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A 'sum-over-paths' approach to diffusion on trees

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Abstract. We use a 'sum-over-paths' method to derive an explicit expression for the Green's function of the diffusion equation on an arbitrary tree, making connection with the conventional Laplace approach but emphasizing the real-time nature of the technique. This provides a general framework for studying both discrete-space and continuous-space diffusion processes on complex one-dimensional topologies.

1. Introduction

The diffusion equation is widely encountered in the physical and biological sciences. A problem of general interest is how to solve this equation on complex topologies, a classical example of which is the one-dimensional process on a branching structure or tree. Many physical systems can be reduced to this problem after suitable approximations. For example, in neurobiology, the diffusion equation with damping (cable equation) has been used to model the passive membrane properties of a neuron's dendritic tree (Rall 1977, Tuckwell 1988). Other examples include the flow of gas through porous media (Dullien 1979), sedimentation processes (Broadbridge and Rogers 1990) and electromigration along the grain boundaries of aluminium tracks on integrated circuits (Shatzes and Lloyd 1986, Dwyer *et al* 1994). Further, as an abstract mathematical problem it is of great importance in its own right, insofar as one is always interested in developing new techniques for solving this and indeed other PDEs on complex structures.

The standard approach to finding the fundamental solution or Green's function of the diffusion equation on a tree would be to take Laplace transforms and solve the resulting set of ODEs (Carlslaw and Jaegar 1959). One derives a set of algebraic equations for the coefficients of the solution to the ODEs by matching boundary conditions. However, there is an obvious difficulty with this approach, namely the inversion of the Laplace transform to extract the behaviour of the system in the time domain. An alternative approach is to exploit the well known relationship between diffusion processes and random walks. For the specific problem of diffusion on a dendritic tree of a neuron, this has been carried out using both path-integral (Abbott *et al* 1991) and space-discretization schemes (Bressloff and Taylor 1993). In both cases, the calculation of the fundamental solution then reduces to the combinatorial problem of summing over paths of an unbiased random walk on the given tree. Using various reflection arguments (analogous to the method of images) an explicit set of rules for performing the path summation can be obtained. The result is a real-time

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expression for the fundamental solution in the form of an infinite series that is useful for studying finite-time behaviour.

In this paper, we develop further the ‘sum-over-paths’ method for solving the diffusion equation on a tree. We follow the space-discretization scheme of Bressloff and Taylor (1993) since it is conceptually simpler than the path-integral approach and, moreover, spatially discrete processes (e.g. continuous-time random walks (Haus and Kehr 1987)) are of interest in their own right. In section 2, we construct the continuous and discrete diffusion equations on a tree and show how the fundamental solution or Green’s function of the latter can be expressed in terms of a path summation. The explicit set of rules for carrying out this path summation is presented in section 3 and the series expansion of the real-time fundamental solution of both the discrete and continuous diffusion processes is given. These series expansions are particularly useful for determining the small-time behaviour of the system. However, in the long-time limit it is still necessary to resort to Laplace transforms in order to sum the series exactly. This is carried out explicitly in section 4. The resulting expression for the Laplace transform of the fundamental solution provides an alternative form to that obtained using the conventional matching boundary approach, and may be more convenient, for example, in the context of configurational averaging.

2. Diffusion on a tree

2.1. Continuous case

Let $c(x, t)$ denote the concentration at time t and position $x \in \Re$ of a single species of particle undergoing diffusion in one dimension. The concentration $c(x, t)$ evolves according to the diffusion equation

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \qquad t > 0 \qquad -\infty < x < \infty \tag{2.1}$$

where D is the diffusion constant, which is assumed to be independent of x and t. Under the initial condition $c(x, 0) = f(x)$, $-\infty < x < \infty$, the solution to equation (2.1) at time $t > 0$ is given by

$$c(x, t) = \int_{-\infty}^{\infty} \mathrm{d}x'\, G(x, t|x', 0) f(x') \tag{2.2}$$

where

$$G(x, t|x', t') = \chi(x - x', t - t') \equiv \frac{1}{\sqrt{4\pi D[t - t']}} \exp\left[-\frac{(x - x')^2}{4D[t - t']}\right]. \tag{2.3}$$

Here $G(x, t|x', t')$ is the fundamental solution of the diffusion equation obtained for the initial data $f(x) = \delta(x - x')$ at $t = t'$.

In this paper we are interested in solving equation (2.1) on an arbitrary tree Γ such as figure 1. In order to proceed, we need to specify boundary conditions for the concentration c at the branching and terminal nodes of the tree. Label the various line segments (edges) of Γ by $i = 1, \ldots, |\Gamma|$ where $|\Gamma|$ is the total number of line segments. The position coordinate along the ith segment is denoted by x with $0 \leqslant x \leqslant L_i$, and L_i is the length of the segment, (for semi-infinite segments, $0 \leqslant x < \infty$). We assume that each segment has the same diffusion constant D. If c_i denotes the concentration on the ith segment then

$$\frac{\partial c_i}{\partial t} = D\frac{\partial^2 c_i}{\partial x^2} \qquad t > 0 \qquad 0 < x < L_i\,. \tag{2.4}$$

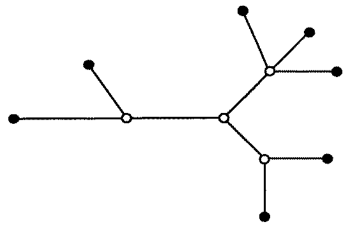

Figure 1. Example of a general tree Γ. Terminal and branching nodes are given by full and open circles, respectively. In this particular example the coordination number at a branching node is either $z_\alpha = 3$ or $z_\alpha = 4$.

All nodes of the tree may be classified as either branching or terminal (see figure 1). Let $\mathcal{B}$ denote the set of branching nodes of Γ. Consider a single branching node $\alpha \in \mathcal{B}$ and label the set of segments radiating from it by $\mathcal{I}_\alpha$. Denote the local coordinate representation of α on the ith segment by $x_i(\alpha)$. Thus $x_i(\alpha) = 0$ or L_i. The boundary conditions are continuity of the concentration at the node,

$$c_i(x_i(\alpha), t) = c_k(x_k(\alpha), t) \qquad \text{for all} \quad i, k \in \mathcal{I}_\alpha \qquad t > 0 \tag{2.5}$$

and conservation of current through the node,

$$\sum_{i \in \mathcal{I}_\alpha} J_i(x_i(\alpha), t)\eta_i = 0 \qquad J_i(x, t) = -D\frac{\partial c_i}{\partial x} \tag{2.6}$$

where $\eta_i = +1 (\eta_i = -1)$ if $x_i(\alpha) = 0$ $(x_i(\alpha) = L_i$.

The boundary conditions at terminal nodes naturally fall into two classes, those where the concentration c is specified and those where the current (density) is specified. We refer to these as boundary conditions of the *first* and *second* kind, respectively. Alternatively, we refer to the boundaries as *open* and *closed*. If a given segment terminates at the point $x_i = 0$ or L_i, then the boundary condition of the first kind requires that

$$c_i(x_i, t) = g_i(t) \tag{2.7}$$

while the second kind has

$$-J_i(x_i, t) \equiv D\frac{\partial c_i}{\partial x}\bigg|_{x=x_i} = h_i(t) \tag{2.8}$$

for given functions g_i and h_i. The set of terminal nodes (or line segments) with boundary conditions of the first and second kind are denoted by $\mathcal{D}$ and $\mathcal{N}$, respectively.

If we are given initial data $c_i(x, 0) = f_i(x), 0 < x < L_i, i = 1, \ldots |\Gamma|$ then we would like to express the solution to equations (2.4)–(2.8) in a similar form to equation (2.2), that is, in terms of the fundamental solution on a tree. This can be achieved using a generalization of Green's theorem (Zauderer 1989). The result is

$$\begin{aligned} c_i(x, t) = \sum_{j=1}^{|\Gamma|} \int_0^{L_j} & \mathrm{d}x'\, G_{ij}(x, t|x', 0) f_j(x') \\ & -D\int_0^t \mathrm{d}t' \sum_{j \in \mathcal{D}} \eta_j \frac{\partial}{\partial x'} G_{ij}(x, t|x', t')\bigg|_{x'=x_j} g_j(t') \\ & + \int_0^t \mathrm{d}t' \sum_{j \in \mathcal{N}} \eta_j G_{ij}(x, t|x_j, t') h_j(t') \end{aligned} \tag{2.9}$$

where $\eta_j = +1$ if $x_j = L_j$ and $\eta_j = -1$ if $x_j = 0$ for terminal nodes and $G_{ij}(x, t|x', 0)$ is the fundamental solution of equation (2.4) with homogeneous boundary conditions $(g_i(t), h_i(t) = 0$ for all $t)$ and initial data $G_{ij}(x, 0|x', 0) = \delta(x - x')\delta_{ij}$. Note that in parabolic equations such as the diffusion equation one should distinguish between the fundamental solution and the Green's function. The latter, denoted by $K_{ij}(x,t|x',t')$ satisfies the backwards diffusion equation

$$-\frac{\partial K_{ij}}{\partial t} - D\frac{\partial^2 K_{ij}}{\partial x^2} = \delta(x-x')\delta(t-t')\delta_{ij} \qquad 0 < x' < L_j \qquad 0 < x < L_i\,. \tag{2.10}$$

However, there is a simple relationship between G and K given by $K_{ji}(x',t'|x,t) = \theta(t-t')G_{ij}(x,t|x',t')$, where θ is the Heaviside function.

The initial boundary value problem for the diffusion equation on a tree thus reduces to the problem of finding the associated Green's function or fundamental solution. Rather than trying to calculate the fundamental solution directly, we shall consider a discrete version of the diffusion equation and determine its fundamental solution using a 'sum-over-paths' approach. The fundamental solution of the original continuous problem will then be generated in the continuum limit (section 3).

2.2. Discrete case

We discretize the tree Γ by taking each line segment i to be subdivided into a set of M_i intervals of length Δx with $M_i\Delta x = L_i$. The continuum limit is given by $\Delta x \to 0$ such that L_i is fixed for each i. This discretization leads to a new tree $\hat{\Gamma}$ of vertices labelled I together with a set of links (IJ) of length Δx (see figure 2). The set of vertices I includes the branching nodes and terminal nodes of the original tree Γ together with the set of internal nodes. In terms of the (discrete) local coordinates of the original line segments, we can set $I = (ni)$ for terminal and internal nodes with n denoting the nth discrete point on the ith segment. On the other hand, for branching nodes, $I = \alpha$ where $\alpha \equiv (n_i(\alpha)i)$ for all $i \in \mathcal{I}_\alpha$. Note that in the discrete case all physics occurs on the vertices of the tree, whereas in the continuous case it occurs on the links.

From the geometry of simplicial lattices (see the appendix) we can write down a discrete version of the diffusion equation in the form

$$\frac{\mathrm{d}c_I}{\mathrm{d}t} = \frac{2D}{z_I\Delta x^2}\sum_{J(I)}[c_J(t) - c_I(t)] \tag{2.11}$$

where the summation is over all neighbours of lattice point I and z_I is the coordination number of I. It is a simple matter to check that equation (2.11) reduces to equations (2.4)–(2.8) in the continuum limit $\Delta x \to 0$. First, if I is an internal node, that is, $I = (ni), 0 < n < M_i$, then $z_I = 2$ and

$$\frac{\mathrm{d}c_{ni}}{\mathrm{d}t} = \frac{D}{\Delta x^2}[c_{n+1,i}(t) - 2c_{ni}(t) + c_{n-1,i}(t)]\,. \tag{2.12}$$

The right-hand side contains the standard finite-difference expression for the Laplacian, and hence we obtain equation (2.4) in the continuum limit. Second, if I is a closed terminal

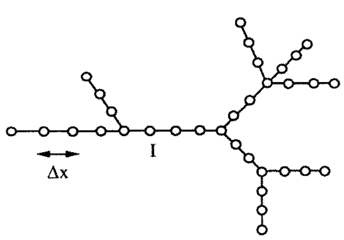

Figure 2. Tree $\hat{\Gamma}$ obtained by discretizing each line segment of the tree Γ (figure 1) into intervals of length Δx.

node with $I = (0i)$ say then

$$\frac{\mathrm{d}c_{0i}}{\mathrm{d}t} = \frac{2D}{\Delta x^2}[c_{1i}(t) - c_{0i}(t)] \tag{2.13}$$

which yields equation (2.8) in the continuum limit (for $h_i = 0$). Finally, consider a branching node $I = \alpha$ such that $c_\alpha \equiv c_{0i}$ for all i. Then

$$\frac{\mathrm{d}c_\alpha}{\mathrm{d}t} = \frac{2D}{z_\alpha \Delta x^2} \sum_{i \in \mathcal{I}_\alpha} [c_{1i}(t) - c_{0i}(t)] \tag{2.14}$$

which reduces to equation (2.6) in the continuum limit. Equations (2.5) and (2.7) are trivially satisfied.

It is useful to rewrite equation (2.11) in the matrix form

$$\frac{\mathrm{d}\mathbf{c}}{\mathrm{d}t} = \rho[\mathbf{Q}\mathbf{c} - \mathbf{c}] \qquad \rho = \frac{2D}{\Delta x^2} \tag{2.15}$$

where

$$\mathbf{Q} = \mathbf{D}^{-1}\mathbf{A} \qquad \mathbf{D} = \mathrm{diag}\ (z_I) \tag{2.16}$$

and $\mathbf{A}$ is the adjacency matrix of the tree $\hat{\Gamma}$. That is, $A_{IJ} = 1$ if (IJ) is a link and $A_{IJ} = 0$ otherwise. The relationship between diffusion and random walks is now clear since $\mathbf{Q}$ generates an unbiased random walk on the lattice $\hat{\Gamma}$. That is, $[\mathbf{Q}^p]_{IJ}$ is the probability that a random walker starting at I reaches J in p steps of length Δx.

It should be noted that equation (2.15) is similar in form to the master equation of a continuous-time random walk with Poissonian waiting-time distributions (Montroll and Weiss 1965, Haus and Kehr 1987). More specifically, if $c_I(t)$ is now interpreted as the probability of a single random walker being at site I at time t then

$$\frac{\mathrm{d}\mathbf{c}}{\mathrm{d}t} = \kappa[\mathbf{Q}^{\mathrm{T}}\mathbf{c} - \mathbf{c}] \tag{2.17}$$

where κ is a transition rate and T indicates transpose. Since $\sum_{J\in\hat{\Gamma}} Q_{IJ} = 1$ for all $I \in \hat{\Gamma}$, it follows from equation (2.17) that the total probability is conserved, that is, $\frac{\mathrm{d}}{\mathrm{d}t}(\sum_{I\in\hat{\Gamma}} c_I) = 0$. On the other hand, the total particle number c_I in the discretized diffusion equation (2.15) is not conserved since $\sum_{I\in\hat{\Gamma}} Q_{IJ} \neq 1$ for J at branching or closed terminal nodes; particle number conservation is recovered, however, in the continuum limit.

The solution of equation (2.15) is

$$c_I(t) = \sum_J G_{IJ}(t) c_J(0) \tag{2.18}$$

where

$$G_{IJ}(t) = \mathrm{e}^{-\rho t}\big[\mathrm{e}^{\rho t \mathbf{Q}}\big]_{IJ} \tag{2.19}$$

is the fundamental solution of the discretized system. Expanding equation (2.19) gives

$$G_{IJ}(t) = \mathrm{e}^{-\rho t} \sum_{p\geqslant 0} \frac{1}{p!}(\rho t)^p [\mathbf{Q}^p]_{IJ}\ . \tag{2.20}$$

Thus the problem of calculating the fundamental solution of the discrete diffusion equation reduces to the combinatorial problem of summing over paths of a random walk on $\hat{\Gamma}$. This 'sum-over-paths' approach is similar in spirit to the treatment of continuous-time random walks by Montroll and Weiss (1965). Having calculated $G_{IJ}(t)$ we can take the continuum limit to determine the fundamental solution of the continuous diffusion equation. In particular, if $I = (ni)$, $J = (mj)$ and $x = n\Delta x$, $x' = m\Delta x$ then

$$G(x, t|x', 0) = \lim_{\Delta x \to 0} \frac{1}{\Delta x} G_{IJ}(t) . \tag{2.21}$$

We shall find that taking the continuum limit is very simple within the 'sum-over-paths' framework (see section 3).

3. Fundamental solution on a tree

Following Bressloff and Taylor (1993), the 'sum-over-paths' approach will now be used to determine a set of rules for constructing the fundamental solution on an arbitrary tree. In order to motivate the rules, it is useful to consider some simple cases first.

3.1. One-dimensional interval $-\infty < x < \infty$

We begin by considering the case of one-dimensional diffusion over the unbounded domain $-\infty < x < \infty$ (see also Haus and Kehr 1987). Dividing the real line into segments of equal length Δx and writing $x = n\Delta x$ for integer n, equation (2.1) reduces to equation (2.12) (without the segment index i). In this simple case

$$[\mathbf{Q}^p]_{nm} = \left(\tfrac{1}{2}\right)^p N[n, m, p] \tag{3.1}$$

where $N[n, m, p]$ is the number of possible paths of p steps from n to m. The latter can be determined using straightforward combinatorics to give (Grimmett and Stirzaker 1988)

$$N[n, m, p] = \begin{pmatrix} p \\ (p + |n - m|)/2 \end{pmatrix} . \tag{3.2}$$

Substitution of equations (3.1) and (3.2) into (2.20) yields

$$G_{nm}(t) = \mathrm{e}^{-\rho t} I_{|n-m|}(\rho t) \tag{3.3}$$

where we have performed the summation over p explicitly to obtain a modified Bessel function of integer order (Abramowitz and Stegun 1970).

Having obtained the fundamental solution to the discrete model, we can take the continuum limit to obtain equation (2.3). First, use an integral representation for I_n to rewrite equation (3.3) as

$$G_{nm}(t) = \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \exp(\mathrm{i}k(n - m) - t\rho(1 - \cos k)) . \tag{3.4}$$

Setting $x = n\Delta x$, $x' = m\Delta x$ and performing a change of variables $k \to k/\Delta x$ gives

$$G_{nm}(t) = \Delta x \int_{-\pi/\Delta x}^{\pi/\Delta x} \frac{\mathrm{d}k}{2\pi} \exp\left(\mathrm{i}k(x - x') - \frac{2tD}{\Delta x^2}(1 - \cos k\Delta x)\right) .$$

Finally, taking the continuum limit $\Delta x \to 0$ according to equation (2.21) yields the desired result. That is,

$$\lim_{\Delta x \to 0} \frac{1}{\Delta x} \mathrm{e}^{-\rho t} I_{|n-m|}(\rho t) = \chi(x - x', t) \tag{3.5}$$

where χ is defined in equation (2.3).

3.2. *Semi-infinite interval* $0 \leqslant x < \infty$

(i) *Open boundary at* $x = 0$. Consider the diffusion equation on the interval $0 \leqslant x < \infty$ with a homogeneous boundary condition of the first kind $c(0, t) = 0$. Discretize the spatial coordinate by setting $x = n\Delta x$ with $n = 0, 1, \ldots$. Then equation (2.12) holds for $n \geqslant 1$ (without the index i) such that $c_0(t) \equiv 0$. In the present example the matrix $\mathbf{Q}$ generates a random walk that is restricted to lie in the positive region $n > 0$, i.e. it involves paths that do not touch the origin. Using a reflection argument (Chandrasekhar 1943, Grimmett and Stirzaker 1988) it can be shown that on an infinite domain there is a one to one correspondence between paths from n to m that touch the origin and paths from n to $-m$. Hence,

$$[\mathbf{Q}^p]_{nm} = \left(\tfrac{1}{2}\right)^p [N[n, m, p] - N[n, -m, p]]\,. \tag{3.6}$$

Substitution into equation (2.20) and the use of equation (3.2) shows that

$$G_{nm}(t) = \mathrm{e}^{-\rho t}[I_{|n-m|}(\rho t) - I_{|m+n|}(\rho t)]\,. \tag{3.7}$$

Finally, taking the continuum limit and using equation (3.5),

$$G(x, t|x', 0) = [\chi(x - x', t) - \chi(x - x', t)]\,. \tag{3.8}$$

(ii) *Closed boundary at* $x = 0$. The calculation of the fundamental solution for the boundary condition of the second kind proceeds along similar lines. One now has the condition that no current flows beyond the end $x = 0$. Discretizing space in the usual manner leads to equation (2.12) for $n \geqslant 1$ and equation (2.13) for $n = 0$. The matrix $\mathbf{Q}$ generates a random walk restricted to lie in the region $n \geqslant 0$; any path that hits the origin is reflected back in the positive x-direction and an additional factor of 2 is picked up (since the coordination number of the terminal node is unity). Thus (for $m \neq 0$)

$$[\mathbf{Q}^p]_{nm} = \left(\tfrac{1}{2}\right)^p \left[N_+^0[n, m, p] + 2N_+^1[n, m, p] + 4N_+^2[n, m, p] + \cdots\right] \tag{3.9}$$

where $N_+^q[n, m, p]$ is the number of paths of length p from n to m on the semi-infinite interval that hit the origin exactly q times. From reflection arguments $N_+^0[n, m, p] = N[n, m, p] - N[n, -m, p]$ and $N_+^q[n, m, p] = 2^{-q+1}N^q[n, -m, p]$ for $q \geqslant 1$ where $N[n, m, p]$ satisfies equation (3.2) and $N^q[n, -m, p]$ is the number of paths from n to $-m$ on the infinite interval that touch the origin exactly q times. It follows that

$$[\mathbf{Q}^p]_{nm} = \left(\tfrac{1}{2}\right)^p [N[n, m, p] + N[n, -m, p]] \tag{3.10}$$

where we have used the identity $\sum_{q=1}^{\infty} N^q[n, -m, p] = N[n, -m, p]$. The above reflection argument is slightly modified if the point m actually lies on the boundary; the result is that the right-hand side of equation (3.10) should be multiplied by a factor of $\frac{1}{2}$ if $m = 0$ (this point was not explicitly addressed in the seminal review of Chandrasekhar (1943), and is easy to overlook). It follows that

$$G_{nm}(t) = \mathrm{e}^{-\rho t}[I_{|n-m|}(\rho t) + I_{|m+n|}(\rho t)]\left(\tfrac{1}{2}\right)^{\delta_{m,0}} \tag{3.11}$$

and

$$G(x, t|x', 0) = [\chi(x - x', t) + \chi(x + x', t)]\,. \tag{3.12}$$

Note the subtle point that the term involving the factor of $\frac{1}{2}$ in equation (3.11) disappears in the continuum limit $\Delta x \to 0$.

3.3. Single branching node

Consider a tree consisting of z_α semi-infinite segments labelled $i = 1, \ldots, z_\alpha$ connected to a single branching node α. Let $c_i(x, t)$, $0 \leqslant x < \infty$, denote the concentration on the ith segment and take the coordinate value of the branching node to be zero for all i. Discretize each segment by setting $x = n\Delta x$ with $n \geqslant 0$. The discretized diffusion equation then takes the form of equation (2.12) for $n \geqslant 1$ and equation (2.14) for $n = 0$. The matrix $\mathbf{Q}$ generates a random walk on the tree such that an additional factor of $2z_\alpha^{-1}$ is picked up each time a path passes from the branching node to any segment radiating from it. The sum over all such paths can be handled using reflection arguments along the lines of Abbott *et al* (1991). Suppose that the initial and final points are on the same segment, that is, $i = j$. Then there is a z_α-independent contribution from paths that do not touch the origin of the form $N[n, m, p] - N[n, -m, p]$. The only z_α-dependent weighting factor that occurs for paths that do touch the branching node arises from the final time the path leaves the branching node before terminating at (mj). This follows from the relation $\sum_\alpha z_\alpha^{-1} = 1$ and is true whether or not $i = j$. In order to understand this more clearly, consider a path that makes an intermediate excursion from the branching node down one of the z_α segments and then returns to the node. The sum over all paths will receive contributions from paths with similar excursions along all of the segments of the branching node. The probability of entering each segment is z_α^{-1} so that when we perform the path summation over all segments we obtain unity. Thus the probability factors associated with excursions that start and end at the branching node are irrelevant in the total sum-over-paths; the only factor that does not sum in this way is the one associated with the last time that the path leaves the branching node. Thus, following the treatment of the closed semi-infinite case, we have (for $m \neq 0$)

$$\begin{aligned}[\mathbf{Q}^p]_{ni,mj} &= \left(\tfrac{1}{2}\right)^p [(N[n, m, p] - N[n, -m, p])\delta_{i,j} \\ &\quad + 2z_\alpha^{-1}(N_+^1[n, m, p] + 2N_+^2[n, m, p] + \cdots)] \\ &= \left(\tfrac{1}{2}\right)^p [(N[n, m, p] - N[n, -m, p])\delta_{i,j} + 2z_\alpha^{-1} N[n, -m, p]] \end{aligned} \tag{3.13}$$

where $N_+^q[n, m, p]$ is defined in section 3.2 (if $m = 0$ then the right-hand side of equation (3.13) is multiplied by an additional factor of $z_\alpha/2$). Again it follows that

$$G_{ni,mj}(t) = \mathrm{e}^{-\rho t}[I_{|n-m|}(\rho t)\delta_{i,j} + (2z_\alpha^{-1} - \delta_{i,j})I_{|m+n|}(\rho t)] \left(\frac{z_\alpha}{2}\right)^{\delta_{m,0}} \tag{3.14}$$

and

$$G_{ij}(x, t|x', 0) = [\chi(x - x', t)\delta_{i,j} + (2z_\alpha^{-1} - \delta_{i,j})\chi(x + x', t)]. \tag{3.15}$$

The validity of the above results (3.13)–(3.15) may be verified by direct enumeration.

3.4. Arbitrary tree

Now consider an arbitrary tree Γ such as figure 1. Discretizing the tree as described in section 2.2 yields the discrete diffusion equation (2.11) or (2.15) defined on the tree $\hat{\Gamma}$ (figure 2). The matrix $\mathbf{Q}$ generates an unbiased random walk on $\hat{\Gamma}$ with the following properties:

(i) An additional factor of 2 occurs whenever a path is reflected from a terminal node with a closed boundary condition.

(ii) Paths cannot touch terminals with open boundary conditions.

(iii) An additional factor of $2z_\alpha^{-1}$ occurs whenever a path passes from the branching node $\alpha \in \mathcal{B}$ to any segment $k \in \mathcal{I}_\alpha$ joining this node.

In order to describe the rules for constructing the fundamental solution on the tree $\hat{\Gamma}$ as given by equation (2.20), it is useful to introduce the notion of a trip (Abbott *et al* 1991). A *trip* from the point (ni) to (mj) on the tree is a path that starts from (ni) in any direction, but subsequent changes in direction can only occur by reflections at branching nodes and terminals; a trip can pass through the points (ni) and (mj) an arbitrary number of times before finally stopping at (mj) and can enter different segments by crossing branching nodes. Each trip μ can be specified by the ordered sequence of segments traversed by the trip. Thus $\mu = \{i, k, k', \ldots, k'', j\}$. The total length of a trip will be $n_\mu + m_\mu + M_\mu$ where

$$n_\mu = \begin{cases} n & \text{if trip starts from } n \text{ in the negative } x\text{-direction} \\ M_i - n & \text{if trip starts from } n \text{ in the positive } x\text{-direction} \end{cases}$$

$$m_\mu = \begin{cases} m & \text{if the final part of the trip reaches } m \text{ in the positive } x\text{-direction} \\ M_j - m & \text{if the final part of the trip reaches } m \text{ in the negative } x\text{-direction} \end{cases}$$

$$M_\mu = M_k + M_{k'} + \cdots + M_{k''} .$$

One exception to the above rule concerns the direct path between two points n, m on the same line segment for which the path length is simply $|n - m|$. Some examples illustrating the definition of a trip are given in figure 3.

Using the above notion of a trip, we can use reflection arguments to reduce the summation over paths on the tree $\hat{\Gamma}$ to a summation over all possible trips of a corresponding one-dimensional random walk. The result is that the fundamental solution (2.20) may be

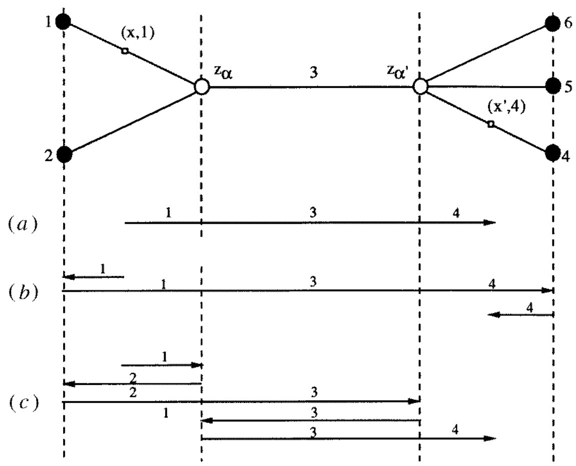

Figure 3. Some examples of trips between two points on a tree with two branching nodes α, α' having coordination numbers $z_\alpha = 3$, $z_{\alpha'} = 4$ and five terminal nodes. The ith line segment has length L_i, $i = 1, \ldots, 6$. Impose open boundary conditions for segments 1, 2 and closed boundary conditions for segments 4, 5, 6. For each segment the positive x-direction is from left to right. The total length of a trip is denoted by L_T. (a) The direct trip between point x on segment 1 and point x' on segment 4. Here $L_T = L_1 - x + L_3 + x'$ and the associated coefficient in equations (3.16) and (3.17) is $b_\mu = 2z_\alpha^{-1} 2z_{\alpha'}^{-1}$. ($b$) A trip that undergoes a single reflection at the terminal node of segment 1 and segment 4. Here $L_T = x + L_1 + L_3 + L_4 + L_4 - x'$ and $b_\mu = (-1)(2z_\alpha^{-1})(2z_{\alpha'}^{-1})(+1)$. ($c$) A trip that reflects twice at left-hand branching node, once at the right-hand branching node and once at the terminal node of segment 2. Here $L_T = (L_1 - x) + 2L_2 + 3L_3 + x'$ and $b_\mu = (2z_\alpha^{-1})(-1)(2z_\alpha^{-1})(2z_{\alpha'}^{-1} - 1)(2z_\alpha^{-1} - 1)(2z_{\alpha'}^{-1})$.

expressed in terms of the infinite series

$$G_{ni,mj}(t) = \mathrm{e}^{-\rho t} \sum_{\mu}^{(ij)} b_\mu I_{|n_\mu + m_\mu + M_\mu|}(\rho t) \tag{3.16}$$

and the sum is restricted to trips starting on segment i and terminating on segment j. The factors contributing to the coefficients b_μ are determined by the following rules:

(i) A factor of $+1$ for every reflection at a closed terminal and a factor -1 for every reflection at an open terminal.

(ii) A factor of $2z_\alpha^{-1}$ whenever a trip crosses branching node α from segment i to segment $k, i \neq k, i, k \in \mathcal{I}_\alpha$.

(iii) A factor of $(2z_\alpha^{-1} - 1)$ whenever a trip is reflected at node α back into the same segment $k \in \mathcal{I}_\alpha$.

(iv) A factor of $2z_\alpha^{-1}$ if a trip starts at a branching node α and a factor 2 if it starts at a closed terminal node.

It is now a very simple matter to obtain the fundamental solution of the continuous diffusion equation on the tree Γ using equation (3.5). First, set $x = n\Delta x$, $x' = m\Delta x$, $x_\mu = n_\mu \Delta x$, $x'_\mu = m_\mu \Delta x$ and $L_\mu = M_\mu \Delta x$. Then the continuum limit of equation (3.16) gives (see also Abbott *et al* 1991)

$$G_{ij}(x, t|x', 0) = \sum_{\mu}^{(ij)} b_\mu \chi(x_\mu + L_\mu + x'_\mu, t) \tag{3.17}$$

where the coefficients b_μ are now determined by rules (i)–(iv) together with an additional rule: (v) A factor $2z_\alpha^{-1}$ if a trip ends at a branching node α and a factor 2 if it ends at a terminal node.

One can view the summation over trips in equation (3.17), or (3.16), as a generalization of the method of images to the case of an arbitrary tree. For non-trivial topologies there is an infinite number of possible trips and hence an infinite number of terms on the right-hand side of (3.17). However, for any fixed time t, trips with lengths much longer than $\sqrt{Dt}$ will only give small contributions so that the sum can be truncated. Hence, using an efficient algorithm for generating trips should provide a new numerical method for directly determining the real-time fundamental solution G.

So far we have restricted our analysis to the case of trees, that is, graphs without loops. However, the results can easily be extended to take into account loops. It is natural to partition the set of trips according to the set of winding numbers of a trip, which specify the number of complete rotations around each loop in an anticlockwise direction minus the corresponding number in the opposite direction. The rules for determining the coefficients b_μ and trip lengths $x_\mu + L_\mu + x_\mu^1$ are unchanged.

4. Summation over trips

In principle, the method presented in section 3 is valid for all times. In practice, for very long times the number of terms in equation (3.16) or (3.17) becomes large and a solution based around Laplace transforms may be more appropriate. In this section, we shall show how one can explicitly perform the summation over trips in Laplace space to yield a closed expression for the Laplace transform $\tilde{G}$ of the fundamental solution. This provides a connection with the conventional Laplace approach of matching boundary conditions.

Laplace transforming equation (3.16) gives

$$\tilde{G}_{ni,mj}(s) = \frac{2}{\rho[\lambda_+(s) - \lambda_-(s)]} \sum_{\mu}^{(ij)} b_\mu [\lambda_-(s)]^{|n_\mu + m_\mu + M_\mu|} \tag{4.1}$$

where

$$\lambda_\pm(s) = 1 + \frac{s}{\rho} \pm \sqrt{\left(1 + \frac{s}{\rho}\right)^2 - 1}\,. \tag{4.2}$$

Similarly, Laplace transforming (3.17) yields

$$\tilde{G}_{i,j}(x, x', s) = \frac{1}{2\sqrt{Ds}} \sum_{\mu}^{(ij)} b_\mu \exp\left(-\sqrt{\frac{s}{D}}(|x_\mu + x'_\mu + L_\mu|)\right). \tag{4.3}$$

Thus in Laplace space the summation over trips involves power series, which can be evaluated explicitly. For concreteness, we shall consider the continuous case, equation (4.3); the discrete case can be handled in an identical fashion. We shall develop the analysis through a number of examples.

(i) *Finite interval* $0 \leqslant x \leqslant L$. Suppose that both ends of the finite interval have boundary conditions of the first kind so that $c_0(t) = c_L(t) = 0$. Without loss of generality, assume that $x > x'$. There are four classes of trips depending on the directions of the initial departure from x and the final arrival at x'. We note these directions by u and v, respectively with $u, v = \pm$. (a) If $u = +, v = -$ then the trip length is $2kL - (x + x')$ with $k \geqslant 1$. (b) If $u = +, v = +$ then the trip length is $2kL + x' - x$ with $k \geqslant 1$. (c) If $u = -, v = -$ then the trip length is $2kL + x - x'$ with $k \geqslant 0$. (d) If $u = -, v = +$ then the trip length is $2kL + x + x'$ with $k \geqslant 0$. Using the fact that a factor of -1 is picked up each time a trip reflects at an open boundary we find that equation (3.17) becomes

$$G(x, t|x', 0) = \sum_{k=-\infty}^{\infty} [\chi(2Lk + x - x', t) - \chi(2Lk + x + x', t)] \tag{4.4}$$

which is the well known result obtained using the method of images. On Laplace transforming equation (4.4) we can perform the summation over k explicitly to obtain the result

$$\tilde{G}(x, x'; s) = \frac{\tilde{\chi}(x - x', s) + \tilde{\chi}(x - 2L - x', s) - \tilde{\chi}(x + x', s) - \tilde{\chi}(x - 2L + x', s)}{[1 - \exp(-2L\sqrt{s/D})]} \tag{4.5}$$

where $\tilde{\chi}(x, s)$ is the Laplace transform of $\chi(x, t)$ defined in equation (2.3),

$$\tilde{\chi}(x, s) = \frac{\exp(-\sqrt{s/D}|x|)}{2\sqrt{Ds}}.$$

(ii) *Single branching node with finite segments.* Next consider the case of a single branching node α with z_α finite segments radiating from it. Consider for concreteness trips that begin and end at the branching node. An arbitrary trip consists of two distinct kinds of contribution: (a) multiple reflections within a segment and (b) transitions across the branching node between segments. A trip undergoing r transitions may be specified by the sequence of integers $n_{i_1} \stackrel{i_2 \neq i_1}{\rightarrow} n_{i_2} \stackrel{i_3 \neq i_2}{\rightarrow} n_{i_3} \cdots \stackrel{i_r \neq i_{r-1}}{\rightarrow} n_{i_r}$, which represents n_{i_1} return journeys to the branching node via internal reflections within segment i_1 followed by a transition to segment i_2, etc. Hence, the Laplace transform (4.3) takes the form (dropping the redundant segment indices ij)

$$\tilde{G}(0,0;s) = \frac{1}{2\sqrt{sD}}\Bigg[1 + \sum_{r=1}^{\infty}\sum_{\{i_1,\cdots,i_r\}}\sum_{\{n_1,\cdots,n_r\}} \exp(-2n_{i_1}L_{i_1}\sqrt{s/D})(\pm\bar{p}_\alpha)^{n_{i_1}}\left(\frac{p_\alpha}{\bar{p}_\alpha}\right) \times \exp(-2n_{i_2}L_{i_2}\sqrt{s/D})(\pm\bar{p}_\alpha)^{n_{i_2}}\left(\frac{p_\alpha}{\bar{p}_\alpha}\right)\cdots \times \exp(-2n_{i_r}L_{i_r}\sqrt{s/D})(\pm\bar{p}_\alpha)^{n_{i_r}}\left(\frac{p_\alpha}{\bar{p}_\alpha}\right)\Bigg]. \tag{4.6}$$

In writing down equation (4.6) we have used the rules presented in section 3.4; each reflection picks up a factor $\bar{p}_\alpha = 2z_\alpha^{-1} - 1$ at the branching node and a factor ± 1 at a terminal node (depending on whether it is closed or open), and each transition across the branching node produces a factor $p_\alpha = 2z_\alpha^{-1}$. Since the integers $n_{i_1}, \cdots, n_{i_r}$ are independent, we can sum over all multiple reflections to obtain the result

$$\tilde{G}(0,0;s) = \frac{p_\alpha}{z\sqrt{sD}}\Bigg[1 + \left(\frac{p_\alpha}{\bar{p}_\alpha}\right)\sum_i f(L_i,s) + \left(\frac{p_\alpha}{\bar{p}_\alpha}\right)^2\sum_i\sum_{j\neq i} f(L_i,s)f(L_j,s) + \left(\frac{p_\alpha}{\bar{p}_\alpha}\right)^3\sum_i\sum_{j\neq i}\sum_{k\neq j} f(L_i,s)f(L_j,s)f(L_k,s) + \cdots\Bigg] \tag{4.7}$$

where

$$f(L,s) = \pm\frac{\bar{p}_\alpha\exp(-2L\sqrt{s/D})}{1\mp\bar{p}_\alpha\exp(-2L\sqrt{s/D})} \tag{4.8}$$

and the choice of signs depends on the boundary condition at the terminal node.

It is important to note that by performing the partial summation over internal reflections to derive equation (4.7) from (4.6) we have spoiled the convergence properties of the latter. To see this assume for simplicity that all segments have the same length L. It turns out that (4.7) is then only convergent if

$$2\frac{z_\alpha - 1}{z_\alpha}\left|\frac{\exp(-2L\sqrt{s/D})}{1\mp\bar{p}_\alpha\exp(-2L\sqrt{s/D})}\right| < 1$$

which implies that $2L\sqrt{s/D} > \ln(3-2z_\alpha^{-1})$. Nevertheless, the series on the right-hand side of equation (4.7) can be summed to give the following closed expression for $\tilde{G}$:

$$\tilde{G}(0,0;s) = \frac{p_\alpha}{z\sqrt{sD}}\{1 + \mathbf{F}_\alpha(s)[1-\boldsymbol{\Phi}_\alpha(s)]^{-1}\mathbf{v}_\alpha\} \tag{4.9}$$

with

$$\mathbf{F}_\alpha(s) = \left(\frac{p_\alpha}{\bar{p}_\alpha}\right)(f(L_1,s),\ldots,f(L_{z_\alpha},s)) \qquad \mathbf{v}_\alpha^{\mathrm{T}} = (1,1,\ldots,1) \tag{4.10}$$

and

$$\boldsymbol{\Phi}_\alpha(s) = \left(\frac{p_\alpha}{\bar{p}_\alpha}\right)\begin{pmatrix} 0 & f(L_2,s) & f(L_3,s) \\ f(L_1,s) & 0 & f(L_3,s) \\ f(L_1,s) & f(L_2,s) & 0 \end{pmatrix}. \tag{4.11}$$

By analytic continuation, equation (4.9) gives the Laplace transform of the fundamental solution throughout the complex domain.

If trips started and ended on the terminal node of segment 1, say, then a similar calculation yields

$$\tilde{G}_{11}(L_1, L_1; s) = \frac{1}{\chi\sqrt{sD}}\left\{1+2f(L_1,s)+2p_\alpha \mathrm{e}^{-2L_1\sqrt{s/D}}(1+f(L_1,s))^2\mathbf{u}_\alpha^1[1-\mathbf{\Phi}_\alpha(s)]^{-1}\bar{\mathbf{u}}_\alpha^1\right\} \tag{4.12}$$

with

$$\mathbf{u}_\alpha^{-1} = (1, 0, \ldots, 0) \qquad \bar{\mathbf{u}}_\alpha^1 = (0, 1, \ldots, 1)^{\mathrm{T}}. \tag{4.13}$$

(iii) *Two branching nodes.* For our third example consider the case of two branching nodes α, α' as given by figure 3 with $\mathcal{I}_\alpha = \{1, 2, 3\}$, $\mathcal{I}_{\alpha'} = \{3, 4, 5, 6\}$. The analysis follows along similar lines to the previous case. That is, we first sum over multiple reflections and then over transitions between segments. The result for trips starting and ending at branching node α is that the Laplace transform (4.3) reduces to the closed expression

$$\tilde{G}(\alpha, \alpha; s) = \frac{p_\alpha}{z\sqrt{sD}}\left\{1 + (\mathbf{F}_\alpha(s), \mathbf{O}_{\alpha'})[1 - \mathbf{\Phi}(s)]^{-1}(\mathbf{v}_\alpha, \mathbf{O}_{\alpha'})^{\mathrm{T}}\right\} \tag{4.14}$$

where $\mathbf{F}_\alpha, \mathbf{v}_\alpha$ are defined by equation (4.10) and $[\mathbf{O}_{\alpha'}]_i = 0$ for all $i \in \mathcal{I}_{\alpha'}$. The matrix $\mathbf{\Phi}(s)$ is an $N \times N$ matrix where $N = z_\alpha + z_{\alpha'}$ and has the structure

$$\mathbf{\Phi}(s) = \begin{pmatrix} \mathbf{\Phi}_\alpha(s) & \mathbf{X}_{\alpha\alpha'}(s) \\ \mathbf{X}_{\alpha'\alpha}(s) & \mathbf{\Phi}_{\alpha'}(s) \end{pmatrix} \tag{4.15}$$

where $\mathbf{\Phi}_\alpha(s)$, $\mathbf{\Phi}_{\alpha'}(s)$ are defined according to equation (4.11) with $f(L_i, s)$ satisfying equation (4.8) for $i \neq 3$ and

$$f(L_3, s) = \frac{\bar{p}_\alpha \bar{p}_{\alpha'} \exp(-2L\sqrt{s/D})}{1 - \bar{p}_\alpha \bar{p}_{\alpha'} \exp(-2L\sqrt{s/D})}. \tag{4.16}$$

The matrix $\mathbf{X}_{\alpha\alpha'}$ and its transport $\mathbf{X}_{\alpha'\alpha}$ are defined by

$$[\mathbf{X}_{\alpha\alpha'}(s)]_{ij} = \begin{cases} p_{\alpha'} \exp(-L_3\sqrt{s/D}) & \text{if } i = 3,\ j \in \mathcal{I}_{\alpha'},\ j \neq i \\ 0 & \text{otherwise} \end{cases} \tag{4.17}$$

and

$$[\mathbf{X}_{\alpha'\alpha}(s)]_{ij} = \begin{cases} p_\alpha \exp(-L_3\sqrt{s/D}) & \text{if } i = 3,\ j \in \mathcal{I}_\alpha,\ j \neq i \\ 0 & \text{otherwise.} \end{cases} \tag{4.18}$$

The corresponding expression for $G(\alpha, \alpha'; s)$ is obtained by replacing the vector $(\mathbf{v}_\alpha, \mathbf{O}_{\alpha'})$ with $(\mathbf{O}_\alpha, \mathbf{v}_{\alpha'})$, etc.

One can extend the above results to arbitrary trees and graphs and for general initial and final points. The basic structure is similar to equation (4.14) and involves a matrix $\mathbf{\Phi}(s)$ with diagonal blocks $\mathbf{\Phi}_\alpha(s)$ for all branching nodes $\alpha \in \mathcal{B}$, off-diagonal blocks $\mathbf{X}_{\alpha\beta}(s), \mathbf{X}_{\beta\alpha}(s)$ for linked branching nodes α, β and zeros elsewhere.

Finally, an interesting notion that emerges from the examples considered above is that of performing partial summations over trips such as multiple internal reflections on a link (see, for example, equation (4.7)). A similar idea was used by Goldhirsch and Geffen (1986, 1987) in their diagrammatic method for analysing the characteristic function of discrete-time random walks on networks. It is also reminiscent of partial summations over ladder diagrams, for example, in quantum field theory. The use of partial summations may be useful in carrying out configurational averaging where the topology of the tree is fixed but the lengths of each segment are generated according to some probability distribution.

5. Discussion

In this paper we have presented an alternative approach to the conventional Laplace transform and matching boundary conditions method of analysing diffusion processes on complex tree structures. By discretizing space and exploiting the connection between diffusion and random walks, the 'sum-over-paths' approach is basically combinatoric in nature and works from the outset with time as the primary variable of interest rather than the Laplace variable s. For certain classes of problem this *obviates the need for inverting any Laplace transform*, a point we would like to emphasize. Thus for the typical problems listed in the introduction our methodology should form the basis for immediate practical applications. A great virtue of the 'sum-over-paths' approach is that, rather like Feynman diagram methods in quantum field theory, the rules presented allow for the *systematic* construction of the solution given an arbitrary tree.

We have also shown how in the present approach one can formally sum the series expansion of the fundamental solution in Laplace space for both discrete-space and continuous-space systems. This provides a connection with the conventional Laplace technique and an underlying unification; further, the representation thus provided may be useful in the context of configurational averaging. The ideas presented may also be helpful in performing partial diagram summations (e.g. multiple internal reflections on a link, which are akin to ladder diagrams in field theory).

This paper has been concerned with developing an underlying mathematical structure for analysing diffusion processes on tree structures, rather than with solving a specific physical problem in great detail. For the latter one is likely to have to develop additional schemes for configurational averaging or exploiting self-similarity (Cayley tree-like topologies for instance, or Bethe lattices). Again, the 'sum-over-paths' solution is a convenient starting point for such calculations.

We would also like to emphasize the possibility of using the 'sum-over-paths' method as a general strategy for solving other linear PDEs on structures with complex spatial topologies. An obvious and important extension would be to include the effects of drift, which can occur in most of the examples listed in the introduction. Suppose (for simplicity) that a constant drift is introduced onto each segment of the tree Γ introduced in section 2.1. We assume that each segment has the same drift speed v but allow the direction of the drift with respect to the local x-coordinate of a segment to be arbitrary (specified by $\epsilon_i = \pm 1$). Equation (2.4) becomes

$$\frac{\partial c_i}{\partial t} = D\frac{\partial^2 c_i}{\partial x^2} - v\epsilon_i\frac{\partial c_i}{\partial x} \qquad t > 0 \qquad 0 < x < L_i \,. \tag{5.1}$$

The boundary conditions (2.5)–(2.8) hold with the modified current

$$J_i(x,t) = -D\frac{\partial c_i}{\partial x} + \epsilon_i v c_i \,. \tag{5.2}$$

Following the analysis of the zero-drift case, one can evaluate the fundamental solution of equation (5.1) using a space-discretization scheme. A discrete version of the drift–diffusion equation defined on the tree $\hat{\Gamma}$ is of the form (see the appendix)

$$\frac{\mathrm{d}c_I}{\mathrm{d}t} = 2z_I^{-1}\sum_{J(I)}\left(\frac{D}{\Delta x^2}[c_J(t) - c_I(t)] - \epsilon_{IJ}\frac{v}{2\Delta x}[c_I(t) + c_J(t)]\right) \tag{5.3}$$

where $\epsilon_{IJ} = +1$ if the link (IJ) is in the direction of drift and $\epsilon_{IJ} = -1$ if (IJ) is in the opposite direction to the drift. Equation (5.3) yields equation (5.1) and the correct boundary conditions in the continuum limit. We can rewrite equation (5.3) in the form of the matrix equation (2.15) where $\mathbf{Q}$ now generates a *biased* random walk on the tree $\hat{\Gamma}$. The calculation of the fundamental solution based on the path-summation approach is now considerably more involved and requires the solution of an integral equation. The results of this analysis will be presented elsewhere.

Besides the drift–diffusion equation, other obvious candidates for solution on tree structures are the wave equation and the Schrödinger equation (quantum mechanics on graphs, a problem of considerable theoretical interest (see e.g. Gratus *et al* 1994 and references therein)). For the latter, the natural variable of interest is energy, but this formally plays an identical role to the Laplace variable s, which we have shown how to analyse. Moreover, the discrete version of the Schrödinger equation is directly related to tight-binding models, which are also of considerable interest.

Appendix

The 'sum-over-paths' method for solving the diffusion equation on a tree involves a discretization of each line segment leading to a set of coupled ODEs. In this appendix we show how the discrete diffusion equation has a natural interpretation in terms of the geometry of simplicial lattices. Our discussion follows closely chapter 11 of Itzykson and Drouffe (1991). We shall restrict ourselves to the one-dimensional case, although all results can be easily extended to higher dimensions (planar lattices, etc).

Consider a simplicial lattice Γ consisting of points (0-simplexes) labelled I together with a set of links (1-simplexes) (IJ) joining neighbouring points on the lattice at a distance $l_{IJ} = l_{JI}$. (Note that in the text we label the lattice by setting $I = (ni)$ with n numbering the nth discrete point on the ith segment of the tree and identifying the endpoints of all line segments radiating from a given branching node. The length of each link is taken to be $l_{IJ} = \Delta x$.) The dual lattice $\tilde{\Gamma}$ consists of 1-cells and 0-cells. The Ith 1-cell consists of all points on the lattice Γ closer to point I than any other point. The total length of this cell is $\sigma_I = \sum_{J(I)} l_{IJ}/2$ where the summation over J is restricted to nearest neighbours of I. The 0-cell dual to the link (IJ) is the point on the lattice Γ located midway on the link. Define $\mathcal{F}_0$ as the set of 0-forms, that is, functions defined at lattice sites, $I \to \phi_I$. Similarly, $\mathcal{F}_1$ is the set of antisymmetric 1-forms defined on links, $\phi_{IJ} = -\phi_{JI}$. On the dual lattice we denote the set of functions ψ_I on 1-cells by $\tilde{\mathcal{F}}_1$ and the set of antisymmetric tensors ψ_{IJ} on 0-cells by $\tilde{\mathcal{F}}_0$. There is a natural duality between $\mathcal{F}_p$ and $\tilde{\mathcal{F}}_{1-p}$ $(p = 0, 1)$ given by

$$\mathcal{F}_p \leftrightarrow \tilde{\mathcal{F}}_{1-p} \qquad \phi \leftrightarrow \psi \qquad \sigma_I \phi_I = \psi_I \qquad l_{IJ}\phi_{IJ} = \psi_{IJ}\,. \tag{A.1}$$

We denote the dual of ϕ and ψ by $\tilde{\phi}$ and $\tilde{\psi}$. There exists a natural scalar product between the dual spaces $\mathcal{F}_p$ and $\tilde{\mathcal{F}}_{1-p}$ given by

$$\langle \phi|\psi\rangle = \sum_I \phi_I \psi_I \qquad \langle \phi|\psi\rangle = \tfrac{1}{2} \sum_{I,J} \phi_{IJ}\psi_{IJ}\,. \tag{A.2}$$

Introduce the operator d (the analogue of exterior derivative) as a mapping from $\mathcal{F}_0 \to \mathcal{F}_1$ such that

$$(\mathrm{d}\phi)_{IJ} = \frac{\phi_I - \phi_J}{l_{IJ}}\,. \tag{A.3}$$

The dual operator $\tilde{\mathrm{d}} : \tilde{\mathcal{F}}_1 \to \tilde{\mathcal{F}}_0$ is defined according to the relation $\langle\, \mathrm{d}\phi|\psi\rangle = \langle \phi|\,\tilde{\mathrm{d}}\psi\rangle$. Thus

$$(\tilde{\mathrm{d}}\psi)_I = \sum_{J(I)} \frac{\psi_{IJ}}{l_{IJ}}\,. \tag{A.4}$$

We can use the definitions of duality and the operator $\tilde{\mathrm{d}}$ to construct the discrete analogue of the divergence operator, namely, $\mathrm{d}^* : \mathcal{F}_1 \to \mathcal{F}_0$. This is obtained by pulling back the operator $\tilde{\mathrm{d}}$ using the duality map (A.1). More specifically, given a 1-form ϕ_{IJ} we have $\mathrm{d}^*\phi = \widetilde{\tilde{\mathrm{d}}\tilde{\phi}}$, that is,

$$(\mathrm{d}^*\phi)_I = \frac{1}{\sigma_I} \sum_{J(I)} \phi_{IJ} \,. \tag{A.5}$$

The divergence operator (A.5) can be used to formulate a discrete version of the drift–diffusion equation on a tree. Let the 0-form $c_I(t)$ represent a scalar quantity at a point I on the lattice at time t. Define the associated current to be the 1-form ϕ where

$$\phi_{IJ} = -D(\mathrm{d}c)_{IJ} + v\epsilon_{IJ}\frac{c_I + c_J}{2} \tag{A.6}$$

where $\epsilon_{IJ} = +1$ if the link (IJ) is in the direction of drift and $\epsilon_{IJ} = -1$ if (IJ) is in the opposite direction to the drift. Then

$$\frac{\mathrm{d}c}{\mathrm{d}t} = \mathrm{d}^*\phi \,. \tag{A.7}$$

Consider a lattice point with coordination number z_I. Setting $l_{IJ} = \Delta x$ for all links we have $\sigma_I = z_I/2$ so that

$$\frac{\mathrm{d}c_I}{\mathrm{d}t} = 2z_I^{-1} \sum_{J(I)} \left(\frac{D}{\Delta x^2}[c_J(t) - c_I(t)] - \epsilon_{IJ}\frac{v}{2\Delta x}[c_I(t) + c_J(t)] \right) \tag{A.8}$$

which gives equations (2.11) and (5.3) used in the text.

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