P_{21} \\ \phi^2 P_{02} & \phi^2 P_{12} & \phi^2 P_{22} \end{pmatrix} \begin{pmatrix} \phi \mathsf{a}_2^{(n-1)} + \phi^2 \mathsf{a}_6^{(n-1)} + \mathsf{a}_7^{(n-1)} \\ \phi^2 \mathsf{c}_2^{(n-1)} + \mathsf{c}_6^{(n-1)} + \phi \mathsf{c}_7^{(n-1)} \\ \mathsf{b}_2^{(n-1)} + \phi \mathsf{b}_6^{(n-1)} + \phi^2 \mathsf{b}_7^{(n-1)} \end{pmatrix} \tag{A.7}$$

$$\begin{pmatrix} \phi^2 \mathsf{a}_3^{(n)} + \mathsf{a}_4^{(n)} + \phi \mathsf{a}_8^{(n)} \\ \mathsf{c}_3^{(n)} + \phi \mathsf{c}_4^{(n)} + \phi^2 \mathsf{c}_8^{(n)} \\ \phi \mathsf{b}_3^{(n)} + \phi^2 \mathsf{b}_4^{(n)} + \mathsf{b}_8^{(n)} \end{pmatrix} = \begin{pmatrix} P_{00} & P_{10} & P_{20} \\ \phi P_{01} & \phi P_{11} & \phi P_{21} \\ \phi^2 P_{02} & \phi^2 P_{12} & \phi^2 P_{22} \end{pmatrix} \begin{pmatrix} \phi^2 \mathsf{a}_3^{(n-1)} + \mathsf{a}_4^{(n-1)} + \phi \mathsf{a}_8^{(n-1)} \\ \mathsf{c}_3^{(n-1)} + \phi \mathsf{c}_4^{(n-1)} + \phi^2 \mathsf{c}_8^{(n-1)} \\ \phi \mathsf{b}_3^{(n-1)} + \phi^2 \mathsf{b}_4^{(n-1)} + \mathsf{b}_8^{(n-1)} \end{pmatrix}. \tag{A.8}$$

The system of equations (A.5), (A.7), (A.8) reduces to the single recursive matrix equation

$$\begin{aligned} &\begin{pmatrix} \mathsf{a}_1^{(n)} + \phi \mathsf{a}_5^{(n)} + \phi^2 \mathsf{a}_9^{(n)} & \phi \mathsf{a}_2^{(n)} + \phi^2 \mathsf{a}_6^{(n)} + \mathsf{a}_7^{(n)} & \phi^2 \mathsf{a}_3^{(n)} + \mathsf{a}_4^{(n)} + \phi \mathsf{a}_8^{(n)} \\ \phi \mathsf{c}_1^{(n)} + \phi^2 \mathsf{c}_5^{(n)} + \mathsf{c}_9^{(n)} & \phi^2 \mathsf{c}_2^{(n)} + \mathsf{c}_6^{(n)} + \phi \mathsf{c}_7^{(n)} & \mathsf{c}_3^{(n)} + \phi \mathsf{c}_4^{(n)} + \phi^2 \mathsf{c}_8^{(n)} \\ \phi^2 \mathsf{b}_1^{(n)} + \mathsf{b}_5^{(n)} + \phi \mathsf{b}_9^{(n)} & \mathsf{b}_2^{(n)} + \phi \mathsf{b}_6^{(n)} + \phi^2 \mathsf{b}_7^{(n)} & \phi \mathsf{b}_3^{(n)} + \phi^2 \mathsf{b}_4^{(n)} + \mathsf{b}_8^{(n)} \end{pmatrix} \\ &\quad = \begin{pmatrix} P_{00} & P_{10} & P_{20} \\ \phi P_{01} & \phi P_{11} & \phi P_{21} \\ \phi^2 P_{02} & \phi^2 P_{12} & \phi^2 P_{22} \end{pmatrix} \\ &\qquad \times \begin{pmatrix} \mathsf{a}_1^{(n-1)} + \phi \mathsf{a}_5^{(n-1)} + \phi^2 \mathsf{a}_9^{(n-1)} & \cdots & \phi^2 \mathsf{a}_3^{(n-1)} + \mathsf{a}_4^{(n-1)} + \phi \mathsf{a}_8^{(n-1)} \\ \phi \mathsf{c}_1^{(n-1)} + \phi^2 \mathsf{c}_5^{(n-1)} + \mathsf{c}_9^{(n-1)} & \cdots & \mathsf{c}_3^{(n-1)} + \phi \mathsf{c}_4^{(n-1)} + \phi^2 \mathsf{c}_8^{(n-1)} \\ \phi^2 \mathsf{b}_1^{(n-1)} + \mathsf{b}_5^{(n-1)} + \phi \mathsf{b}_9^{(n-1)} & \cdots & \phi \mathsf{b}_3^{(n-1)} + \phi^2 \mathsf{b}_4^{(n-1)} + \mathsf{b}_8^{(n-1)} \end{pmatrix}, \\ &\quad = \begin{pmatrix} P_{00} & P_{10} & P_{20} \\ \phi P_{01} & \phi P_{11} & \phi P_{21} \\ \phi^2 P_{02} & \phi^2 P_{12} & \phi^2 P_{22} \end{pmatrix}^{n-1} \begin{pmatrix} P_{00} & \phi P_{10} & \phi^2 P_{20} \\ \phi P_{01} & \phi^2 P_{11} & P_{21} \\ \phi^2 P_{02} & P_{12} & \phi P_{22} \end{pmatrix}, \\ &\quad = \begin{pmatrix} P_{00} & P_{10} & P_{20} \\ \phi P_{01} & \phi P_{11} & \phi P_{21} \\ \phi^2 P_{02} & \phi^2 P_{12} & \phi^2 P_{22} \end{pmatrix}^{n} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \phi & 0 \\ 0 & 0 & \phi^2 \end{pmatrix}. \end{aligned} \tag{A.9}$$

References

[1] Weiss G H 1994 *Aspects and Applications of the Random Walk* (Amsterdam: North-Holland)
[2] Haus J W and Kehr K W 1987 Diffusion in regular and disordered lattices *Phys. Rep.* **150** 263–406
[3] Fürth R 1920 Die Brownsche Bewegung bei Berücksichtigung einer Persistenz der Bewegungsrichtung. Mit Anwendungen auf die Bewegung lebender Infusorien *Zeit. f. Phys.* **2** 244
[4] Taylor G I 1922 Diffusion by continuous movements *Proc. London Math. Soc.* **20** 196
[5] Kuhn W 1934 *Kolloid Z.* **68** 2
Kuhn W 1936 *Kolloid Z.* **76** 258
[6] Manning J R 1959 Correlation effects in impurity diffusion *Phys. Rev.* **116** 819
[7] Weiss G H 2002 Some applications of persistent random walks and the telegrapher's equation *Physica* A **311** 381
[8] Montroll E W 1950 Markoff chains and excluded volume effect in polymer chains *J. Chem. Phys.* **18** 734
[9] Bender E A and Richmond L B 1984 Correlated random walks *Ann. Prob.* **12** 274
[10] Renshaw E and Henderson R 1981 The correlated random walk *J. Appl. Probab.* **18** 403
Renshaw E and Henderson R 1994 The general correlated random walk *J. Appl. Probab.* **31** 869
[11] Gilbert T and Sanders D P 2009 Persistence effects in deterministic diffusion *Phys. Rev.* E **80** 041121 (arXiv:0908.0600v1)
[12] Larralde H 1997 Transport properties of a two-dimensional 'chiral' persistent random walk *Phys. Rev.* E **56** 5004
[13] Fink T M and Mao Y 1999 Designing tie knots using random walks *Nature* **398** 31