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Title: Skew Brownian Motion and Branching Processes Applied to
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Abstract approved: ______________________________

Enrique Thomann - Edward Waymire

This thesis contains three manuscripts addressing the application of stochastic processes to the analysis and solution of partial differential equations (PDEs) in mathematical physics.

In the first manuscript, one dimensional diffusion and Burgers equation are considered. The Fourier transform of the solution to each PDE is represented as the expected value of a multiplicative functional on a branching stochastic process. Monte Carlo simulation schemes are then developed to perform accurate numerical calculations of the solution.

The second manuscript considers an advection-diffusion PDE in a cylinder where the diffusion coefficient and flow velocity are constant in the direction of fluid flow, but are arbitrarily non-smooth in the transversal direction. The stochastic process associated with the PDE is constructed as a diffusion process with the appropriate infinitesimal generator. The properties of ergodic Markov processes are then used to obtain a homogenization result for the solution of the PDE.

The third manuscript studies the stochastic process associated with the one-dimensional diffusion equation in the case where the diffusion coefficient is piecewise constant with a countable set of discontinuities. The resulting process generalizes skew Brownian motion to the case of countable many interfaces. Finally, some applications to advection-diffusion phenomena in two-dimensional layered media are outlined.

Skew Brownian Motion and Branching Processes Applied to Diffusion-Advection in Heterogenous Media and Fluid Flow

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I understand that my thesis will become part of the permanent collection of Oregon State University libraries. My signature below authorizes release of my thesis to any reader upon request.

Jorge M. Ramirez, Author

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1 INTRODUCTION

Profound connections between certain aspects of probability theory and partial differential equations (PDEs) have been identified ever since A. Kolmogorov established a measure theoretical framework for studying continuous time stochastic processes. Very generally, a PDE is connected/associated with a stochastic process, when the solution to the equation is given by certain average over realizations of the random process. In this thesis, I consider PDEs describing the phenomena of solute diffusion and fluid motion, and study their association with certain random branching processes and regular diffusions closely related to Brownian motion. In each instance, I use the analytical tools provided by the theories of probability and PDEs to investigate quantitative and qualitative properties of both, the solution to the PDE and the associated stochastic process.

As usual in mathematics, the discovery of the connections between probability theory and partial differential equations was led by the study of natural processes through mathematical models. In this particular chapter of the history of science, these roles were respectively played by the phenomenon of solute diffusion and the concept of Brownian motion. Indeed, considering the motion of a solute molecule as it is randomly displaced by frequent collisions with the molecules of the surrounding liquid, Einstein (1905) showed that if the motion of individual molecules are independent, and the rate of change of their mean-square displacements is a constant D, then the concentration of molecules $c(t, x)$ must obey the diffusion PDE,

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}. \tag{1.1}$$

Concerning the structure of the paths followed by the particles, Einstein adds: "it is possible that the motions to be treated here are identical to what is known as 'Brownian molecular motion'". This comment, of course, refers to the motion of pollen particles suspended in water observed by Brown (1828). Attempts at mathematically describing Brownian motion as a random process in continuous time were undertaken by Bachelier (1900, 1912) and von Smoluchowski (1906), but the required description of Brownian motion via a measure in path space had to wait for the work of Wiener (1923). This development serves as a prototype for the foundational work by Kolmogorov (1931) where measure theoretical probability was used to arrive at the Chapman-Kolmogorov equations, generalize the Markov property to processes in continuous time, and show that the transition probabilities of certain stationary Markov processes satisfy the Fokker-Planck differential equation. This, and other works leading to the publication of Kolmogorov (1933), gave birth to the modern theory of stochastic processes and its intimate relationship with PDEs in mathematical physics.

The material presented in this thesis relies on many crucial, and some recent, developments in the theories of stochastic processes and PDEs. These include K. Itô's representation of diffusions via integrals with respect to Brownian paths, and the application by W. Feller of the theory of E. Hille and K. Yosida on semigroups associated with the Cauchy problem. My favorite references for these classical results include Mandl (1968), Yosida (1971), Freedman (1971), Itô and McKean (1974), Breiman (1992), Bhattacharya and Waymire (1990b) and Kallenberg (2002). The study of the fine structure of Brownian paths, its local time process and other additive functionals, pioneered by A. Levy and explained thoroughly in Itô and McKean (1974) and Revuz and Yor (1991), will also play a very important role in the analysis of diffusion phenomena presented here. Other notable available tools are the work of Stroock and Varadhan (1979) relating continuous time martingales and differential operators, and the probabilistic reformulation via the Feymann-Kac formula of basic problems in potential theory. In the discussion on diffusion in heterogenous media presented here, I study stochastic processes associated with generalizations of equation (1.1) where D is a non-smooth function of x. Of fundamental importance for that discussion is the treatment of Dirichlet forms in Fukushima (1980) and Ma and Röckner (1991), where the authors successfully bridge the gap between the formulation of PDEs in the weak sense, and the Markov processes governing the motion of the diffusing particles. Finally, for the application of multiplicative cascades and branching processes to the diffusion and Burgers equation, my starting point is the probabilistic representation for the Navier-Stokes equations in LeJan and Sznitman (1997) and the later generalization by Bhattacharya et al. (2003). I am then, proud and thankful to continue a tradition of "standing on the shoulder of giants", and hopefully contribute with novel developments to this interesting subject.

Each problem considered in this thesis arises from the study of physical phenomena and involves a PDE and an associated stochastic process. In general, the PDEs I consider are evolution equations of the form

$$\frac{\partial u}{\partial t} = \mathcal{A}u, \quad t \geqslant 0, \quad u(0) = u_0, \tag{1.2}$$

for u in a appropriate function space $\mathscr{L}$, and where $\mathcal{A}$ is an operator on $\mathscr{L}$. A stochastic process with state space S and index set Λ, is a sequence of random variables $X = \{X_\lambda : \lambda \in \Lambda\}$ defined on the same probability space $\{\Omega, \mathscr{F}, \mathbb{P}\}$, namely $X_\lambda : \Omega \to S$ for all $\lambda \in \Lambda$. For instance, throughout my treatment on diffusion processes, S is Euclidean space $\mathbb{R}^d$ and the index set Λ is the positive real line $[0, \infty)$; the process X being then a model for the motion of particles. In my considerations about diffusion and Burgers equation in Fourier space, Λ is the set of vertices of a tree, and the state space is a subset of $\mathbb{Z} \times [0, \infty) \times \{0, 1\}$. For problems in this thesis, I say that the process X is "associated" to the problem (1.2) if there is a (random) functional F such that the solution to (1.2) is given by

$$u(t) = \mathbb{E}\{F(X, t, u_0)\}, \quad 0 \leqslant t < T, \tag{1.3}$$

for some $T > 0$, where $\mathbb{E}$ denotes expectation with respect to the measure $\mathbb{P}$, and the equality is defined in the sense of functions in $\mathscr{L}$.

Equation (1.3) gives a mathematical characterization of the association between stochastic processes and PDEs for the problems considered in this thesis. As it will be shown for each particular problem, however, a probabilistic formulation of the form (1.2) usually involves more than the representation of the solution u via (1.3). At a first glance, such a representation has the following three advantages:

i. Whenever X is also a model for a physical process, equation (1.3) explicitly shows how the deterministic quantity u is the result of the average behavior of the system described by X. This observation is at the heart of the reasoning in Einstein (1905): if X is the right model for the position of individual solute molecules, then the concentration of the solute at any point must equal the average fraction of particles that occupy a small neighborhood around the point.

ii. Equation (1.3) gives a way of estimating u via Monte Carlo methods. Namely, if enough realizations of X can be accurately performed, then the average of the simulated values of $F(X, t, u_0)$ gives an approximation for $u(t)$.

iii. One may apply results from ergodic theory, large deviations and convergence of random processes to X, and gain information about the behavior of u under different limit scenarios.

The above list is by no means complete, and mostly reflects the general intention of the topics treated in this thesis. In what follows, I explain the organization of this document and give a general outline of the problems considered in subsequent chapters.

This dissertation is written in the “manuscript document format” as specified by the Oregon State University Thesis Guide 2006-2007. Each of the three subsequent chapters contains a manuscript on the common general subject of applications of stochastic processes to the analysis of PDEs. The publication status of each manuscript is specified in the respective chapter heading page. In the last chapter of this dissertation the reader can find some concluding remarks, afterthoughts and open problems that did not make it into the submitted manuscripts.

I apologize in advance for the difficulties the reader might encounter due to the difference in notation and style between the manuscripts. It suffices to say that each of the documents was written at different stages of my academic formation and is intended for different audiences. Also, I will not go into detail in this introduction about the material presented in each manuscript, for each of them contains a proper introduction section. It is pertinent, however, to describe the accomplishments of each work viewed under the light of the general subject.

Manuscript number one considers the diffusion equation with a potential, and Burgers equation in a periodic medium. The goal is to obtain numerical approximations as described in item (***ii***) of the list above. The motivation comes from the work by LeJan and Sznitman (1997) and Bhattacharya et al. (2003) on random multiplicative cascade representations for PDEs in Fourier space. My results include particular stochastic processes amenable to numerical simulation, and some algorithms to numerically approximate the solution to the associated PDEs by Monte Carlo and classical Picard iteration methods.

The work in manuscript number two arose from multidisciplinary discussions on the effect medium heterogeneities have over the transport of solutes undergoing advection and diffusion. As a first approximation, we considered a cylindrical medium filled with a fluid moving parallel to the axes of the cylinder, and containing a passive solute. The heterogenous nature of the media is modeled by a diffusion coefficient that might be discontinuous in the direction transverse to the flow. In the sprit of item (***iii***) above, we extend the work by Bhattacharya and Gupta (1984) and use central limit theory techniques to establish the effect of the fluid velocity on the asymptotic longitudinal dispersion of the solute. Our result generalizes the classical formulation by Taylor (1953) and Aris (1956) on effective dispersion in Poiseuille flow, to the case of a non-smooth diffusion coefficient and an arbitrary velocity profile. A second result aims, in view of item (***i***), at determining the effect that sharp discontinuities of the diffusion coefficient have on the paths of individual particles. We consider a piecewise constant diffusion coefficient, and prove that the stochastic process modeling the motion of particles is locally a re-scaling of skew Brownian motion, a process introduced in Itô and McKean (1963). In particular, the right model for particle motion is one in which sample paths behave like Brownian motion until they reach a point where the diffusion coefficient is discontinuous, once there, the path experiences a skewness and tends to move in the direction where the diffusion coefficient is higher.

The third manuscript explores mathematical questions motivated by the problem considered in the second manuscript. In particular, I analyze a generalization of skew Brownian motion to the case of an infinite set of interfaces, each of them with a given value of skewness. Classical probabilistic techniques are then used to establish the local and the long term behavior of the process as a function of the values of the skewness. The process is then associated with the appropriate advection diffusion PDE on two-dimensional space. Finally, I consider a particular example in which the structure of the stochastic process is tractable, and use its properties to establish the long term behavior of a solute in an infinite two-dimensional layered medium.

Finally, some acknowledgments are in order. It is my pleasure to thank those people involved in the preparation of this dissertation, in particular my major professors Edward Waymire and Enrique Thomann, for their relentless support, guidance and encouragement. The discussion and collaboration with my coauthors on the second manuscript is also greatly appreciated. Special thanks are also in order for the helpful comments and corrections made by the editors and reviewers of each of the submitted manuscripts. Lastly, I am thankful to the rest of my graduate committee, professors Ralph E. Showalter, John W. Lee, Yevgeniy Kovchegov, and James Liburdy, for taking the time to review this final version.

2 MULTIPLICATIVE CASCADES APPLIED TO PARTIAL DIFFERENTIAL EQUATIONS

(TWO NUMERICAL EXAMPLES)

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2.1 Introduction

Stochastic processes have been found to have important connections to deterministic partial differential equations (PDEs), most notable being the relationship between the linear diffusion equation and Brownian motion through the Feynman-Kac formula (e.g. see van Kampen (1981), Bhattacharya and Waymire (1990b)). In later developments, probabilistic representations have been found to solutions of semilinear and quasilinear equations. Important examples include the well-known example by H. P. McKean McKean (1975) for the solution to the KPP equation as the expected value of a functional of branching Brownian motion, and more recently the work in Ossiander (2005), where the solution to the incompressible Navier-Stokes equations is written in terms of a jumping and branching Brownian motion.

In each of the three works cited above, the solution to the PDE is represented as the expected value of a functional acting on the sample paths of certain stochastic process evolving in physical space. This paper deals with the analogous idea in *Fourier space*, along the lines of the method introduced in LeJan and Sznitman (1997) for the Navier-Stokes equations. Namely, multiplicative functionals of tree-like stochastic models are used to give probabilistic representation of the Fourier transform of the solution to the PDE. Two particular examples are considered: simple linear diffusion with a potential, and viscous Burgers equation. Further restrictions are imposed to the Fourier transform of the data in each PDE to achieve the probabilistic representation.

The main emphasis is on the design of *Monte Carlo simulation* schemes to numerically approximate the solution of each PDE in Fourier space. The initial approximations are further improved by means of numerical *Picard iteration.*

In order to fix the main ideas of the methods used in subsequent sections of this paper, consider the simple example of the diffusion equation with Fickian flux and a sink term of constant rate $c > 0$,

$$u_t = u_{xx} + cu,\, t > 0, \quad u(0^+) = u_0. \tag{2.1}$$

Feynman-Kac's formula gives the following explicit probabilistic representation of the solution u in physical space,

$$u(t,x) = \int_{-\infty}^{\infty} e^{-ct}\, \tfrac{1}{\sqrt{2\pi t}}\, e^{-\frac{1}{2t}(x-y)^2}\, u_0(y)\,\mathrm{d}y = \mathbb{E}_x\{\mathbb{1}_{S>t}\, u_0(B_t)\}, \tag{2.2}$$

where $B = \{B_t : t \geqslant 0\}$ is a standard Brownian motion and S is an exponentially distributed random variable independent of B, namely $\mathbb{P}(S > t) = e^{-ct}, \quad t > 0$. The symbol $\mathbb{E}_x$ denotes expectation conditioned to the event $[B_0 = x]$ and $\mathbb{1}_{S>t}$ denotes the indicator function of the event $[S > t]$, i.e. $\mathbb{1}_{S>t}$ is 1 or 0 depending on wether $[S > t]$ occurs or not.

The probabilistic representation in (2.2) helps create a very clear and intuitive physical picture of the solution to the PDE: for $t > 0$, particles initially distributed according to u_0, start moving (diffusing) following the paths of B and are "killed" at a random time S; $u(x,t)$ is the expected fraction of surviving particles that occupy the point x at time t.

A generalization of the example (2.1) will be revisited in Section 2.2, but in contrast to the description above, the solution is now represented probabilistically in Fourier space. Namely, the Fourier transform of u

$$\hat{u}(t,\xi) = \tfrac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-ix\xi} u(t,x)\,\mathrm{d}x,$$

which from (2.1) satisfies

$$\hat{u}_t(t,\xi) = -\xi^2\, \hat{u}(t,\xi) + c\hat{u}(t,\xi),\, t > 0, \quad \hat{u}(0^+) = \hat{u}_0, \tag{2.3}$$

is expressed as the expected value of a functional of some process that takes values in time-frequency space.

The problem in (2.3) can be solved exactly in a variety of ways. One non-obvious method that illustrates the main ideas used in this paper is outlined below.

Multiply both sides of (2.3) by $e^{\xi^2 t}$ and integrate on $(0,t)$ to get,

$$\begin{aligned}\hat{u}(t,\xi) &= e^{-\xi^2 t}\hat{u}_0(\xi) + \frac{c}{\xi^2}\int_0^t \xi^2 e^{-\xi^2 s}\hat{u}(t-s,\xi)\,\mathrm{d}s && (2.4)\\ &= \mathbb{E}\left\{\hat{u}_0(\xi)\mathbb{1}_{S_0>t} + \frac{c}{\xi^2}\hat{u}(t-S_0,\xi)\mathbb{1}_{S_0<t}\right\}, && (2.5)\end{aligned}$$

where S_0 is an exponentially distributed with

$$\mathbb{P}(S_0 > t) = e^{-\xi^2 t}. \tag{2.6}$$

The goal is now to use (2.5) to construct a stochastic model τ and a functional $\mathsf{X} = \mathsf{X}(\tau)$ such that

$$\hat{u}(t,\xi) = \mathbb{E}\mathsf{X}(\tau). \tag{2.7}$$

Consider a root vertex $\langle 0\rangle$. Assign to it a frequency (or type) ξ, and compare a realization of the random time S_0 to the termination time of $\langle 0\rangle$ denoted by $T_0 = t$. In the event that $S_0 \geqslant t$, the process stops and the multiplier $M_0 = u_0(\xi)$ is assigned to $\langle 0\rangle$. If $S_0 < t$, a new vertex $\langle 1\rangle$ of τ is created. In this example, the frequency of the vertex $\langle 1\rangle$ remains equal to ξ, i.e. is selected according to the Dirac delta distribution δ_ξ. The respective multiplier is $M_1 = \frac{c}{\xi^2}$. The construction of τ is continued by generating an exponential time S_1 independent of, and with the same distribution (2.6), as S_0. The termination time of the vertex $\langle 1\rangle$ is set to $T_1 = t - S_0$.

Let N be the number of vertices in τ, and define X as the following *multiplicative functional*

$$\mathsf{X}(\tau) = \prod_{i=0}^{N-1} M_i. \tag{2.8}$$

The formulation is then completed by showing that indeed (2.7) holds. This can be done following the lines of the proof of Theorem (2.2.1).

The probabilistic formulations given in (2.5) or (2.7) do not immediately point to a physical picture as clear as the one obtained by Feynman-Kac's formula (2.2) in physical space. Nevertheless, the stochastic model (2.8) gives a useful way of studying solutions in Fourier space and, in particular, is amenable to numerically estimation of

$\hat{u}$. Two techniques are used in this paper to achieve this, and can be illustrated with the derivations in the example above. The first is direct Monte Carlo simulation of the expected value in (2.7). The second is more classical and stems from understanding (2.4) as the fixed point equation $\hat{u}(t,\xi) = F(\hat{u},t,\xi)$, where F is the linear operator given by the right hand side of (2.4) on an appropriate Banach space. Provided that F is a contraction in the norm of the space under consideration, a solution is given by $\hat{u} = \lim_{n\to\infty} \hat{u}^{(n)}$ with $\hat{u}^{(n+1)} = F(\hat{u}^{(n)},t,\xi)$, $n = 0,1,2\ldots$ (see Folland (1999) for more details). This latter method is referred to in this paper as Picard iteration.

A probabilistic formulation along the lines of the illustrative example (2.1), is available for a diverse class of evolution equations, including reaction-diffusion, Schrödinger, Burgers and Navier-Stokes equations (see Waymire (2002), Thomann (2002), Orum (2004), Kolokoltsov (2002)). In the seminal work of LeJan and Sznitman (1997), the authors show that the Fourier transformed solution to the incompressible Navier-Stokes equations in three dimensions satisfies an equation of the form of (2.7) with τ having tree graph structure. The branching at the vertices of τ is produced by the quadratic nonlinearity in the PDE, very much like the branching necessary for McKean's solution to KPP equation in physical space (see McKean (1975)).

The stochastic process involved in the probabilistic representation of Navier-Stokes in Fourier space is difficult to model due to the three degrees of freedom in the frequencies assigned to the vertices of τ. Fortunately, the main features of the associated multiplicative random functional, appear also in the probabilistic formulation of the one-dimensional Burgers equation in Fourier space. The branching at the vertices of τ is linked to the nonlinear term common to both equations. The example of Burgers equation is worked out in detail in Section 2.3.

In the probabilistic formulation for Burgers and the Navier-Stokes equations, the branching structure requires that one specifies the probability distribution of the frequency of the offspring vertices given the frequency of the parent vertex. In the case of the diffusion equation (2.1), where τ has no branching, this distribution was a Dirac delta distribution.

Admissible distributions are referred to as *majorizing kernels*, and were studied thoroughly in Bhattacharya et al. (2003) for the case of incompressible Navier-Stokes equations. The authors also show how the majorizing kernel can be used in establishing existence and regularity of solutions.

Although the theory and numerical schemes explored here are mathematically motivated, there is hope for a physically intuitive picture for the branching stochastic model in the probability formulation of Burgers or Navier-Stokes equations in Fourier space. The branching process τ, together with the multipliers associated to its vertices, is referred to as a *stochastic cascade* (see Waymire (2002) and references therein). This name is appropriate, especially when viewed in terms of Kolmogorov's statistical theory of turbulence. Identifying the actual link between the probabilistic formulation and Kolmogorov's cascade is still a very important open problem. It is conceivable that the majorizing kernels that determine the branching in τ are related to the physical rates of transport of energy between frequencies in turbulent flows. The numerical models reported in this paper are simple tools that might help to shed light on this relationship.

The organization is as follows. The rest of this introduction sets down some terminology about the main tools to be used, namely Fourier transform and tree graphs. The linear diffusion equation with potential

$$u_t = \tfrac{a^2}{2} u_{xx} + c(x)u$$

is considered in Section 2.2, and Burgers equation

$$u_t + \sqrt{2\pi}\, u u_x = \nu u_{xx} + f(t,x)$$

is treated on Section 2.3.

Some remarks on notation are in order. All partial differential equations are assumed to hold in the Schwartz class of tempered distributions $\mathcal{S}'$. The Fourier transform on $\mathcal{S}'$ is defined through its action on test functions as

$$\hat{\phi}(\xi) = \tfrac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-ix\xi} \phi(x)\, \mathrm{d}x, \quad \xi \in \mathbb{R}, \quad \phi \in C_0^\infty(\mathbb{R}).$$

In the case of periodic distributions, the Fourier series representation is available,

$$u = \tfrac{1}{\sqrt{2\pi}} \sum_{k\in\mathbb{Z}} \hat{u}(k)\, e^{ikx}, \quad u \in \mathcal{S}',\ u \text{ periodic}. \tag{2.9}$$

Details on the construction of the Fourier transform on $\mathcal{S}'$ and its properties can be found in Folland (1999) or Zemanian (1987).

Tree graphs are used in this paper as a suitable frame to define certain multiplicative processes, and only a bit of special notation is required. A tree graph τ is a connected graph of vertices with no cycles, and with vertex set containing a unique root vertex coded as $\langle 0\rangle$. The edges of a tree are determined by the relation "belongs to the offspring of". The $n_{\langle 0\rangle}$ vertices in the offspring of $\langle 0\rangle$ are coded by $\langle 1\rangle, \langle 2\rangle, \ldots, \langle n_{\langle 0\rangle}\rangle$. The vertices of second generation, i.e. the offspring of some $\langle i\rangle$, are coded as $\langle i1\rangle, \langle i2\rangle, \ldots, \langle in_{\langle i\rangle}\rangle$. Inductively, a vertex of the n-th generation of τ has the form $\langle v\rangle = \langle i_1 i_2 \ldots i_n\rangle$, where i_k is a positive integer for each k. For a vertex $\langle v\rangle = \langle i_1 i_2 \ldots i_n\rangle$ its length is defined as $|\langle v\rangle| = n$ with the convention $|\langle 0\rangle| = 0$. For $j = 1, 2, \ldots, |\langle v\rangle|$, the j-th level of $\langle v\rangle$ is the vertex let $\langle v\rangle|j = \langle i_1, \ldots, i_j\rangle$, $\langle v\rangle|0 = \langle 0\rangle$. The sequence $\{\langle v\rangle|0, \langle v\rangle|1, \ldots, \langle v\rangle\}$ can be viewed as a path connecting $\langle 0\rangle$ with $\langle v\rangle$.

2.2 Linear diffusion equation

Consider the one-dimensional linear diffusion equation in $(-\infty, \infty)$ with constant diffusion coefficient $\frac{1}{2}a^2 > 0$, potential $c = c(x)$ and initial condition $u_0 = u_0(x)$,

$$u_t(t) = \tfrac{a^2}{2} u_{xx}(t) + c\, u(t), t > 0 \quad u(0^+) = u_0. \tag{2.10}$$

Assume that c and u_0 have Fourier series with a finite number of terms, and that the Fourier coefficients of c are all nonnegative. In particular c and u_0 are periodic and there exist finite sets of frequencies $\{\alpha_i\}_{i=1}^{m_c}$ and $\{\beta_j\}_{j=1}^{m_u}$, such that

$$c(x) = \tfrac{1}{\sqrt{2\pi}} \sum_{i=1}^{m_c} \hat{c}(\alpha_i)\, e^{i\alpha_i x}, \quad u_0(x) = \tfrac{1}{\sqrt{2\pi}} \sum_{j=1}^{m_u} \hat{u}_0(\beta_j)\, e^{i\beta_j x}. \tag{2.11}$$

Assume furthermore that

$$\hat{c}(\alpha_i) > 0,\ i = 1, \ldots, m_c, \quad \hat{u_0}(\beta_j) \neq 0,\ j = 1, \ldots, m_u.$$

Take Fourier transform on both sides of equation (2.10) and use the integrating factor $e^{\frac{a^2}{2}\xi^2 s}$ to get

$$\hat{u}(t,\xi) = e^{-\frac{a^2}{2}\xi^2 t}\,\hat{u}_0(\xi) + \int_0^t e^{-\frac{a^2}{2}\xi^2 s}\left\{\sum_{i=1}^{m_c} \hat{c}(\alpha_i)\,\hat{u}(t-s,\xi-\alpha_i)\right\} \mathrm{d}s. \tag{2.12}$$

The integral equation (2.12) can readily be written as the expected value of some multiplicative process, however, for computational reasons described in (2.2.1), is more convenient to introduce an exponential factor whose argument does not depend on ξ, for example e^{-t}. Define

$$m(t,\xi) = e^{-\frac{a^2}{2}\xi^2 t + t}, \quad m'(t,\xi) = m(t,\xi)\sum_{i=1}^{m_c} \hat{c}(\alpha_i) \tag{2.13}$$

and write

$$\hat{u}(t,\xi) = m(t,\xi)\,e^{-t}\hat{u}_0(\xi) + \int_0^t e^{-s}\,m'(s,\xi)\sum_{k=1}^{m_c}\left[\frac{\hat{c}(\alpha_k)}{\sum_{i=1}^{m_c}\hat{c}(\alpha_i)}\hat{u}(t-s,\xi-\alpha_i)\right] \mathrm{d}s, \tag{2.14}$$

The representation in (2.14) suggests the following stochastic model for $\hat{u}$. For each $t > 0$, $\xi \in \mathbb{R}$, consider the linear tree graph

$$\tau(t,\xi) = \{\langle 0\rangle, \langle 1\rangle, \langle 11\rangle, \langle 111\rangle \ldots\} = \{\langle 0\rangle, \langle 1\rangle, \langle 2\rangle, \langle 3\rangle \ldots\}$$

and let $(\Omega, \mathcal{F}, \mathbb{P}_\xi)$ be a probability space. To each vertex $\langle i\rangle$ associate a Fourier wavenumber (or type) $\xi_{\langle i\rangle}$ and a exponential random time $S_{\langle i\rangle}$ with $\mathbb{P}_\xi(S_{\langle i\rangle} > s) = e^{-s}$, $s > 0$. Equip the sequence of types $\{\xi_{\langle i\rangle}\}_{i=0}^{\infty}$ with a random walk structure with mutually independent and identically distributed increments $\eta_{\langle i\rangle} = \xi_{\langle i+1\rangle} - \xi_{\langle i\rangle}$ satisfying

$$\mathbb{P}_\xi(\eta_{\langle i\rangle} = -\alpha_k) = \frac{\hat{c}(\alpha_k)}{\sum_{j=1}^{m_c}\hat{c}(\alpha_j)}, \quad k = 1, \ldots, m_c. \tag{2.15}$$

Then equation (2.14) can be written as,

$$\hat{u}(t,\xi) = \mathbb{E}_\xi\left\{\mathbb{1}_{S_{\langle 0\rangle} > t}\, m(t,\xi)\,\hat{u}_0(\xi) + \mathbb{1}_{S_{\langle 0\rangle} \leq t}\, m'(S_{\langle 0\rangle},\xi)\,\hat{u}(t - S_{\langle 0\rangle}, \xi + \eta_{\langle 0\rangle})\right\} \tag{2.16}$$

hinting that $\hat{u}$ can be represented as the expected value of a random product. Define termination times by

$$T_{\langle 0\rangle} = t, \quad T_{\langle i+1\rangle} = t - (S_{\langle 0\rangle} + \cdots + S_{\langle i\rangle}), \quad i = 0, 1 \ldots$$

and let $N = N(\tau(t,\xi)) = \inf\{i : S_{\langle i\rangle} > T_{\langle i\rangle}\}$. The random variable N gives the total number of vertices of τ and has a Poisson distribution with mean t, namely $\mathbb{P}(N = n) = \frac{1}{n!}e^{-t}t^n$. Define the multiplicative functional $\mathsf{X}(t,\xi) = \mathsf{X}(\tau(t,\xi))$ of the random collections $\{\xi_{\langle i\rangle}\}_{i=0}^N$, $\{S_{\langle i\rangle}\}_{i=0}^N$ by:

$$\mathsf{X}(\tau(t,\xi)) = \left(\prod_{i=0}^{N-1} m'(S_{\langle i\rangle}, \xi_{\langle i\rangle})\right) m(T_{\langle N\rangle}, \xi_{\langle N\rangle})\, \hat{u}_0(\xi_{\langle N\rangle}), \tag{2.17}$$

where for $N = 0$ the product in parenthesis is taken to be one. The following holds

Theorem 2.2.1. *For $t > 0, \xi = \xi_{\langle 0\rangle}$,*

$$\hat{u}(t,\xi) = \mathbb{E}_\xi\, \mathsf{X}(\tau(t,\xi))$$

is a solution to the integral equation (2.14).

Proof. The finiteness of the expected value has to be established first. Let $\sigma \geqslant \sum_{i=1}^{m_c} \hat{c}(\alpha_k)$, $U \geqslant \max\{\hat{u}(b_j), j = 1, \ldots, m_u\}$, and note that for each ξ, $m(t,\xi) \leqslant e^t$ and $m'(t,\xi) \leqslant \sigma e^t$. Then

$$\begin{aligned} \mathbb{E}_\xi \mathsf{X}(\tau(t,\xi)) &\leqslant Ue^t\, \mathbb{E}_\xi \left\{\prod_{i=0}^{N-1} \sigma e^{S_{\langle i\rangle}}\right\} = Ue^t \sum_{n=0}^{\infty} \frac{t^n e^{-t}}{n!} \sigma^n e^{S_{\langle 0\rangle} + \cdots + S_{\langle n-1\rangle}} \\ &\leqslant Ue^t \sum_{n=0}^{\infty} \frac{t^n e^{-t}}{n!} \sigma^n e^t = Ue^{t(\sigma+1)}. \end{aligned}$$

Let $t > 0$, $\xi = \xi_{\langle 0\rangle}$. By the lack of memory of the exponential distribution, (2.17) can be written recursively as

$$\mathsf{X}(\tau(t,\xi)) = \begin{cases} m(t, \xi_{\langle 0\rangle})\, \hat{u}_0(\xi_{\langle 0\rangle}) & \text{if } S_{\langle 0\rangle} > t, \\ m'(S_{\langle 0\rangle}, \xi_{\langle 0\rangle})\, \mathsf{X}(\tau(t - S_{\langle 0\rangle}, \xi_{\langle 1\rangle})) & \text{if } S_{\langle 0\rangle} \leq t. \end{cases} \tag{2.18}$$

Use the mutual independence of $S_{\langle i\rangle}$ and $\eta_{\langle i\rangle}$ to get

$$\begin{aligned}
\mathbb{E}_\xi \mathsf{X}(t,\xi) &= m(t,\xi)\hat{u}_0(\xi)\mathbb{P}(S_{\langle 0\rangle} > t) + \mathbb{E}_\xi \left\{ m'(S_{\langle 0\rangle},\xi)\,\mathsf{X}(t - S_{\langle 0\rangle}, \xi + \eta_{\langle 0\rangle})\mathbb{1}_{S_{\langle 0\rangle}\leqslant t} \right\} \\
&= m(t,\xi)e^{-t}\hat{u}_0(\xi) + \int_0^t e^{-s} m'(s,\xi)\ \mathbb{E}_\xi \left\{ \mathsf{X}(t-s, \xi + \eta_{\langle 0\rangle}) \middle| S_{\langle 0\rangle} = s \right\} \mathrm{d}s \\
&= m(t,\xi)e^{-t}\hat{u}_0(\xi) + \int_0^t e^{-s} m'(s,\xi)\ \mathbb{E}_\xi \left\{ \mathsf{X}(t-s, \xi + \eta_{\langle 0\rangle}) \middle| S_{\langle 0\rangle} = s \right\} \mathrm{d}s \\
&= m(t,\xi)e^{-t}\hat{u}_0(\xi) + \int_0^t e^{-s} m'(s,\xi) \sum_{i=1}^{m_c} \left\{ \frac{\hat{c}(\alpha_k)}{\sum_{i=1}^{m_c} \hat{c}(\alpha_k)} \mathbb{E}_\xi \mathsf{X}(t-s, \xi - \alpha_i) \right\} \mathrm{d}s.
\end{aligned}$$

□

Heuristically, the underlying stochastic process can be thought of as a "construction" of $\tau(t,\xi)$ as follows: fix $\xi_{\langle 0\rangle} = \xi$, generate $S_{\langle 0\rangle}$ and compare its value to the termination time $T_{\langle 0\rangle} = t$. In the event $[S_{\langle 0\rangle} > t]$ the tree has no further vertices. If $[S_{\langle 0\rangle} \le t]$, the vertex $\langle 1\rangle$ is created and it is assigned a random type $\xi_{\langle 1\rangle} = \xi_{\langle 0\rangle} + \eta_{\langle 0\rangle}$ (see figure 2.1). Repeat this process at $\langle 1\rangle, \langle 2\rangle, \ldots$ until no more new vertices arise. Assign the correct multipliers to the N resulting nodes, and evaluate (2.17).

2.2.1 Modeling

As a first step, $\hat{u}(t,\xi)$ is approximated by a Monte Carlo estimation of $\mathbb{E}\,\mathsf{X}(\tau(t,\xi))$ given by equation (2.17). Let ξ and t be fixed. The construction of $\tau(t,\xi)$ can be modified in such a way that only realizations that contribute to the mean of $\mathsf{X}(t,\xi)$ are preformed, i.e. realizations with $\hat{u}_0(\xi_{\langle N\rangle}) \neq 0$. For this, condition the expected value of (2.17) on $\xi_{\langle 0\rangle} = \xi$, $N = n$ and $\xi_{\langle n\rangle} = \beta_j$, to get

$$\hat{u}(t,\xi) = \sum_{j=1}^{m_u} \sum_{n=0}^{\infty} \mathbb{E}_\xi \left\{ \left[\prod_{i=0}^{n-1} m'(S_{\langle i\rangle}, \xi_{\langle i\rangle}) \right] m(T_{\langle n\rangle}, \beta_j)\, \hat{u}_0(\beta_j) \right\} \frac{e^{-t} t^n}{n!} \mathbb{P}_\xi(\xi_{\langle n\rangle} = \beta_j). \quad (2.19)$$

The Monte Carlo simulation of the expected value in equation (2.19) can be done as follows. For each t, n, and β_j, perform an appropriate number of random "backward walks" $\{\xi_{\langle i\rangle}\}_{i=n}^{0}$ with $\xi_{\langle n\rangle} = \beta_j$, $\xi_{\langle i\rangle} = \beta_j - \eta_{\langle n-1\rangle} - \cdots - \eta_{\langle i\rangle}$, $i = n-1, \ldots, 0$, and generate

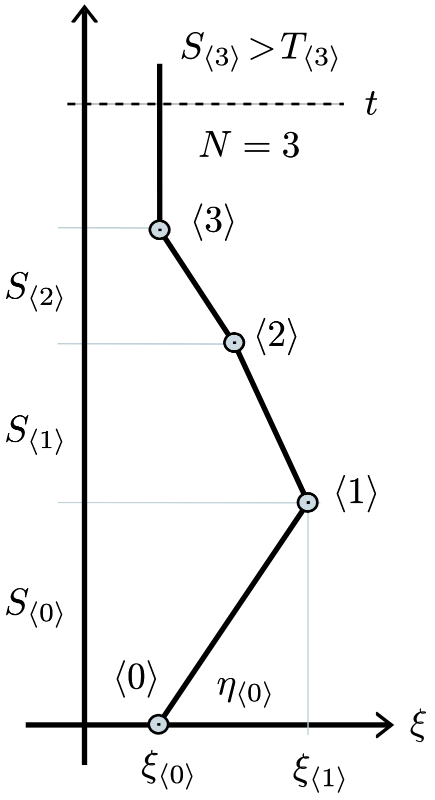

Figure 2.1: Diagram of a realization of a tree τ for the diffusion equation with $N = 3$. The value of the multiplicative functional is $\mathsf{X}(t,\xi) = m(S_{\langle 0\rangle},\xi_{\langle 0\rangle})m(S_{\langle 1\rangle},\xi_{\langle 1\rangle})m(S_{\langle 2\rangle},\xi_{\langle 2\rangle})m'(T_{\langle 3\rangle},\xi_{\langle 3\rangle})$.

exponential times $\{S_{\langle i\rangle}\}_{i=0}^{n-1}$ conditioned to $[S_{\langle 0\rangle}+\cdots+S_{\langle n-1\rangle}<t]$. Then calculate the average of the product

$$\left[\prod_{i=0}^{n-1} m'(S_{\langle i\rangle},\xi_{\langle i\rangle})\right] m(t-(S_{\langle 0\rangle}+\cdots+S_{\langle n\rangle}),\beta_j)\,\hat{u}_0(\beta_j)$$

over all walks with $\xi_{\langle 0\rangle}=\xi$.

The probabilities $\mathbb{P}_\xi(\xi_{\langle n\rangle}=\beta_j)$, $j=1,\dots,m_u$, can be computed from the n-th power of the transition probability matrix of the Markov process $\{\xi_{\langle i\rangle}=\xi+\eta_{\langle 0\rangle}+\cdots+\eta_{\langle i-1\rangle}\}_{i\geq 1}$. The entries of this matrix are obtained from (2.15).

Some remarks are in order. First, recall that the conditional distribution of $(S_{\langle 0\rangle}, S_{\langle 0\rangle}+S_{\langle 1\rangle},...,S_{\langle 0\rangle}+\cdots+S_{\langle n\rangle})$ given $[S_{\langle 0\rangle}+\cdots+S_{\langle n\rangle}<t]$ is the same as the distribution of n increasingly ordered independent random variables each having the uniform distribution on $(0,t]$, (see Bhattacharya and Waymire (1990b) pg. 280). Secondly, although the summation over n in (2.19) is over all positive integers, the probability $\frac{e^{-t}t^n}{n!}\mathbb{P}_\xi(\xi_{\langle n\rangle}=\beta_j)$ decreases to zero very fast for moderate values of t, so only small trees have to be considered. For example, for values of t close to 1, trees with $N\geqslant 15$ have probability of the order 10^{-8}, and so their contribution to the mean can be neglected.

A Picard iteration of the integral equation (2.12) can be used to assess the accuracy of the Monte Carlo simulation and improve the results. Let $\hat{u}^{(0)}$ be the approximation of $\mathbb{E}_k\,\mathsf{X}(\tau(t,\xi))$, and for $n\geqslant 0$, define

$$\hat{u}^{(n+1)}(t,\xi)=e^{-\frac{a^2}{2}\xi^2 t}\,\hat{u}_0^{(n)}(\xi)+\int_0^t e^{-\frac{a^2}{2}\xi^2 s}\left\{\sum_{i=1}^{m_c}\hat{c}(\alpha_i)\,\hat{u}^{(n)}(t-s,\xi-\alpha_i)\right\}\mathrm{d}s, \tag{2.20}$$

a sequence in the space of almost everywhere bounded functions $L^\infty(\mathbb{R})$. A solution to the diffusion equation in Fourier space is a fixed point of equation (2.20), and the error of the n-th approximation to the solution can be measured by

$$E_n=\frac{\|\hat{u}^{(n+1)}-\hat{u}^{(n)}\|_\infty}{\|\hat{u}^{(n)}\|_\infty}.$$

Crucial to the algorithm presented here is the introduction of the multipliers in (2.13). Previous attempts using random times $S_{\langle i\rangle}$ with frequency-dependent mean and time-independent multipliers $m(\xi)$, led to very unstable and non-convergent simulations (S. Dobson, E. Thomann, personal communication). This problem is corrected by the definition of $m(\xi, t)$ used here.

2.2.2 Example

Consider equation (2.10) with data $c(x) = \cos x$, $u_0(x) = \sin x$. The problem in Fourier space is

$$\hat{u}_t(t,\xi) = -\tfrac{a^2}{2}\xi^2\hat{u}(t,\xi) + \tfrac{1}{2}(\delta_1 + \delta_{-1}) * \hat{u}(t,\xi), \quad \hat{u}_0(\xi) = \tfrac{1}{2}(\delta_1 - \delta_{-1}). \tag{2.21}$$

Only trees (walks) with $\xi_{\langle N \rangle} = \pm 1$ have to be constructed, and the solution is expected to be an odd function. The number of generated walks of length N for each finishing should be large enough so all accessible values of $\xi_{\langle 0 \rangle}$ are well sampled, and the values of the aggregates $S_{\langle 0 \rangle}, S_{\langle 0 \rangle} + S_1, \ldots, S_{\langle 0 \rangle} + \cdots + S_{N-1}$ exhibit a good approximation to a uniform distribution on $(0, t]$. A simple heuristic rule is, for each N and t, to generate a number of trees proportional to Nt. The error for this particular example showed little change for values of the constant of proportionality over 1000, so this value was used. The iterates of (2.20) were computed for ten equally spaced time points in $[0, 1]$, and the integration in time was performed with a simple trapezoidal rule. A comparison between the consecutive iterates $n = 0, 1$ and $n = 4, 5$ is shown in figures (2.2) and (2.3). The observed errors listed below indicate a linear rate of convergence.

n	0	1	2	3	4	5
E_n	6.7×10^{-3}	5.9×10^{-4}	1.6×10^{-4}	7.0×10^{-5}	1.6×10^{-5}	3.2×10^{-6}

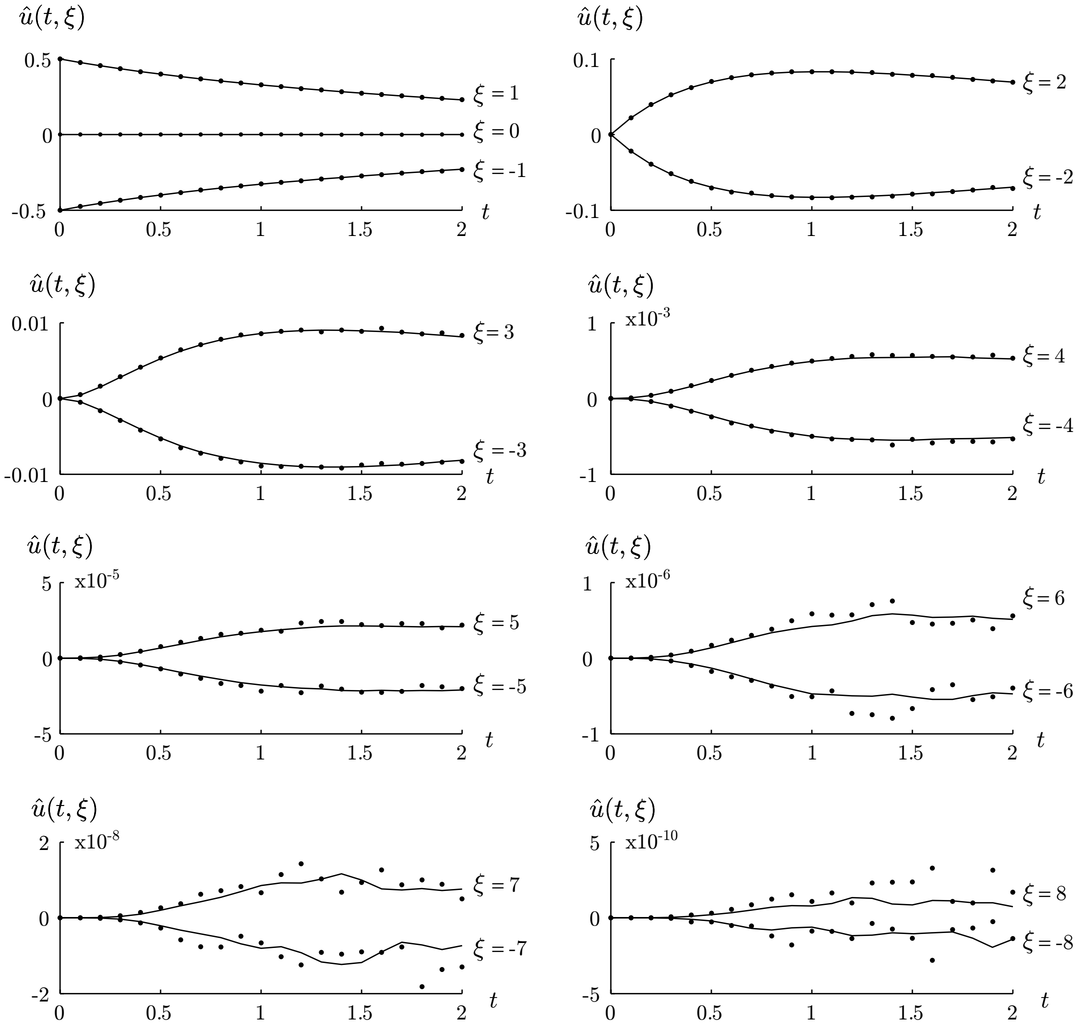

Figure 2.2: Comparison between $\hat{u}^{(0)} = \mathbb{E}_\xi \mathsf{X}$ (dots) and $\hat{u}^{(1)}$ (lines) for the diffusion equation with data given by (2.21).

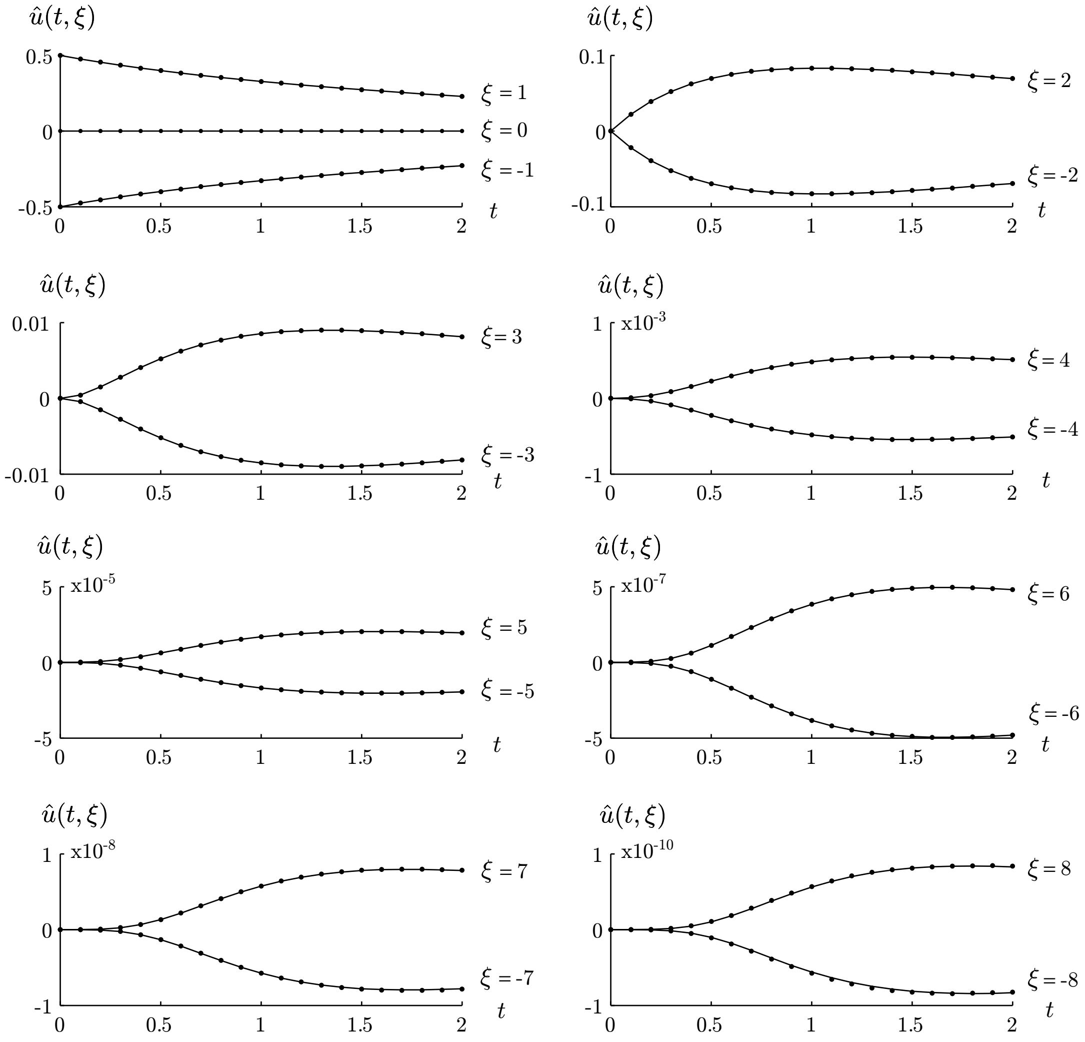

Figure 2.3: Comparison between $\hat{u}^{(4)}$ (dots) and $\hat{u}^{(5)}$ (lines) for the diffusion equation with data given by (2.21).

2.3 Viscous Burgers equation

Consider the viscous Burgers equation in $\mathbb{T} = [0,1)$ with periodic initial condition $u_0 = u_0(x)$, periodic forcing term $f = f(t,x)$, periodic boundary conditions, and viscosity $\nu > 0$,

$$\begin{aligned} &u_t(t) + \sqrt{2\pi}\, u(t)\, u_x(t) = \nu u_{xx}(t) + f,\ t > 0, \\ &u(0^+, x) = u_0(x), \quad u(t,0) = u(t,1). \end{aligned} \tag{2.22}$$

A solution to equation (2.22) will remain periodic for $t > 0$, and therefore one has Fourier series representations for u_0, f, and u, with coefficients $\hat{u}_0(k,t)$, $\hat{f}(k,t)$ and $\hat{u}(k,t)$ respectively, $k \in \mathbb{Z}$.

Write $uu_x = \frac{1}{2}(u^2)_x$ and take Fourier transform of both sides of (2.22). Use the integrator factor $e^{\nu k^2 s}$, and multiply and divide by νk^2 inside the resulting integral, then

$$\hat{u}(t,k) = \hat{u}_0(k)\, e^{-\nu k^2 t} + \int_0^t \nu k^2 e^{-\nu k^2 s} \left[\frac{1}{2}\frac{1}{i\nu}\, \frac{\hat{u} * \hat{u}(t-s,k)}{k} + \frac{1}{2}\frac{2\hat{f}(t-s,k)}{\nu k^2} \right] \mathrm{d}s. \tag{2.23}$$

Now, make the following change of variables

$$\hat{w}(t,k) = \frac{1}{i\nu}\, \hat{u}(t,k), \quad \hat{w}_0(k) = \hat{w}(0,k), \quad \hat{g}(t,k) = \frac{2\hat{f}(t,k)}{i\nu^2 k^2}. \tag{2.24}$$

Then $\hat{w}$ satisfies the following equation

$$\hat{w}(t,k) = \hat{w}_0(k)\, e^{-\nu k^2 t} + \int_0^t \nu k^2 e^{-\nu k^2 s} \left[\frac{1}{2}\frac{\hat{w} * \hat{w}(t-s,k)}{k} + \frac{1}{2}\, \hat{g}(t-s,k) \right] \mathrm{d}s, \tag{2.25}$$

where the convolution $\hat{w} * \hat{w}$ is to be understood over $\mathbb{Z}$ as

$$\hat{w} * \hat{w}(t-s,k) = \sum_{j \in \mathbb{Z}} \hat{w}(t-s,j)\, \hat{w}(t-s,k-j). \tag{2.26}$$

The form of (2.25) is similar to that of (2.12), and the initial structure of the appropriate stochastic process can be guessed. Let $S_{\langle 0 \rangle}$ be an exponentially distributed random variable of parameter νk^2, and let $c_{\langle 0\rangle}$ be a fair coin tossing with values in $\{0,1\}$. Equation (2.25) can be written as

$$\hat{w}(t,k) = \mathbb{E}\left\{\mathbb{1}_{S_{\langle 0\rangle}>t}\hat{w}_0(k) \;+\mathbb{1}_{S_{\langle 0\rangle}\leq t}\left[c_{\langle 0\rangle}\,\frac{\hat{w}*\hat{w}(t-S_{\langle 0\rangle},k)}{k} \;+\;(1-c_{\langle 0\rangle})\,\hat{g}(t-S_{\langle 0\rangle},k)\right]\right\}. \tag{2.27}$$

Note that if a discrete probability density function on $j\in\mathbb{Z}$ is introduced in the summation (2.26), the convolution could be interpreted (for each k) as an average of products of $\hat{w}$ evaluated at random frequencies. The problem of finding such a density appears whenever stochastic cascades are used to solve partial differential equations in Fourier space, and is linked to the more general problem of establishing existence and regularity of solutions. In the more general case of the Navier-Stokes equations, the characterization of admissible densities for the frequencies of offspring vertices was solved with the introduction of “majorizing kernels” in Bhattacharya et al. (2003), Chen et al. (2003) and Bhattacharya et al. (2004).

It follows from equation (2.26) that any function decreasing as $o(j^{-\frac{1}{2}})$ can be used to give a full probabilistic representation of (2.25). This will provide the existence of solutions without restrictions on the support of $\hat{u}_0$ and $\hat{f}$. Some attempts to numerically model this problem have been made by S. Dobson, E. Thomann, A. Chorin A. and P. Stinis (personal communications).

Here the simplest possible probabilistic representation of the convolution (2.26) is used through the following assumption:

$$\text{there exists } K>0 \text{ such that } \hat{f}(t,k)=\hat{u}_0(k)=0, \text{ for all } k<K. \tag{2.28}$$

It is due to a theorem of F. and M. Riesz (see Rudin (1973), p.335) that property (2.28) implies that f and u_0 belong to the Hardy space H^1, namely, the Banach space of functions with holomorphic extension to the unit disc with the norm

$$\|f\|_{H^p} = \lim_{r\to 1}\left\{\frac{1}{2\pi}\int_{-\pi}^{\pi}|f(r\,e^{i\theta})|\,\mathrm{d}\theta\right\}^{\frac{1}{p}}.$$

Assume (2.28) holds and let $J_{\langle 0\rangle}$ be a uniformly distributed random variable taking values in $\{K,\dots,k-K\}$, then

$$\hat{w}*\hat{w}(t,k)=\begin{cases}0, & K\leqslant k<2K,\\ (k-2K+1)\ \mathbb{E}\left\{\hat{w}(t,J_{\langle 0\rangle})\,\hat{w}(t,k-J_{\langle 0\rangle})\right\}, & k\geqslant 2K.\end{cases}$$

Denote $p_{\langle 0\rangle}=(k-2K+1)^{-1}$, and write equation (2.27) as

$$\begin{aligned}\hat{w}(t,k)=\mathbb{E}\Bigg\{&\mathbb{1}_{S_{\langle 0\rangle}>t}\hat{w}_0(k)\ +\mathbb{1}_{S_{\langle 0\rangle}\leq t}\left[c_{\langle 0\rangle}\,\frac{1}{p_{\langle 0\rangle}k}\,\hat{w}(t-S_{\langle 0\rangle},J_{\langle 0\rangle})\,\hat{w}(t-S_{\langle 0\rangle},k-J_{\langle 0\rangle})\right.\\ &\left.+\ (1-c_{\langle 0\rangle})\,\hat{g}(t-S_{\langle 0\rangle},k)\right]\Bigg\}\,\mathbb{1}_{k\geq 2K}\\ &+\mathbb{E}\left\{\mathbb{1}_{S_{\langle 0\rangle}>t}\hat{w}_0(k)\ +\mathbb{1}_{S_{\langle 0\rangle}\leq t}\left[\frac{1}{2p_{\langle 0\rangle}k}\hat{g}(t-S_{\langle 0\rangle},k)\right]\right\}\,\mathbb{1}_{k<2K}.\end{aligned}\tag{2.29}$$

From the construction of the appropriate stochastic process associated to (2.27), it will follow that $\hat{w}(t,k)$ satisfies (2.28) for all $t>0$.

For $k>0$ and $t>0$ consider a binary tree $\tau=\tau(t,k)$ with a particle of type k assigned to its root vertex $\langle 0\rangle$. Let $(\Omega,\mathcal{F},\mathbb{P}_k)$ be a probability space. Define a vertex-indexed stochastic process $\{k_{\langle v\rangle}\}_{\langle v\rangle\in\tau}$ with $k_{\langle 0\rangle}=k$, satisfying the conservation rule

$$k_{\langle v\rangle}=k_{\langle v1\rangle}+k_{\langle v2\rangle},\quad \langle v\rangle\in\tau,\tag{2.30}$$

and with increments $k_{\langle v1\rangle}-k_{\langle v\rangle}=J_{\langle v\rangle}$ conditionally distributed as,

$$\mathbb{P}_k(J_{\langle v\rangle}=j|k_{\langle v\rangle},c_{\langle v\rangle})=\frac{1}{k_{\langle v\rangle}-2K+1}\mathbb{1}_{k_{\langle v\rangle}\geqslant 2K}\mathbb{1}_{c_{\langle v\rangle}=1}:=p_{\langle v\rangle}.\tag{2.31}$$

Let $c_{\langle v\rangle}$ be fair coin tosses taking values on $\{0,1\}$. Introduce "waiting times" $S_{\langle v\rangle}$ with conditional exponential distributions given by

$$\mathbb{P}_k(S_{\langle v\rangle}>s\,|k_{\langle v\rangle})=e^{-\nu k^2_{\langle v\rangle}s},\quad s>0.$$

Finally, for $\langle v\rangle\in\tau$, define termination times as

$$T_{\langle v\rangle}=t-\sum_{j=0}^{|\langle v\rangle|-1}S_{\langle v\rangle|j},\quad T_{\langle 0\rangle}=t,\tag{2.32}$$

where $|\langle v\rangle|$ and $\langle v\rangle|j$ are defined in Section (2.1).

A multiplicative functional of $\{k_{\langle v\rangle}, S_{\langle v\rangle}, c_{\langle v\rangle}\}_{\langle v\rangle\in\tau}$ related to $\hat{w}$ can now be constructed in a similar way as in Section (2.2). Consider

$$\mathsf{X}(\tau(t,k)) = \mathsf{X}(t,k) = \prod_{\langle v\rangle\in\tau} M_{\langle v\rangle} \tag{2.33}$$

with multipliers given by

$$M_{\langle v\rangle} = \begin{cases} \hat{w}_0(k_{\langle v\rangle}) & \text{if } S_{\langle v\rangle} > T_{\langle v\rangle}, \\ \frac{1}{2}\,\hat{g}(T_{\langle v\rangle}, k_{\langle v\rangle}) & \text{if } k_{\langle v\rangle} < 2K, S_{\langle v\rangle} \leq T_{\langle v\rangle}, \\ \hat{g}(T_{\langle v\rangle}, k_{\langle v\rangle}) & \text{if } k_{\langle v\rangle} \geq 2K, S_{\langle v\rangle} \leq T_{\langle v\rangle}, c_{\langle v\rangle} = 0, \\ \frac{1}{k_{\langle v\rangle} p_{\langle v\rangle}} & \text{if } k_{\langle v\rangle} \geq 2K, S_{\langle v\rangle} \leq T_{\langle v\rangle}, c_{\langle v\rangle} = 1. \end{cases} \tag{2.34}$$

Then the following holds,

Theorem 2.3.1. *Assume* $\hat{f}(t,k) = \hat{u}_0(k) = 0$ *for all* $k < K$*, and that there is* $\alpha \geqslant 0$ *such that* $|\hat{u}_0(k)| \leqslant \nu e^{-\alpha k}$, $\left|\hat{f}(t,k)\right| \leqslant \frac{\nu^2 k^2}{2} e^{-\alpha k}$, *for* $k \geqslant K, t > 0$*. Then Burgers equation (2.22) has a unique solution* $\hat{u}$*. Moreover,*

$$\hat{u}(t,k) = 0,\ k < K, \quad \textit{and} \quad |\hat{u}(t,k)| \leqslant \nu e^{-\alpha k},\ k \geqslant K,\ t > 0,$$

and $\hat{u}(t,k)$ *is explicitly given by*

$$\hat{u}(t,k) = i\nu\, \mathbb{E}_k\, \mathsf{X}(\tau(t,k)).$$

Proof. The bounds on $\hat{u}$ and $\hat{f}$ combined with (2.24), and the definition of $p_{\langle v\rangle}$ give the following bound for the random product in (2.34),

$$\mathsf{X}(t,k) \leqslant \exp\Big\{ -\alpha \sum_{\langle v\rangle\in\tau\setminus\tau_B} k_{\langle v\rangle}\Big\} \prod_{\langle v\rangle\in\tau_B} \frac{k_{\langle v\rangle} - 2K + 1}{k_{\langle v\rangle}}$$

where τ_B is the set of vertices where branching occurs, namely,

$$\tau_B = \{\langle v\rangle \in \tau : k_{\langle v\rangle} \geq 2K \text{ or } S_{\langle v\rangle} \leq T_{\langle v\rangle} \text{ or } c_{\langle v\rangle} = 1\}.$$

Since $\alpha \geqslant 0$ and $0 < K \leqslant k_{\langle v\rangle}$, then $|\mathbb{E}_k \mathsf{X}(\tau(t,k))| < \infty$. Moreover, the conservation rule (2.30) gives $\sum_{\langle v\rangle \in L} k_{\langle v\rangle} = k$, so the estimate for $|\hat{u}(t,k)|$ holds and $\hat{u}(t,k) = 0$ for $k < K$. Due to the Markovian character of the waiting times $S_{\langle v\rangle}$, and the mutual independence between $c_{\langle v\rangle}$ and $J_{\langle v\rangle}$, the following recursive representation of X is available,

$$\mathsf{X}(\tau(t,k_{\langle 0\rangle})) = \begin{cases} \hat{w}_0(k_{\langle 0\rangle}) & \text{if } S_{\langle 0\rangle} > T_{\langle 0\rangle}, \\ \frac{1}{2}\,\hat{g}(T_{\langle 0\rangle}, k_{\langle 0\rangle}) & \text{if } k_{\langle 0\rangle} < 2K, S_{\langle 0\rangle} \leq T_{\langle 0\rangle} \\ \hat{g}(T_{\langle 0\rangle}, k_{\langle 0\rangle}) & \text{if } k_{\langle 0\rangle} \geq 2K, S_{\langle 0\rangle} \leq T_{\langle 0\rangle}, c_{\langle 0\rangle} = 0, \\ \frac{1}{k_{\langle 0\rangle} p_{\langle 0\rangle}}\,\mathsf{X}(\tau(T_{\langle 0\rangle}, k_{\langle 1\rangle}))\,\mathsf{X}(\tau(T_{\langle 0\rangle}, k_{\langle 2\rangle})) & \text{if } k_{\langle 0\rangle} \geq 2K, S_{\langle 0\rangle} \leq T_{\langle 0\rangle}, c_{\langle 0\rangle} = 1, \end{cases} \tag{2.35}$$

Conditioning on the cases of (2.35) gives that $\mathbb{E}_k \mathsf{X}(\tau(t,k))$ satisfies equation (2.23). □

2.3.1 Modeling

Because of the binary tree structure of τ, conditioning on the frequencies at the terminating vertices does not simplify the computation of $\mathsf{X}(\tau)$ as it did for the example in Section (2.2). Here, the realizations of the multiplicative functional can be done constructing trees from the root vertex following equation (2.35) (see figure 2.4). The root particle of type $k_{\langle 0\rangle} = k$ holds for the exponential time $S_{\langle 0\rangle}$ which is compared to $T_{\langle 0\rangle} = t$. If $[S_{\langle 0\rangle} > t]$, then no further vertices are used. If $[S_{\langle 0\rangle} < t]$ occurs, a coin $c_{\langle 0\rangle}$ is tossed. In the event $c_{\langle 0\rangle} = 0$, again the construction stops. If $c_{\langle 0\rangle} = 1$, branching occurs, and the new vertices $\langle 1\rangle$ and $\langle 2\rangle$ are created with random types $k_{\langle 1\rangle} = J_{\langle 0\rangle}$ and $k_{\langle 2\rangle} = k_{\langle 0\rangle} - J_{\langle 0\rangle}$ respectively. The same process is followed independently with trees rooted in $\langle 1\rangle$ and $\langle 2\rangle$. Whenever a vertex $\langle v\rangle$ has type $k_{\langle v\rangle} < 2K$, then $S_{\langle v\rangle}$ is compared to the respective termination time but no coin is tossed, and no branching occurs. The multipliers are then assigned to the vertices according to (2.34).

The integral equation (2.23) can be used to test the error in any numerical estimation of the expected value in Theorem (2.3.1). Define $\hat{u}^{(0)}$ to be the approximation provided by Monte Carlo algorithm, and define the following iterates,

$$\hat{u}^{(n+1)}(t,k) = \hat{u}_0(k)\, e^{-\nu k^2 t} + \int_0^t \nu k^2 e^{-\nu k^2 s} \left[\frac{\hat{u}^{(n)} * \hat{u}^{(n)}(t-s,k)}{2i\nu k} + \frac{\hat{f}(t-s,k)}{\nu k^2} \right] \mathrm{d}s. \quad (2.36)$$

The sequence $\{\hat{u}_{(n)}\}_{n\geqslant 0}$ forms a Picard iteration of which the solution $\hat{u}$ is a fixed point. The error at each term can be measured with

$$E_n = \frac{\|\hat{u}^{(n+1)} - \hat{u}^{(n)}\|_\infty}{\|\hat{u}^{(n)}\|_\infty}.$$

2.3.2 Example

Consider the Fourier transformed Burgers equation with data given by

$$\hat{u}_0(k) = i\nu, \quad \hat{f}(t,k) = \frac{i\nu^2 k^2}{2}(1-t)^2, \quad t \in (0,1),\, k \geqslant 1. \qquad (2.37)$$

By Theorem 2.3.1, $\hat{u}(t,k) = i\nu\, \mathbb{E}_k\, \mathsf{X}(\tau(t,k))$ is the unique solution to this equation. A numerical approximation to $\hat{u}$ was calculated for $k = 1, \dots 8$ and ten discrete time points in $[0,1]$. The number of computed realizations of $\mathsf{X}(\tau)$ was proportional to t for frequencies $k_{\langle 0\rangle} < 2K$, and proportional to $(t+k-2K)$ for frequencies $k_{\langle 0\rangle} \geq 2K$. The proportionality constant used was 3000. Some terms of the sequence $\{\hat{u}^{(n)}\}$ defined by (2.36) were calculated using a simple trapezoidal rule for the integration in time. A comparison between the complex norm of the consecutive iterates for $n = 0, 1$ and $n = 4, 5$ is shown in figures (2.5) and (2.6). The observed errors, as defined by (2.3.1), are listed below.

n	0	1	2	3	4	5
E_n	1.8×10^{-2}	2.1×10^{-3}	4.0×10^{-4}	1.0×10^{-4}	2.1×10^{-5}	2.2×10^{-6}

2.4 Concluding remarks

Monte Carlo techniques are developed to model the random multiplicative cascades associated with two partial differential equations: linear diffusion and viscous Burgers

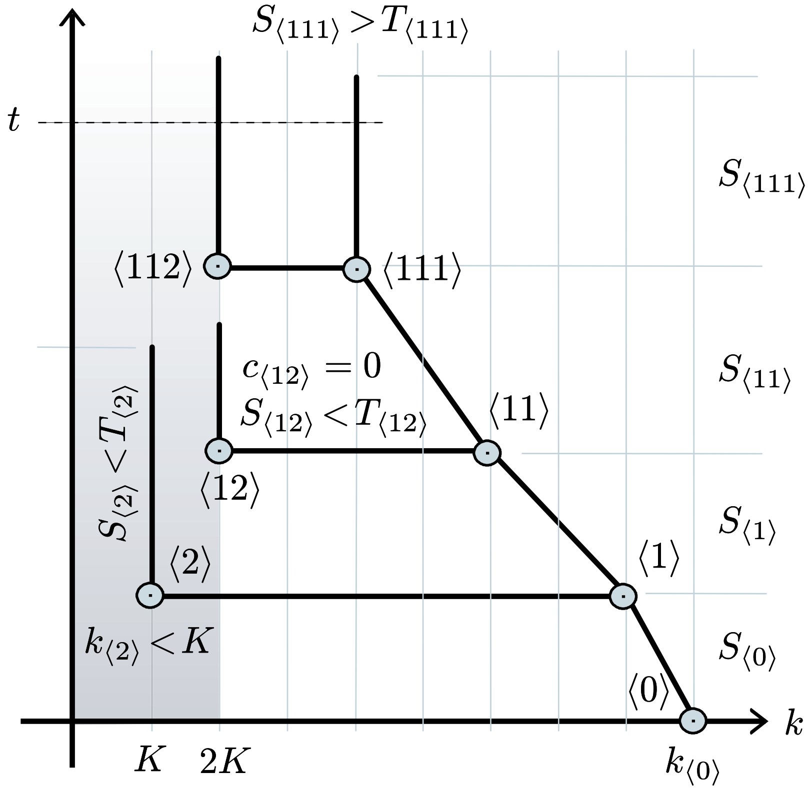

Figure 2.4: Diagram of a realization of a tree τ for Burgers equation with $N = 3$. The value of the multiplicative functional is $\mathsf{X}(t,k) = \frac{1}{k_{\langle 0\rangle}p_{\langle 0\rangle}}\frac{1}{k_{\langle 1\rangle}p_{\langle 1\rangle}}\frac{\hat{g}(T_{\langle 2\rangle},k_{\langle 2\rangle})}{2}\frac{1}{k_{\langle 11\rangle}p_{\langle 11\rangle}}\hat{g}(T_{\langle 12\rangle},k_{\langle 12\rangle})\frac{1}{k_{\langle 111\rangle}p_{\langle 111\rangle}}\hat{w}_0(k_{\langle 112\rangle})\hat{w}_0(k_{\langle 111\rangle})$.

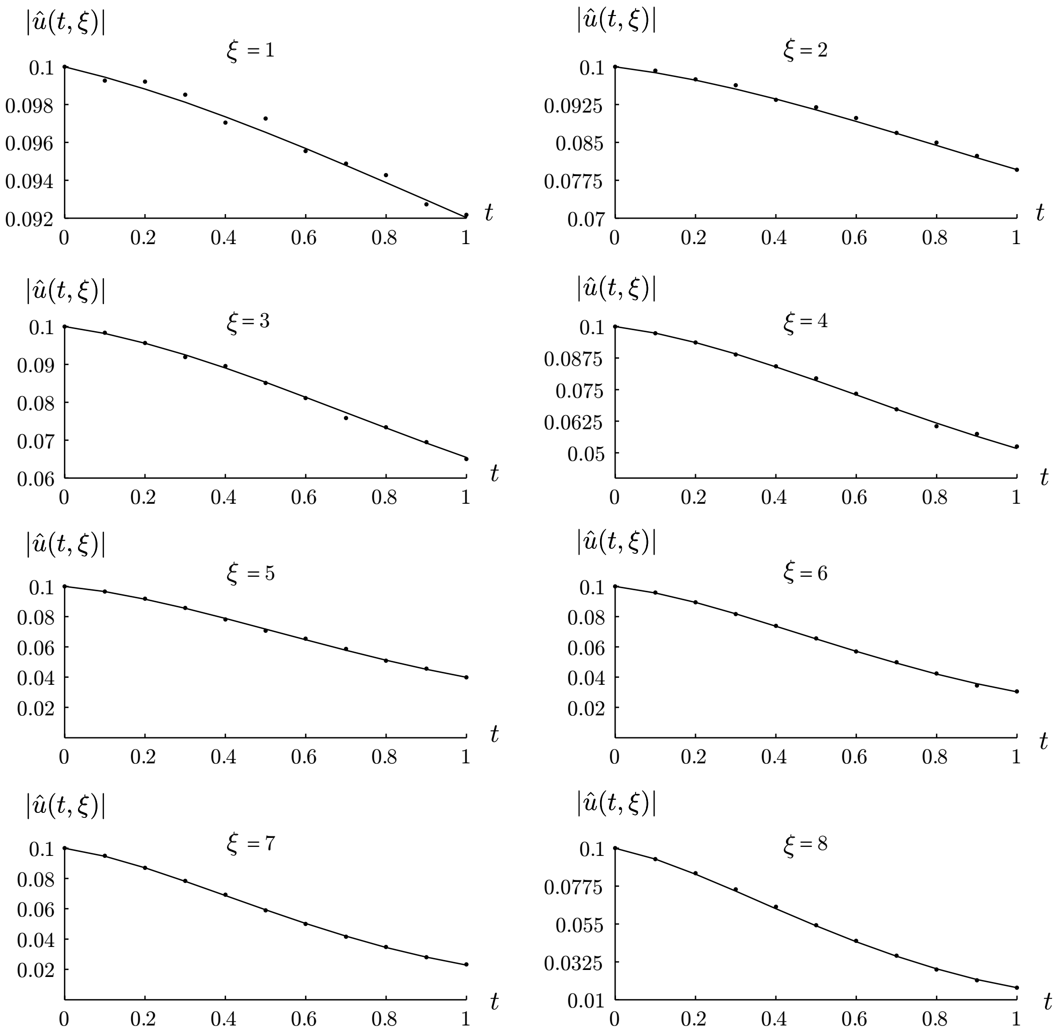

Figure 2.5: Comparison between $\hat{u}^{(0)} = \mathbb{E}_\xi \mathsf{X}$ (dots) and $\hat{u}^{(1)}$ (lines) for Burgers equation with data given by (2.37).

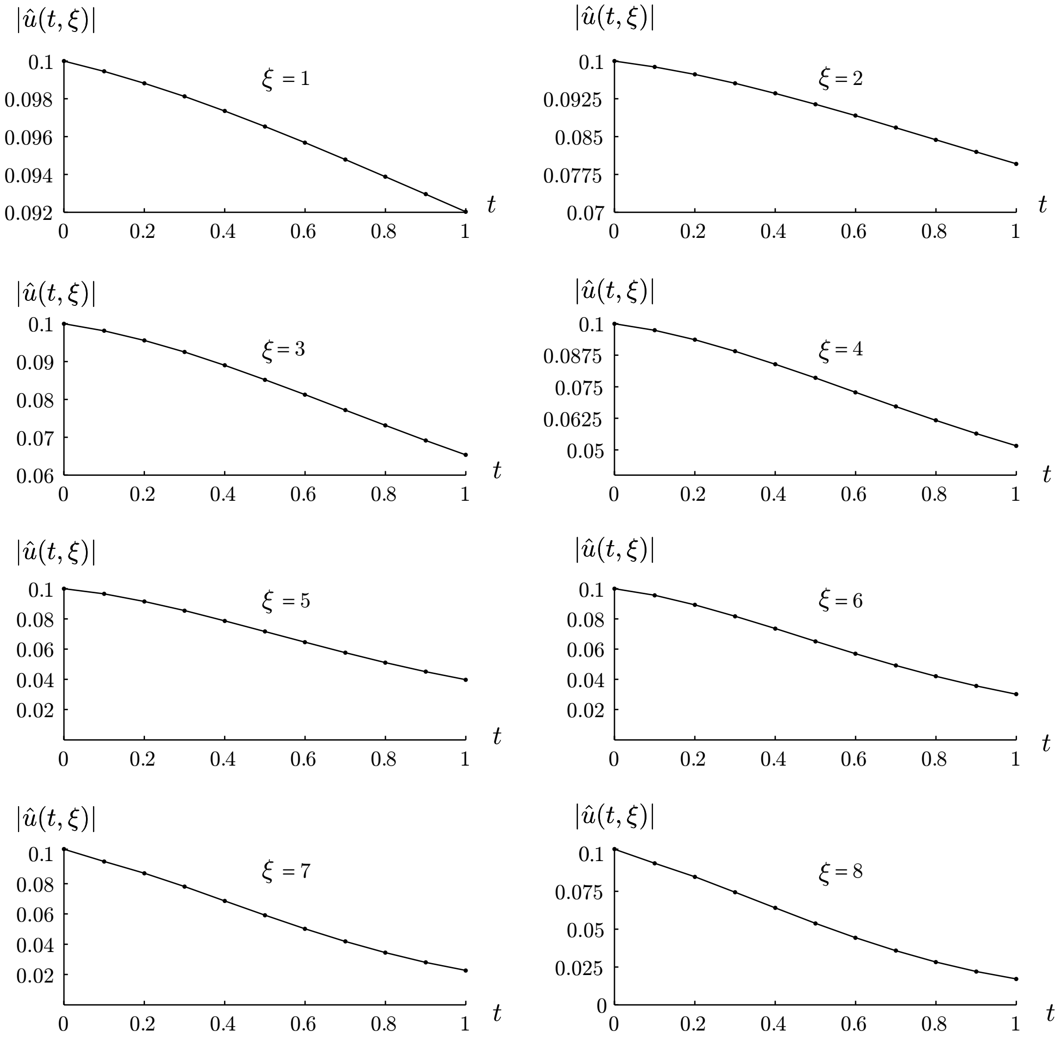

Figure 2.6: Comparison between $\hat{u}^{(4)}$ (dots) and $\hat{u}^{(5)}$ (lines) for Burgers equation with data given by (2.37).

equation. The Fourier transformed solution of the PDE is written as the expected value of a random aggregate of its main components, i.e. initial condition, nonlinear terms and forcing terms. These aggregates are evaluated at random frequencies $\xi_{\langle v\rangle}$ (or $k_{\langle v\rangle}$), and random times $S_{\langle v\rangle}$, indexed by $\langle v\rangle \in \tau$, where τ has a tree structure. The choice on the distributions of $\xi_{\langle v\rangle}$ and $S_{\langle v\rangle}$ determine the limitations and scope of the multiplicative cascade representation.

Exponential waiting times $S_{\langle v\rangle}$ with parameter dependent on $k_{\langle v\rangle}$, arose naturally in both examples presented here (see equations (2.12) and (2.23)). Computational stability considerations led to the removal of this dependence for the case of the diffusion equation. The exponential distribution has the advantage of giving Markov structure to the resulting stochastic process, (see proof of Theorem 2.2.1), and it also simplifies the numerical modeling. Multiplicative cascade representations using distributions for the waiting times different than exponential are considered in Bhattacharya et al. (2004).

In the examples presented here, the transition distributions for the frequency process $\{\xi_{\langle v\rangle}\}_{\langle v\rangle\in\tau}$ are chosen so both the analytical and the modeling problem are considerably simplified. This selection imposes restrictions on the PDE's data for which a multiplicative cascade representation gives a solution. There is however, no "physical" reason behind the choices made here. The identification of processes $\{\xi_{\langle v\rangle}\}_{\langle v\rangle\in\tau}$ that correspond with the physical situations the partial differential equations arise from, is still unexplored. Simulations such as those presented here, can be used to study the relationship between this processes in frequency space, and known qualitative features of the solutions.

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3 A GENERALIZED TAYLOR-ARIS FORMULA AND SKEW DIFFUSION.

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3.1 Introduction

The seminal paper by Taylor (1953) together with the refinements by Aris (1956) describe the dispersion of a solute concentration immersed in Poiseuille flow directed along the horizontal axis of a cylindrical tube in terms of the *tube radius* R, *molecular diffusion coefficient* D, and the *maximum flow* U (or *cross-sectional average* $U/4$) of the parabolic flow profile. In the case $U = 0$ the dispersion coincides with molecular diffusion, and when $D = 0$ the dispersion of solute is aligned with the parabolic profile of the flow. The relative contributions of these combined effects $(D > 0, U > 0)$ are captured in Taylor's remarkable insights leading to the formula

$$\bar{D} = 2D + \frac{R^2U^2}{96D}. \tag{3.1}$$

Motivated by considerations of the stability of a viscous liquid to two-dimensional disturbances in a porous-medium, Wooding (1960) adapted their analysis to obtain the corresponding formula for dispersion of a solute in a unidirectional parabolic flow between two parallel planes separated by a distance R. Accordingly, in this setting

$$\bar{D} = 2D + \frac{8R^2U^2}{945D}. \tag{3.2}$$

In either case, the significance of such dispersion rates for the spread of solute concentration was demonstrated by the derivation of the time-asymptotic (homogenized) equation for the solute concentration averaged over the cross section.

In subsequent mathematical work, Fife and Nicholes (1975) used perturbation methods for this derivation, while later Bhattacharya and Gupta (1984) obtained these results using central limit theory techniques from probability. While their approach can be applied to quite more general diffusion (or dispersion) and velocity coefficients than originally formulated by Taylor (1953) and Aris (1956), they restrict to the case of smoother coefficients than those considered here. Specifically we consider highly heterogeneous media allowing for characteristically *sharp interfaces,* and analyze these effects on effective dispersion rates in the case of longitudinal flow in a cylindrical region. Moreover, we will see that new physical insights into the role of heterogeneities in dispersion emerge from these results, which should be useful in analyzing more complex heterogeneous flow problems. In addition to interest among geophysicists for solute transport in highly heterogeneous porous media (e.g. see Berentsen et al. (2005)), examples occur in micro-reactor engineering and liquid-liquid extraction (see Ueno et al. (2002)), as well as in biological processes at cellular levels, see Saxton and Jacobsen (1997).

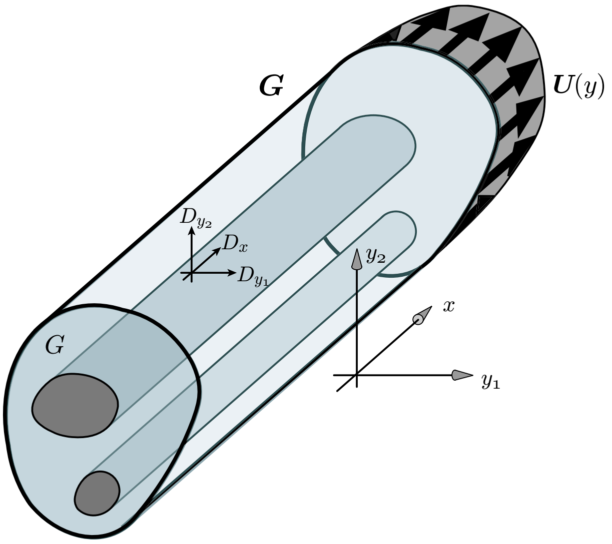

Figure 3.1: Three dimensional advection dispersion in a cylinder $\boldsymbol{G} = G \times \mathbb{R}$ with heterogenous diffusion coefficient. Coordinates are given by $\boldsymbol{x} = (x, y) = (x, y_1, y_2)$

Our focus is two-fold: (i) Calculation of the longitudinal effective dispersion coefficient, and (ii) determination of the probability laws governing the (stochastic) motion of the underlying solute particles. The model we consider has the following structure. Consider diffusion of a dilute solute on the region $\boldsymbol{G} = \{\boldsymbol{x} = (x, y) \in \mathbb{R}^d : x \in \mathbb{R},\ y \in G\}$, where the constant cross section G is a connected compact subset of $\mathbb{R}^{d-1}$ with smooth boundary and d is equal to either 2 or 3 (see Figure 3.1). The velocity profile is a bounded measurable vector function of the form $\boldsymbol{U}(\boldsymbol{x}) = (U(y), \boldsymbol{0})$, and the diffusion coefficient is uniformly bounded and elliptic tensor $\boldsymbol{D}(\boldsymbol{x}) = \boldsymbol{D}(y)$ in diagonal form with entries $D_x(y)$

and $D_y(y)$. According to Fick's law, the concentration $c(\boldsymbol{x}, t)$ at location $\boldsymbol{x} = (x, y)$ at time $t > 0$ satisfies

$$\begin{cases} \partial_t c = \nabla\cdot(\boldsymbol{D}\,\nabla c) - \nabla\cdot(c\,\boldsymbol{U}), \quad \text{in}\,\boldsymbol{G}, \\ (\boldsymbol{D}\nabla c)\big|_{\partial\boldsymbol{G}}\cdot\boldsymbol{n} = 0, \quad c\big|_{t=0} = c_0, \end{cases} \tag{3.3}$$

An effective diffusion coefficient is derived through a general homogenization result for this problem.

Homogenization problems continue to provide an active area of research in applied mathematics and probability. The general theory involves a form of averaging that typically depends on some assumptions of repeatability throughout the domain of the model parameters, e.g. periodicity, almost periodicity, or stationary ergodic coefficients. The literature for such theory and its applications is quite extensive, e.g. see Bensoussan et al. (1978), Majda and Kramer (1999), Winter et al. (1984). The main focus of the problems of the type considered here are on the time asymptotics of transversely averaged cross sections of concentration in the longitudinal direction under both convection and dispersion. Neither periodicity nor smoothness conditions are available for the parameters in the present applications.

As a very interesting special case of the formulation, we consider longitudinal flow between parallel plates through a layered medium. Namely, the diffusion coefficient $\boldsymbol{D}$ is assumed to be a piecewise constant function of the transverse spatial variable. The presence of sharp interfaces between regions of different diffusivity, creates interesting effects on the motion of the solute particles that can be studied through the structure of the associated diffusion process governing the motion of individual solute particles. For this case, the effective diffusion coefficient is found to be a weighted average of the diagonal values of $\boldsymbol{D}$ and its inverses.

Although our approach follows closely the probabilistic techniques developed by Bhattacharya (1982), the mild conditions allowed for $\boldsymbol{U}$ and $\boldsymbol{D}$ lead to new mathematically interesting technical considerations in the identification of the underlying diffusion process associated with the solution to (3.3). This is further resolved through a combination of the theory of Dirichlet forms, partial differential equations, and the Sroock-Varadahn martingale problem and Itô-Tanaka stochastic calculus. The organization of the paper is as follows. In the next section the problem is re-cast in terms of stochastic processes associated with L^2-semigroups defined from the Dirichlet form corresponding to the operator $\nabla\cdot(\boldsymbol{D}\,\nabla c) - \nabla\cdot(c\boldsymbol{U}), \quad \nabla c\big|_{\partial\boldsymbol{G}}\cdot\boldsymbol{n} = 0$. We then apply the central limit theorem and asymptotic variance formula of Bhattacharya (1982) to obtain the generalized Taylor-Aris formula for dispersion. We include the special case of layered media with sharp interfaces as a corollary. The last section of the paper is devoted to a more detailed description of the stochastic motion (i.e. physical process) of the underlying solute particles in the presence of sharp interfaces.

3.2 Heterogenous dispersion in longitudinal flow

3.2.1 The model.

Let $G \subset \mathbb{R}^{d-1}$, $(d = 2, 3)$ be a compact domain with smooth boundary in the sense of Davies (1989), pp. 46-47. Consider the cylinder $\boldsymbol{G} = \{\boldsymbol{x} = (x, y) \in \mathbb{R}^d :, x \in \mathbb{R}, y \in G\}$. In the case $d = 3$, y denotes the planar vector $y = (y_1, y_2)$. For time $t > 0$, let $c(\boldsymbol{x}, t)$ be the concentration of a solute at $\boldsymbol{x} \in \boldsymbol{G}$ which is diffusing in a fluid with velocity $\boldsymbol{U}(\boldsymbol{x})$ and through a medium with diffusion tensor $\boldsymbol{D}(\boldsymbol{x})$. We make the following assumptions on $\boldsymbol{U}$ and $\boldsymbol{D}$:

- the velocity in the cylinder is parallel to the x coordinate, and

$$\boldsymbol{U}(\boldsymbol{x}) = (U(y), \boldsymbol{0}), \tag{3.4}$$

  is bounded and measurable;

- $\boldsymbol{D}(\boldsymbol{x})$ is bounded and uniformly positive definite on $\boldsymbol{G}$, and has the form

$$\boldsymbol{D}(\boldsymbol{x}) = \begin{bmatrix} D_x(y) & 0 \\ 0 & D_y(y) \end{bmatrix}, \tag{3.5}$$

  where in the case $d = 3$, $D_y(y)$ denotes the diagonal matrix with entries $D_{y_1}(y_1, y_2)$ and $D_{y_2}(y_1, y_2)$.

These assumptions cover the especially interesting case of diffusion in a medium with sharp interfaces as defined by a piecewise constant cross-sectional diffusion coefficient. Note also that the form (3.4) makes the velocity $\boldsymbol{U}$ *incompressible.* This property is essential to many of the computations, though we do not always make special note when it occurs. Notice for example that one may write $\nabla\cdot(v\,\boldsymbol{U}) \equiv \boldsymbol{U}\cdot\nabla v$.

Modeling the flux of the concentration c by Fick's law leads to the conservation equation

$$\begin{cases} \partial_t c = \nabla\cdot(\boldsymbol{D}\,\nabla c) - \nabla\cdot(c\,\boldsymbol{U}), \quad \text{in } \boldsymbol{G}, \\ (\boldsymbol{D}\nabla c)\big|_{\partial\boldsymbol{G}}\cdot\boldsymbol{n} = 0, \quad c\big|_{t=0} = c_0, \end{cases} \tag{3.6}$$

where spatial derivatives are to be understood in the weak sense. Specifically, we look for $c(\boldsymbol{x}, t) \in \mathcal{C}^0([0,\infty), H^1(\boldsymbol{G})) \cap \mathcal{C}^1([0,\infty), L^2(\boldsymbol{G}))$ such that $c(\boldsymbol{x}, 0) = c_0(\boldsymbol{x})$ and for $t \geqslant 0$,

$$\partial_t(u, c(t,\cdot))_{L^2(\boldsymbol{G})} = -\boldsymbol{\mathcal{E}}(u, c(t,\cdot)) \tag{3.7}$$

where $\boldsymbol{\mathcal{E}}$ is the bilinear form naturally associated with the differential equation (3.6),

$$\boldsymbol{\mathcal{E}}(u, v) = \int_{\boldsymbol{G}} \boldsymbol{D}\nabla u\cdot\nabla v - (\boldsymbol{U}\cdot\nabla u)v\,\mathrm{d}\boldsymbol{x}, \tag{3.8}$$

and $(u, v)_{L^2(\boldsymbol{G})}$ denotes the usual inner product in $L^2(\boldsymbol{G})$.

3.2.2 Generalized Taylor-Aris problem

Let $c(\boldsymbol{x}, t)$ be a solution to problem (3.6), and consider the cross-sectional total,

$$C(x, t) = \int_G c(x, y, t)\,\mathrm{d}y. \tag{3.9}$$

We seek large scale parameters $\bar{U}, \bar{D}$ such that on space-time scales λx, $\lambda^2 t$, the weak limit

$$\widetilde{C}(\tilde{x}, \tilde{t})\,\mathrm{d}\tilde{x} = \lim_{\lambda\to\infty} C(\lambda\tilde{x} + \bar{U}\lambda^2\tilde{t}, \lambda^2\tilde{t})\lambda\,\mathrm{d}\tilde{x}$$

provides a solution

$$\bar{C}(x,t) = \widetilde{C}(x - \bar{U}t, t)$$

to the homogenized partial differential equation,

$$\partial_t\bar{C} = \bar{D}\,\partial_x^2\bar{C} - \bar{U}\,\partial_x\bar{C}. \tag{3.10}$$

Thus the goal is to prove the following theorem.

Theorem 3.2.1. *(Generalized Taylor-Aris Formula) Let* $\pi(\,\mathrm{d}y)$ *be the uniform probability measure on* G*, and let* h *be a solution in* $L^2(G,\pi)$ *to the boundary value problem*

$$\begin{cases} \nabla_y\cdot(D_y\,\nabla_y h) = U(y) - \bar{U}, & \text{in}\,G, \\ (D_y\nabla_y h)\cdot\boldsymbol{n}_y = 0 & \text{in } \partial G. \end{cases} \tag{3.11}$$

Then, for any $t > 0$*,* $x \in \mathbb{R}$*, and Borel measurable* $A \subseteq \mathbb{R}$ *with boundary* ∂A *such that* $\pi(\partial A) = 0$*,*

$$\lim_{\lambda\to\infty}\int_A C(\lambda x + \bar{U}\lambda^2 t, \lambda^2 t)\lambda\,\mathrm{d}x = \int_A \bar{C}(x + \bar{U}t, t)\,\mathrm{d}x \tag{3.12}$$

with homogenized parameters

$$\bar{U} = \int_G U(y)\,\pi(\,\mathrm{d}y), \quad \bar{D} = \int_G \{D_x(y) + (D_y\nabla_y h)\cdot\nabla_y h(y)\}\;\pi(\,\mathrm{d}y). \tag{3.13}$$

In the case $d = 2$ and D_y is piecewise constant, we get (see Figure 3.2)

Corollary 3.2.2. *(Diffusion in a layered medium) Assume* $d = 2$*,* $G = [a, b]$ *and* $\boldsymbol{D}$ *has the form*

$$\boldsymbol{D}(\boldsymbol{x}) = \boldsymbol{D}(y) = \sum_{k=-m}^{M} \mathsf{D}^{(k)}\,\mathbb{1}_{[l_k, l_{k+1})}(y), \quad \mathsf{D}^{(k)} = \begin{bmatrix} D_x^{(k)} & 0 \\ 0 & D_y^{(k)} \end{bmatrix}$$

where $a = l_{-m} < l_{-m+1} < \cdots < l_M < l_{M+1} = b$ *is a collection of interfaces partitioning* $[a, b]$. *If* $D_x^{(k)} > 0$ *and* $D_y^{(k)} > 0$ *for all* k*, then the limit (3.12) of Theorem (3.2.1) holds with homogenized diffusion coefficient*

$$\bar{D} = \sum_{k=-m}^{M} \left\{ D_x^{(k)} \frac{l_{k+1} - l_k}{b - a} + \frac{1}{D_y^{(k)}} \int_{l_k}^{l_{k+1}} g(y)^2 \, \pi(\,\mathrm{d}y) \right\} \tag{3.14}$$

where g *is given by*

$$g(y) = \int_a^y \left(U(z) - \bar{U} \right) \pi(\,\mathrm{d}z). \tag{3.15}$$

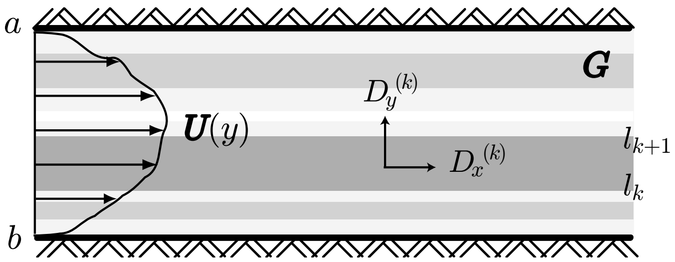

Figure 3.2: Two dimensional advection-diffusion in a layered medium.

3.2.3 Probabilistic reformulation

The physical justification for probabilistic reformulations traces back to Einstein's conception of molecular diffusion, and its general extension relating linear parabolic PDEs of the form (3.6) and Brownian motion via stochastic differential equations and central limit theory. In particular, for smooth coefficients one may exploit continuity of particle paths and coefficients to view the displacement of a suspended particle $X(t + dt) - X(t)$ locally in time as that of (approximately) a Brownian motion with drift $U(X(t))dt$ and variance $2D(X(t))dt$. This reasoning clearly fails in the presence of discontinuities. Thus, from a physical perspective, we are left to determine the appropriate stochastic particle motions in the presence of sharp interfaces. Once the appropriate stochastic process is established, the formulation in terms of central limit theory can be obtained.

The following lemma provides the technical basis for the construction of the stochastic process associated with the Dirichlet form (3.8). Let $D[0,\infty)$ be the space of right-continuous functions on $[0,\infty)$ with left-hand limits.

Lemma 3.2.3. *For each path $y \in D[0,\infty)$, define a process $X^{(y)} \equiv \{X_t^{(y)} : t \geqslant 0\}$ by*

$$X_t^{(y)} = x_0 + \int_0^t \mu(y(s))\,\mathrm{d}s + \int_0^t \sigma(y(s))\,\mathrm{d}B_s,$$

where μ and σ are bounded measurable functions with $\sigma(z) \geqslant \delta > 0$ for all $z \in \mathbb{R}$. Let $Y = \{Y_t : t \geqslant 0\}$ be a Markov process with sample paths in $D[0,\infty)$ having stationary transition probabilities with infinitesimal generator $(A, \mathscr{D}_A)$. Also assume Y is independent of $\{B_t : t \geqslant 0\}$. Define $\boldsymbol{X}_t = (X_t^{(Y)}, Y_t)$, $t \geqslant 0$. Then $\{\boldsymbol{X}_t : t \geqslant 0\}$, is a Markov process with stationary transition probabilities whose generator $\boldsymbol{A}$ acts on a core of functions of the form $f(x_1,x_2) = g(x_1)h(x_2)$, where g is twice continuously differentiable, $h \in \mathscr{D}_A$, by

$$\boldsymbol{A}f(x_1,x_2) = g(x_1)\,Ah(x_2) + h(x_2)\left\{\mu(x_2)\,g'(x_1) + \tfrac{1}{2}\sigma^2(x_2)\,g''(x_1)\right\}$$

Proof. The Markov property follows immediately from the decomposition for $0 \leqslant t' < t$

$$X_t^{(Y)} = X_{t'}^{(Y)} + \int_{t'}^t \mu(Y_s)\,\mathrm{d}s + \int_{t'}^t \sigma(Y_s)\,\mathrm{d}B_s,$$

the independence of Y, B, and the Markov property for Y. Consider the following σ-fields,

$$\mathcal{G}_t := \sigma(B_s, Y_s, s \leqslant t), \quad \bar{\mathcal{G}}_t := \sigma(Y, X_s^{(Y)}, s \leqslant t), \quad \mathcal{H}_t := \sigma(Y_s, s \leqslant t).$$

By an application of Itô's lemma one may first write

$$\begin{aligned} g(X_t^{(Y)}) &= g(x_1) + \int_0^t \left\{\mu(Y_s)\,g'(X_s^{(Y)}) + \tfrac{1}{2}\sigma^2(Y_s)\,g''(X_s^{(Y)})\right\}\mathrm{d}s \\ &\quad + \int_0^t \sigma(Y_s)\,g'(X_s^{(Y)})\,\mathrm{d}B_s. \end{aligned}$$

In particular,

$$G_t := g(X_t^{(Y)}) - \int_0^t \{\mu(Y_s)\,g'(X_s^{(Y)}) + \tfrac{1}{2}\sigma^2(Y_s)\,g''(X_s^{(Y)})\}\,\mathrm{d}s$$

is the martingale $\int_0^t \sigma(Y_s)g'(X_s^{(Y)})\,\mathrm{d}B_s$, $t \geqslant 0$, with respect to $\bar{\mathcal{G}}_t$. Similarly,

$$H_t := h(Y_t) - \int_0^t Ah(Y_s)\,\mathrm{d}s, \quad t \geqslant 0,$$

is a martingale with respect to $\mathcal{H}_t$. Combining this martingale structure with projective properties of conditional expectations based on $\mathcal{H}_t \subseteq \mathcal{G}_t \subseteq \bar{\mathcal{G}}_t$, one may check that

$$\begin{aligned} M_t \quad := \quad & g(X_t^{(Y)})\,h(Y_t) - \int_0^t h(Y_s)\left\{\mu(Y_s)\,g'(X_s^{(Y)}) + \tfrac{1}{2}\sigma^2(Y_s)\,h''(X_s^{(Y)})\right\}\,\mathrm{d}s \\ & - \int_0^t g(X_s^{(Y)})\,Ah(Y_s)\,\mathrm{d}s \end{aligned}$$

is a martingale with respect to the filtration $\mathcal{G}_t$. The result now follows by an application of theory; see Stroock and Varadhan (1979). □

Remark 3.2.4. It is interesting to note that a direct calculation of the generator formally involves the computation of the limit as $t \downarrow 0$ in the following expression:

$$\begin{aligned} \frac{1}{t}\left\{\mathbb{E}g(X_t^{(Y)})h(Y_t) - g(x_1)h(x_2)\right\} \quad &= \quad g(x_1)\frac{1}{t}\,\mathbb{E}\left\{h(Y_t) - h(x_2)\right\} \\ + \frac{1}{t}\int_0^t \mathbb{E}\{\mu(Y_s)\,g'(X_s^{(Y)})\,h(Y_t)\}\,\mathrm{d}s \quad & + \frac{1}{2t}\int_0^t \mathbb{E}\left\{\sigma^2(Y_s)\,g''(X_s^{(Y)})\,h(Y_t)\right\}\,\mathrm{d}s \\ \to g(x_1)\,Ah(x_2) + \mu(x_2)\,g'(x_1)\,h(x_2) + \tfrac{1}{2}\sigma^2(x_2)\,g''(x_1)\,h(x_2). \end{aligned}$$

However direct justification of such an approach does not seem possible in the absence of (spatial) continuity of the coefficients μ and σ. The Stroock-Varadahn theory beautifully exploits the construction of the underlying Markov processes in replacing the calculation of derivatives by calculations of integrals.

In accordance with Lemma 3.2.3 and as suggested by the differential equation (3.6) in the transversal directions, consider the differential operator A with domain $\mathscr{D}_A$ given by

$$\begin{aligned} & Au = \nabla_y \cdot (D_y \nabla_y u), \quad u \in \mathscr{D}_A, \\ & \mathscr{D}_A = \{u \in H^1(G) : D_y \nabla_y u \in H^1(G),\, D_y \nabla_y u\big|_{\partial G} \cdot n_y = 0\}. \end{aligned} \tag{3.16}$$

The bilinear form associated to A is given by

$$\mathcal{E}(u,v) = \int_G D_y \, \nabla_y u \cdot \nabla_y v \, \mathrm{d}y, \quad u, v \in D_{\mathcal{E}} = H^1(G), \tag{3.17}$$

Standard considerations, see e.g. Example 2.b, page 45 in Ma and Röckner (1991), or Nash (1958), show that there exists a (strong) Markov process $Y = \{Y_t : t \geqslant 0\}$ with right continuous paths with left limits (Hunt process) defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and associated with $\mathcal{E}$. Observe that $\pi(y) = 1/|G|$ is the unique invariant probability for Y, uniquely solving the differential equation $A\pi = 0$ (up to non-normalized constants), In particular

$$T_t f(y) = \mathbb{E}_y f(Y_t), \quad t \geq 0, f \in L^2(G). \tag{3.18}$$

defines an L^2-semigroup. Some of the technical properties of this process and its infinitesimal generator are summarized in the following lemma

Lemma 3.2.5. *Let A be the operator with domain $\mathscr{D}_A$ defined in (3.16). Then the corresponding Markov process Y is an ergodic process. Furthermore, if $f \in L^2(G)$ and $\int_G f(y)\,\mathrm{d}y = 0$, then $f \in Ran(A) := \{Au : u \in \mathscr{D}_A\}$.*

Proof. The first property follows immediately since, as noted above, $\pi(y) = 1/|G|$ is the unique solution, up to non-normalized constants, of the differential equation $A\pi = 0$. The identification of the range follows from Bhattacharya (1982), Proposition 2.3 (c) since, in view of the smooth Neumann boundary ∂G, $(\lambda - A)^{-1}$ is a compact operator for any $\lambda > 0$, (Davies (1989), p. 48, Theorem 1.7.12), and 0 is a simple eigenvalue of A. □

Next, let $B = \{B_t : t \geqslant 0\}$ be a standard Brownian motion independent of Y and define the Itô process X by

$$\mathrm{d}X_t = U(Y_t)\,\mathrm{d}t + \sqrt{2D_x(Y_t)}\,\mathrm{d}B_t. \tag{3.19}$$

Then, to complete the construction of the stochastic process associated with the differential equation (3.6) via Lemma 3.2.3, we consider the process defined by

$$\boldsymbol{X} = \{\boldsymbol{X}_t = (X_t, Y_t) : t \geqslant 0\}. \tag{3.20}$$

Remark 3.2.6. The decomposition $\boldsymbol{X} = (X, Y)$ implies that the lifetime of $\boldsymbol{X}$ is a.s. infinite; i.e. the process is non-explosive. Specifically, $\mathbb{P}_{\boldsymbol{x}}$ almost surely one has,

$$|X_t - x| \leqslant \|U\|_{L^\infty(G)} t + \sqrt{2\|D_x\|_{L^\infty(G)}}\ |B_t|, \quad t \geqslant 0,$$

and the process in the right hand side does not explode in finite time. Also explosion does not occur for Y by ergodicity.

The stochastic process defined by (3.20) defines a semigroup whose infinitesimal generator coincides with that defining the bilinear form $\boldsymbol{\mathcal{E}}$. In particular the asymptotic homogenization problem may be viewed as the asymptotic (marginal) distribution of the rescaled longitudinal process $X^{(Y)}$. This is the topic of the next section.

3.2.4 Proof of main results.

The homogenization result will follow from an application of the following central limit theorem and formula for the variance for ergodic Markov processes due to Bhattacharya (1982).

Theorem 3.2.7. *Let* $Y = \{Y_t : t \geq 0\}$ *be a progressively measurable stationary Markov process on* G*, having invariant measure* π *and infinitesimal generator* $A : \mathscr{D}_A \to L^2(G, \pi)$*. Let* $U_0 \in$ *Ran*(A) *and consider the process* $Z_t = \int_0^t U_0(Y_s)\,\mathrm{d}s$*,* $t \geqslant 0$*. Then, as* $n \to \infty$*, the distribution of the scaled process* $\left\{n^{-\frac{1}{2}} Z_{nt} : t \geq 0\right\}$ *converges weakly to the Wiener measure with zero drift and variance parameter*

$$-(U_0, h)_{L^2(G,\pi)} = -\int_G U_0(y)\, h(y)\, \pi(\,\mathrm{d}y), \tag{3.21}$$

where h *is a solution to* $Ah = U_0$*.*

The result in Theorem (3.2.1) now follows easily. By Lemma (3.2.3), the longitudinal component of $\boldsymbol{X}$ is given by

$$X_t = x + \int_0^t U(Y_s)\,\mathrm{d}s + \int_0^t \sqrt{2D_x(Y_s)}\,\mathrm{d}B_s.$$

Let $\bar{U}$ be the mean of U with respect to π (see equation 3.13), and denote the centered drift of Y by

$$U_0(y) = U(y) - \bar{U}. \tag{3.22}$$

Let $\widetilde{X}_t = (X_t - \bar{U}t - x)$, and for $n \geqslant 0$, consider the scaled process $\widetilde{X}^{(n)} = \{n^{-\frac{1}{2}}\widetilde{X}_{nt} : t \geq 0\}$,

$$\widetilde{X}^{(n)}_t = n^{-\frac{1}{2}} \int_0^{nt} U_0(Y_s)\,\mathrm{d}s + n^{-\frac{1}{2}} \int_0^{nt} \sqrt{2D_x(Y_s)}\,\mathrm{d}B_s := Z^{(n)}_t + W^{(n)}_t. \tag{3.23}$$

For the process $W^{(n)}$, note that if $W^{(n)}_0$ has distribution equal to the invariant probability π, then for each n and $t > 0$, $\mathbb{E}W^{(n)}_t = 0$. The Itô isometry gives

$$\mathbb{E}_\pi\big[W^{(n)}_t\big]^2 = n^{-1} \int_0^{nt} \mathbb{E}_\pi[2D_x(Y_s)]\,\mathrm{d}s = t \int_G D_x(y)\pi(\,\mathrm{d}y). \tag{3.24}$$

Now, conditionally given Y up to time t, $W^{(n)}$ is a linear functional of the Brownian motion B. The characteristic function of $W^{(n)}$ can be then computed for each n, and the limit is taken using the ergodicity of Y,

$$\begin{aligned}
\mathbb{E}_\pi \exp\Big(i\xi W^{(n)}_t\Big) &= \mathbb{E}_\pi\,\mathbb{E}\Big[\exp\Big(i\xi W^{(n)}_t\Big)\,\big|\{Y_s : 0 \leqslant s \leqslant t\}\Big] \\
&= \mathbb{E}_\pi \exp\Big(-\frac{\xi^2 t}{nt}\int_0^{nt} D_x(Y_s)\,\mathrm{d}s\Big) \\
&\to \exp\Big(-\xi^2 t \int_G D_x(y)\pi(\,\mathrm{d}y)\Big), \quad \text{as}\, n \to \infty.
\end{aligned}$$

Therefore $W^{(n)}$ is asymptotically a Brownian motion with diffusion coefficient

$$\bar{D}_W = \int_G D_x(y)\pi(\,\mathrm{d}y). \tag{3.25}$$

To establish the convergence of process $Z^{(n)}$, note first that by Lemma (3.2.5), $U_0 \in \mathrm{Ran}(A)$. Now apply Lemma (3.2.7) to get that for any initial distribution of $W^{(n)}_0$, as $n \to \infty$, $Z^{(n)}$ converges weakly to a Brownian motion with zero drift and diffusion coefficient given by

$$\bar{D}_Z = -\int_G U_0(y)\,h(y)\,\pi(\,\mathrm{d}y) = -\int_G Ah(y)\,h(y)\,\pi(\,\mathrm{d}y) = \int_G (D_y\nabla_y h)\cdot\nabla_y h(y)\,\pi(\,\mathrm{d}y). \tag{3.26}$$

From here we obtain the convergence of $\tilde{X}^{(n)}$ to a Brownian motion with the asserted dispersion coefficient as follows.

Proposition 3.2.8. *$\tilde{X}^{(n)}$ converges weakly to a Brownian motion with diffusion coefficient*

$$\bar{D} = \bar{D}_W + \bar{D}_Z.$$

Proof. Since we have shown that each of the two processes $Z^{(n)}$ and $W^{(n)}$ converge weakly to Brownian motions, it suffices to show that for each pair of times $0 \le s \le t$, $(Z_s^{(n)}, W_t^{(n)})$ converges weakly to a pair of independent Gaussian random variables. For this consider the bivariate moment generating function along the above lines. Specifically,

$$\begin{aligned} \mathbb{E}\exp\Big(\lambda_1 Z_s^{(n)} + \lambda_2 W_t^{(n)}\Big) &= \mathbb{E}\Big\{\exp\Big(\lambda_1 Z_s^{(n)}\Big)\ \mathbb{E}\Big[\exp\Big(\lambda_2 W_t^{(n)}\Big)\,|\{Y_r : r \le t\}\Big]\Big\} \\ &= \mathbb{E}\left\{\exp\Big(\lambda_1 Z_s^{(n)}\Big)\ \exp\left(\frac{\lambda_2^2}{n}\int_0^{nt} D_x(Y_\tau)d\tau\right)\right\} \\ &= \mathbb{E}\exp\left(\lambda_1\left(Z_s^{(n)} + \frac{\lambda_2^2 t}{\lambda_1 n t}\int_0^{nt} D_x(Y_\tau)d\tau\right)\right). \end{aligned} \tag{3.27}$$

Now, since by the Ergodic Theorem the random variable $\frac{\lambda_2^2 t}{\lambda_1 n t}\int_0^{nt} D_x(Y_\tau)d\tau$ converges a.s. to a constant (for fixed t), namely $\gamma := \frac{\lambda_2^2 t}{\lambda_1}\int_G D_x(y)\pi(dy)$, it follows that the sum $Z_s^{(n)} + \frac{\lambda_2^2 t}{\lambda_1 n t}\int_0^{nt} D_x(Y_\tau)d\tau$ converges in distribution to the sum of the limit distributions; see Billingsley (1999), Chapter 1, Section 4. In particular, therefore, the moment generating function of the sum (as a function of λ_1) has the following asymptotic factorization

$$\begin{aligned} \lim_{n\to\infty}\mathbb{E}\exp\Big(\lambda_1 Z_s^{(n)} + \lambda_2 W_t^{(n)}\Big) &= \lim_{n\to\infty}\mathbb{E}\exp\left(\lambda_1\left(Z_s^{(n)} + \frac{\lambda_2^2 t}{\lambda_1 n t}\int_0^{nt} D_x(Y_\tau)d\tau\right)\right) \\ &= \exp\left(\frac{\lambda_1^2 2s\bar{D}_Z}{2} + \lambda_1\gamma\right) \\ &= \exp\left(\frac{\lambda_1^2 2s\bar{D}_Z}{2}\right)\exp\left(\frac{\lambda_2^2 2t\bar{D}_W}{2}\right). \end{aligned} \tag{3.28}$$

Since the two limit Brownian motions are independent at any two time points, the processes are independent. □

To relate the convergence of X to Theorem 3.2.1, consider an initial longitudinal concentration $C_0(x)$ and define

$$v_0(\boldsymbol{x}) = C_0(x)\frac{1}{|G|}, \quad \boldsymbol{x} \in \boldsymbol{G}.$$

This amounts to Y_0 having v_0 as its distribution. Let $C(x,t)$ be the cross-sectional concentration defined in (3.9) and I an interval. Since

$$\int_I C(x,t)\,\mathrm{d}x = \int_{G\times I} v(\boldsymbol{x},t)\,\mathrm{d}x = \mathbb{P}(\boldsymbol{X}_t \in G\times I) = \mathbb{P}(X_t \in I),$$

the homogenization result follows.

For the particular case treated in Corollary (3.2.2) consider the one dimensional diffusion with $G = [a,b]$ and

$$\boldsymbol{D}(y) = \begin{bmatrix} D_x(y) & 0 \\ 0 & D_y(y) \end{bmatrix},$$

where D_x and D_y are positive and bounded away from zero and infinity. Let g be as in (3.15), and define

$$h(y) = \int_a^y \frac{g(z)}{D_y(z)}\pi(\,\mathrm{d}y).$$

Then h solves the two dimensional version of problem (3.11). Using this solution in (3.13), gives

$$\bar{D} = \int_G \{D_x(y) + \frac{g(y)^2}{D_y(y)}\}\ \pi(\,\mathrm{d}y). \tag{3.29}$$

The result of Corollary (3.2.2) now follows by applying (3.29) to the case of $\boldsymbol{D}$ given by (3.5).

3.3 One dimensional diffusion in heterogenous media.

3.3.1 Skew Brownian motion and skew diffusion.

Consider first the case of a solute immersed in a medium without boundary in which $G = \mathbb{R}$. Assume zero drift, and a diffusion (dispersion) coefficient having a single interfacial point of discontinuity at $l_0 = 0$, namely, $D(y) = D^{(-1)}\mathbb{1}_{(-\infty,0)}(y) + D^{(0)}\mathbb{1}_{[0,\infty)}(y)$, $y \in \mathbb{R}$. To simplify notation write

$$D^{(-1)} \equiv D^{-} \qquad D^{(0)} \equiv D^{+}.$$

In this case the equations governing solute concentration $c(y,t)$ are given by

$$\begin{aligned}
&\frac{\partial c}{\partial t} = \frac{\partial}{\partial y}\left(D(y)\frac{\partial c}{\partial y}\right), \quad t > 0, \\
&c(0^-,t) = c(0^+,t), \qquad D^-\frac{\partial c}{\partial x}(0^-,t) = D^+\frac{\partial c}{\partial x}(0^+,t), \quad t > 0, \\
&c(y,0^+) = c_0(y).
\end{aligned} \tag{3.30}$$

For this problem one may explicitly compute the fundamental solution $p(t,x,y)$ by solving the half-space problems on $[0,\infty)$ and $(-\infty,0]$ with (apriori unknown) Neumann boundary fluxes at 0. One then may use the continuity of concentration and fluxes to match the values at the interface and determine $c(y,t)$. In particular, it follows that

$$p(x,y;t) = \begin{cases}
\frac{1}{\sqrt{4\pi D^+ t}}\left[\exp\left\{-\frac{(y-x)^2}{4D^+t}\right\} + \frac{\sqrt{D^+}-\sqrt{D^-}}{\sqrt{D^-}+\sqrt{D^+}}\exp\left\{-\frac{(y+x)^2}{4D^+t}\right\}\right] & \text{if } x > 0, y > 0 \\
\frac{1}{\sqrt{4\pi D^- t}}\left[\exp\left\{-\frac{(y-x)^2}{4D^-t}\right\} - \frac{\sqrt{D^+}-\sqrt{D^+}}{\sqrt{D^-}+\sqrt{D^-}}\exp\left\{-\frac{(y+x)^2}{4D^-t}\right\}\right] & \text{if } x < 0, y < 0 \\
\frac{1}{\sqrt{D^+}+\sqrt{D^-}}\frac{1}{\sqrt{\pi t}}\exp\left\{-\frac{(y\sqrt{D^-}-x\sqrt{D^+})^2}{4D^-D^+t}\right\} & \text{if } x \le 0, y > 0 \\
\frac{1}{\sqrt{D^+}+\sqrt{D^-}}\frac{1}{\sqrt{\pi t}}\exp\left\{-\frac{(y\sqrt{D^+}-x\sqrt{D^-})^2}{4D^-D^+t}\right\} & \text{if } x \ge 0, y < 0.
\end{cases} \tag{3.31}$$

One may identify the underlying stochastic process as a function of the *skew-Brownian motion with parameter* $\alpha \in [0,1]$ introduced by Itô and McKean (1963), and here with the particular skew parameter

$$\alpha^* = \frac{\sqrt{D^+}}{\sqrt{D^+}+\sqrt{D^-}}.$$

Specifically,

Proposition 3.3.1. *Let* $B^{(\alpha)} = \{B_t^{(\alpha)} : t \ge 0\}$ *denote skew Brownian motion with parameter* $\alpha \in (0,1)$,[1] *and let* $Y^{(\alpha^*)} = \{Y_t^{(\alpha^*)} : t \ge 0\}$ *be the diffusion on* $\mathbb{R}$ *defined by*

$$Y_t^{(\alpha^*)} := \sqrt{2D\left(B_t^{(\alpha^*)}\right)}\, B_t^{(\alpha^*)}, \quad \alpha^* = \frac{\sqrt{D^+}}{\sqrt{D^+}+\sqrt{D^-}},$$

---

[1] $\alpha = 0$ or 1 is permitted but corresponds to reflecting boundary at 0. This is a somewhat degenerate case and will be excluded from the general discussion.

Then $Y^{(\alpha^*)}$ is the diffusion with transition probabilities given by (3.31). In particular, the solution to (3.30) is given by

$$c(y,t) = \mathbb{E}_y \, c_0\left(Y_t^{(\alpha^*)}\right), \quad t \geq 0.$$

Proof. Since the function $\varphi(y) = \sqrt{2D(y)}y$, $y \in \mathbb{R}$, is continuous and one-to-one, it follows that for any $\alpha \in (0,1)$, $\{\varphi(B_t^{(\alpha)}) : t \geq 0\}$ is a diffusion, i.e. strong Markov process with continuous sample paths, as this is directly inherited from $B^{(\alpha)}$. One may directly compute the transition probabilities of $\{\varphi(B_t^{(\alpha)}) : t \geq 0\}$ in terms of those for skew Brownian motion given by Walsh (1978) . A comparison with (3.31) then yields the determination of $\alpha = \alpha^*$ as asserted. ☐

Remark 3.3.2. We refer to the stochastic process $Y^{(\alpha^*)}$ as the *physical skew diffusion* corresponding to the problem (3.30).

There are now a number of alternative ways in which to describe the motion of solute particles. For example, Walsh (1978) characterized skew Brownian motion by the property

$$\mathrm{Law}(|B_t^{(\alpha)}|) = \mathrm{Law}(|B_t|), \quad \mathbb{P}_0(B_t^{(\alpha)} > 0) = \alpha, \tag{3.32}$$

and used this to calculate the transition probability densities. Harrison and Shepp (1981) obtained skew Brownian motion as a weak limit of rescaled birth-death processes on the integer lattice with transition probabilities $p_{i,j} = \frac{1}{2}, |i-j| = 1$, $i \neq 0$, and $p_{0,1} = \alpha, p_{0,-1} = 1 - \alpha$. They also showed that skew Brownian motion is a solution to the stochastic differential equation

$$\mathrm{d}B_t^{(\alpha)} = (2\alpha - 1)\,\mathrm{d}l_0^{(\alpha)}(t) + \mathrm{d}B_t, \tag{3.33}$$

where $B \equiv B^{(\frac{1}{2})}$ is standard Brownian motion and $\{l_0^{(\alpha)}(t) : t \geq 0\}$ is the local-time (at 0) for the (unknown) solution process $B^{(\alpha)}$. The stochastic processes $B^{(\alpha)}$ were later shown by Le Gall (1984) to be a strong solutions to (3.33). In any case, it follows from this and the Itô-Tanaka lemma that $Y^{(\alpha^*)}$ satisfies the stochastic differential equation

$$\mathrm{d}Y_t^{(\alpha^*)} = K\,\mathrm{d}l_0^{(\alpha^*)} + \varphi(Y_t^{(\alpha^*)})\,\mathrm{d}B_t, \tag{3.34}$$

for a constant K depending on α, D^+, D^-, and where $l_0^{(\alpha)}$ is the local time at 0 of the process $Y^{(\alpha)}$. Ouknine (1990a) obtained the class of processes $Y^{(\alpha)}$, for $\alpha \in (0,1)$, in an extension of Le Gall (1984) to a theory of strong solutions to the corresponding stochastic differential equation. The transition semigroup of $Y^{(\alpha)}$ was also shown by Ouknine (1990a) to have a functional-valued (generalized) infinitesimal generator, namely

$$\lim_{t \to 0} \tfrac{1}{t} \mathbb{E}_y \left\{ u(Y_t^{(\alpha)}) - u(y) \right\} = \{\partial(D\partial) + [D\partial]_0 \, \delta_0\} \, u, \quad u \in H^1(\mathbb{R}). \tag{3.35}$$

Here δ_0 and $[\,\cdot\,]_0$ denote the Dirac delta distribution and the jump at point zero respectively, and the term $[D\partial]_0 \, \delta_0$ gives explicitly the propagation of the discontinuity of D as a generalized drift coefficient. The idea of a infinitesimal generator with generalized coefficients has been extended in Portenko (1990), Mastrangelo and Mouloud (1990), Kopytko (1992) and others, to analytically describe diffusion processes.

In their original construction Itô and McKean (1963) defined the skew Brownian motion process B^α by independently assigning ± signs to the excursions around zero of a Brownian motion with respective probabilities $\alpha, 1-\alpha$. The probabilistic behavior of the skew Brownian motion process was then described in terms of the probabilities and rates of escape from arbitrary intervals via computation of its scale function and speed measure. From this one may easily obtain the corresponding scale function and speed measure for the physical skew diffusion since the transformation $y \mapsto \varphi(y) = \sqrt{2D(y)}y$ is invertible. This is the approach that we will follow in the next subsection to obtain a probabilistic description of the underlying solute particles in the generalized Taylor-Aris problem in a layered medium. In particular the picture that emerges is that particles behave locally as in a regular diffusion, but are perturbed at the interfaces. The strength of this perturbations depend on the size of the jump of the diffusion coefficient at the interface, and have the net effect of directing the particles to the regions of higher diffusivity.

3.3.2 Diffusion in a layered medium.

We now turn our attention to the layered medium described in Corollary (3.2.2). The process Y is a one-dimensional diffusion in the interval $G = [a, b]$, experiencing sharp discontinuities of the diffusion coefficient at discrete interfaces l_k in the interior of G, and reflecting boundaries at the endpoints [2] By Lemma (3.2.3), Y is the diffusion process associated with the Dirichlet form

$$\mathcal{E}(u, v) = \int_G D(y)\, \partial u(y)\, \partial v(y)\, \mathrm{d}y, \quad u, v \in D_{\mathcal{E}} = H^1(G),$$

where D is the piecewise constant function,

$$D(y) = \sum_{k=-m}^{M} D^{(k)}\, \mathbb{1}_{[l_k, l_{k+1})}(y)$$

for some positive local diffusion coefficients $D^{(k)}$ and interfaces $a = l_{-m} < \cdots < l_{M+1} = b$. We now seek to obtain the basic probabilistic structure of Y in terms of its scale function and speed measure as computed below. Our approach is to first "guess" the scale function and speed measure of Y by informal consideratons of the expected relationship to skew Brownian motion, and then give proofs (see Theorem 3.3.3 below) using the said relationship and known properties of skew-Brownian motion. The basis for this guess is that since the speed measure and scale function measure the time to escape a sufficiently small interval and the probabilities to escape to the right or left of the interval respectively, it is enough to consider the process started in one of two types of intervals: an interval containing a single interface and an interval in which there is no interface. For these one may apply the results noted in the previous subsection on the speed measure and scale function of skew Brownian motion.

First, for $c \in G = [a, b]$, let $\tau(c)$ be the hitting time of c by the process Y, if $c < d$, denote $\tau(c, d) = \min\{\tau(c), \tau(d)\}$, the exit time of the interval (c, d). The scale function

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[2] Although in general interfaces are not boundaries, as noted earlier reflecting boundaries may be regarded as cases of degenerate interfaces.

(or scale measure) of Y is a continuous strictly increasing function $s : (a, b) \to \mathbb{R}$ such that for each y, c, d with $a \leqslant c < y < d \leqslant b$,

$$\mathbb{P}_y(\tau(c,d) = \tau(d)) = \frac{s(y) - s(c)}{s(d) - s(c)}. \tag{3.36}$$

The scale function is unique up to an additive constant and is characterized by its associated positive measure $s(\,\mathrm{d}x)$ (see, e.g. Revuz and Yor (1991), Sec. VII.3.) If $(c, d) \subset (l_k, l_{k+1})$, then up to $\tau(c, d)$ the process behaves as if it was in natural scale, namely

$$\mathbb{P}_y(\tau(c,d) = \tau(d)) = \frac{y - c}{d - c}.$$

This gives

$$s(\,\mathrm{d}y) = s_k \,\mathrm{d}y, \quad y \in (l_k, l_{k+1}), \tag{3.37}$$

for some positive constants s_k, $k = -m, \dots, M$. Now fix an interface l_k and set $c = l_k - \delta\sqrt{2D^{(k-1)}}$, $d = l_k + \delta\sqrt{2D^{(k)}}$ for some $\delta > 0$ such that $(c, d) \subset (l_{k-1}, l_{k+1})$. In view of (3.32), we must have

$$\alpha_k := \frac{\sqrt{D^{(k)}}}{\sqrt{D^{(k)}} + \sqrt{D^{(k-1)}}} = \mathbb{P}_{l_k}(\tau(c,d) = \tau(d)) = \frac{s_{k-1}(\delta\sqrt{2D^{(k-1)}})}{s_{k-1}(\delta\sqrt{2D^{(k-1)}}) + s_k(\delta\sqrt{2D^{(k)}})}.$$

Solving gives $s_k D^{(k)} = s_{k-1} D^{(k-1)}$. Set $s_{-m} = 1$ to get

$$s_k = \frac{D^{(k-1)}}{D^{(k)}}, \quad k = -m-1, \dots, M. \tag{3.38}$$

The speed measure of A is the unique Radon measure m on (a, b) such that for any y, c, d with $y \in (c, d) \subset G$,

$$\mathbb{E}_y \tau(c,d) = \int_G G_{c,d}(y, y')\; m(\,\mathrm{d}y'), \tag{3.39}$$

where $G_{c,d}$ is the Green's function of Y for the interval (c, d) (see Revuz and Yor (1991), Sec. VII.3)

$$G_{c,d}(y, y') = \begin{cases} \frac{(s(y)-s(c))(s(d)-s(y'))}{s(d)-s(c)} & \text{if} \quad c \leqslant y \leqslant y' \leqslant d, \\ \frac{(s(y')-s(c))(s(d)-s(y))}{s(d)-s(c)} & \text{if} \quad c \leqslant y' \leqslant y \leqslant d, \\ 0 & \text{otherwise.} \end{cases}$$

Assume a speed measure of the form $m(\,\mathrm{d}y) = m_k\,\mathrm{d}y$ for $y \in (l_k, l_{k+1})$ and consider an interval $(y-\delta, y+\delta) \subset (l_k, l_{k+1})$. On such an interval, the diffusion coefficient is constant and equal to $D^{(k)}$, therefore

$$\begin{aligned}\frac{\delta^2}{2D^{(k)}} &= \mathbb{E}_y \tau(y-\delta, y+\delta) = \int_{y-\delta}^{y+\delta} G_{y-\delta,y+\delta}(y,y')\, m(\,\mathrm{d}y') \\ &= s_k\, m_k \left\{ \int_{y}^{y+\delta} \frac{\delta(y+\delta-y')}{2\delta}\,\mathrm{d}y' + \int_{y-\delta}^{y} \frac{(y'-\delta+y)\delta}{2\delta}\,\mathrm{d}y' \right\} \\ &= s_k\, m_k \frac{\delta^2}{2}\end{aligned}$$

Solving for m_k, gives that $m(\,\mathrm{d}y)$ is constant and equal to

$$m(\,\mathrm{d}y) = \frac{1}{D^{(k)} s_k}\,\mathrm{d}y, \quad y \in (l_k, l_{k+1}). \tag{3.40}$$

The behavior at the boundaries is determined by the value of the speed measure at a and b. In particular, for instantaneously reflecting endpoints, m must satisfy (see Revuz and Yor (1991), Def. 3.3.11)

$$m(\{a\}) = m(\{b\}) = 0. \tag{3.41}$$

Theorem 3.3.3. *Y is a Feller process on $G = [a,b]$ with scale function s given by (3.37) and (3.38), and speed measure m given by (3.40) and (3.41).*

Proof. The Feller property follows from noting that the process Y can be written as $Y = F(\widetilde{Y})$ where F is a continuous function that folds $\mathbb{R}$ onto $[a,b]$, and $\widetilde{Y}$ is a diffusion process on $\mathbb{R}$ with diffusion coefficient function given by the appropriate periodic extension of D to all $\mathbb{R}$; see Bhattacharya and Waymire (1990a). The Feller property of $\widetilde{Y}$ can be obtained by the classical bounds on solutions to parabolic partial differential equations developed in Nash (1958). To check that s and m are indeed the scale and speed measures of Y, we use the representation of the infinitesimal generator as a second derivative with respect to this measures (See, e.g., Revuz and Yor (1991), Theorem 3.3.12.) Let $\mathscr{D}_{A_0} = \{u \in \mathscr{D}_A : D\partial_y u \text{ is absolutely continuous}\}$ and A_0 the restriction of A to $\mathscr{D}_{A_0}$. One has to check first that for $u \in \mathscr{D}_{A_0}$ and x in the interior of G, the s-derivative of u exists. Note that

$$\frac{\mathrm{d}u}{\mathrm{d}s}(y) = \frac{1}{s_k}\partial_y u(y), \quad \text{for } x \in (l_k, l_{k+1}),$$

which clearly exists at each point away from the interfaces and boundaries of G. At an interface l_k this condition is equivalent to

$$\frac{1}{s_{k-1}}\partial_y u(l_k^-) = \frac{1}{s_k}\partial_y u(l_k^+),$$

which by (3.38), is satisfied since $D\partial_y u$ is continuous. Now let y, y' be such that $l_{k-1} < y < l_k < y' < l_{k+1}$ for some k, and use (3.38) and the absolute continuity of $D\partial_y u$ to compute,

$$\begin{aligned} \frac{\mathrm{d}u}{\mathrm{d}s}(y) - \frac{\mathrm{d}u}{\mathrm{d}s}(y') &= \frac{1}{s_{k-1}}\partial_y u(y) - \frac{1}{s_k}\partial_y u(y') = \frac{1}{s_k D^{(k)}}\left(D^{(k-1)}\partial_y u(y) - D^{(k)}\partial_y u(y')\right) \\ &= \frac{1}{s_k D^{(k)}}\int_y^{y'} \partial_y(D\,\partial_y u)\,\mathrm{d}y = \int_y^{y'} A_0 u(y)\ m(\,\mathrm{d}y). \end{aligned}$$

Lastly, the conditions $\frac{\mathrm{d}u}{\mathrm{d}s}(a) = m(\{a\})A_0 u(a)$ and $\frac{\mathrm{d}u}{\mathrm{d}s}(b) = m(\{b\})A_0 u(b)$ hold trivially by the boundary condition imposed to functions in $\mathscr{D}_A$. We then have that m and s satisfy $A = \frac{\mathrm{d}}{\mathrm{d}m}\frac{\mathrm{d}}{\mathrm{d}s}$ on $\mathscr{D}_{A_0}$, and therefore these are the speed and scale measures of Y. $\square$

4 MULTI-SKEW BROWNIAN MOTION AND DIFFUSION IN LAYERED MEDIA.

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Manuscript to be submitted.

4.1 Introduction

Skew Brownian motion was introduced by Itô and McKean (1963, p. 222) in an effort to construct certain stochastic processes associated with W. Feller's classification of one-dimensional second order (generalized) differential operators for diffusion processes. Their original construction consisted of independently assigning to the excursions about zero of reflected Brownian motion a positive sign with probability α, and a negative sign with probability $1-\alpha$, for some $\alpha \in [0,1]$. The resulting process B^α behaves like standard Brownian motion when away from the "interface" at zero, but its sample paths are skewed, namely $\mathbb{P}(B_t^\alpha > 0 \big| B_0^\alpha = 0) = \alpha$ for all $t \geqslant 0$. Thus corresponding to the differential operator $\mathcal{A}^\alpha f = \frac{1}{2} f''(u \cdot \mathbb{1}_{(0,\infty)}) + \frac{1}{2} f''(u \cdot \mathbb{1}_{(-\infty,0)})$ for f twice differentiable on $\mathbb{R} \setminus \{0\}$ and satisfying $\alpha f'(0^+) = (1-\alpha) f'(0^-)$.

Since its introduction, skew Brownian motion has been applied as a model for transport in heterogenous media and in the presence of membranes (Mastrangelo and Mouloud, 1990; Lang, 1995; Portenko, 2000; Ueno et al., 2002; Berentsen et al., 2005; Ramirez et al., 2006). In Lejay (2006) the reader can find a recent and thorough survey of the large body of work by many authors devoted to the study of alternative characterizations, properties and some generalizations of skew Brownian motion.

Le Gall (1983, 1984) proved existence and uniqueness of a strong solution to

$$X_t = X_0 + B_t + \int_{\mathbb{R}} L^X(t,x)\,\mathrm{d}\mu(x) \tag{4.1}$$

where L^X is the symmetric local time of the unknown process X, and μ is a signed measure such that $|\mu(\{x\})| < 1$ for all $x \in \mathbb{R}$. Skew Brownian motion solves (4.1) for μ concentrated on $\{0\}$ with $\mu(\{0\}) = 2\alpha - 1$. For a general signed measure μ on the Borel measure space $(\mathbb{R}, \mathscr{B})$, its Lebesgue decomposition gives $\mu = \mu_c + \mu_s$ where

μ_c is absolutely continuous with respect to Lebesgue measure, say $\mu(\mathrm{d}x) = g(x)\,\mathrm{d}x$, and μ_s is orthogonal to μ_c. By the occupation times formula (see (4.7) below) equation (4.1) reads,

$$X_t = X_0 + B_t + \int_0^t \tfrac{1}{2} g(X_s)\,\mathrm{d}s + \int_{\mathbb{R}} L^X(t,x)\,\mathrm{d}\mu_s(x) \tag{4.2}$$

The focus here is the solution $B^{\boldsymbol{\alpha}} = \{B^{\boldsymbol{\alpha}}_t : t \geqslant 0\}$ to (4.1) in the case $\mu = \mu_s$ supported on a set $S = \{x_k : k \in \mathbb{Z}\}$ with no accumulation points and $0 < |\mu(\{x_k\})| < 1$, $k \in \mathbb{Z}$. Writing $\mu(\{x_k\}) := 2\alpha_k - 1$, gives that such a solution can be constructed for $\alpha_k \in (0,1) \setminus \{1/2\}$, $k \in \mathbb{Z}$.

The process $B^{\boldsymbol{\alpha}}$ is referred to as *multi-skew Brownian motion* and generalizes skew Brownian motion to the case of a countable set of interfaces $S = \{x_k : k \in \mathbb{Z}\}$ with skewness values $\boldsymbol{\alpha} = \{\alpha_k : k \in \mathbb{Z}\}$. Namely, $B^{\boldsymbol{\alpha}}$ behaves like standard Brownian motion inside each interval (x_k, x_{k+1}), and at each x_k, experiences a skewness α_k, $k \in \mathbb{Z}$. We restrict ourselves to the case in which S has no accumulation points and $\alpha_k \in (0,1) \setminus \{1/2\}$, $k \in \mathbb{Z}$. The case of finite interfaces and reflecting boundaries is considered in Ramirez et al. (2006).

Our approach is to construct $B^{\boldsymbol{\alpha}}$ as a regular diffusion by specifying its infinitesimal generator according to the desired local behavior of the process. In particular, the measure m with piecewise constant density $m'(x) = \prod_{j=1}^{k} \alpha_j/1-\alpha_j$ for $x \in (x_k, x_{k+1})$, is invariant for $B^{\boldsymbol{\alpha}}$, and on $L^2(\mathbb{R}, m)$ the infinitesimal generator of the process is

$$\boldsymbol{A}u = \sum_{k\in\mathbb{Z}} \tfrac{1}{2}\,\partial^2 \left(u \cdot \mathbb{1}_{(x_k,x_{k+1})}\right), \quad \alpha_k\,\partial u(x_k^+) = (1-\alpha_k)\,\partial u(x_k^-), \quad k \in \mathbb{Z}. \tag{4.3}$$

For the sample path description of $B^{\boldsymbol{\alpha}}$, we exploit the representation of regular diffusions as scaled versions of Brownian motion under a random time change. Our second goal is to associate $B^{\boldsymbol{\alpha}}$ to a model for the motion of solute particles undergoing diffusion in a medium with piecewise constant diffusion coefficient.

Motivated by applications to solute diffusion in heterogeneous media, we consider the following initial value problem in $L^2(\mathbb{R}^2)$,

$$\partial_t c = \nabla\cdot(\tfrac{1}{2}\boldsymbol{D}\nabla c) + \nabla\cdot(\boldsymbol{U}c), \quad c(0) = c_0, \tag{4.4}$$

where $\boldsymbol{D}(\boldsymbol{x}) = \mathrm{diag}(D_x(x), D_y(x))$, $\boldsymbol{U}(x, y) = (0, U(x))$ for $\boldsymbol{x} = (x, y) \in \mathbb{R}^2$. We assume $\boldsymbol{D}$ is elliptic on compact sets of $\mathbb{R}^2$ and bounded everywhere, and ${}^{U}/\sqrt{D_y}$ is bounded. Furthermore D_x is piecewise constant, with values $D_x(x) = D_k$ for $x \in (z_k, z_{k+1})$ where $\{z_k : k \in \mathbb{Z}\}$ is a set of interfaces with no accumulation points. The goal is to construct and analyze a diffusion process $\boldsymbol{X}$ associated to (4.4), namely $c(t, \boldsymbol{x}) = \mathbb{E}_{\boldsymbol{x}} c_0(\boldsymbol{X}_t)$, $t \geqslant 0$, $\boldsymbol{x} \in \mathbb{R}^2$. We prove that $\boldsymbol{X}$ is of the form $\boldsymbol{X} = (X, Y)$, where Y is given by a stochastic integral depending on the path of X, and X is a suitable re-scaling of multi-skew Brownian motion $B^{\boldsymbol{\alpha}}$ with the following choice of skewness

$$\alpha_k = \frac{\sqrt{D_k}}{\sqrt{D_k} + \sqrt{D_{k-1}}}, \quad k \in \mathbb{Z}.$$

In the case of a single point (or hyperplane) of discontinuity of $\boldsymbol{D}$, the process associated to (4.4) can be constructed from an explicit calculation of its semigroup (Portenko, 1990; Mastrangelo and Mouloud, 1990; Kopytko, 1992). In the one-dimensional case, stochastic differential equations with local time terms may be considered (Ouknine, 1990b; Le Gall, 1983). For more general situations (including ours), the theory of Dirichlet forms provides the tools to establish the existence of such a process (Fukushima, 1980; Ma and Röckner, 1991; Lang, 1995). The properties of $\boldsymbol{X}$ can then be deduced by solving the appropriate martingale problem as in Ramirez et al. (2006).

The organization of this article is as follows. In Section (4.2) we construct multi-skew Brownian motion, identify its semigroup on the space of continuous bounded functions, and give conditions on the skewness $\boldsymbol{\alpha}$ for recurrence, positive recurrence, and existence of an invariant measure. In order to formulate a forward equation in the weak sense for $B^{\boldsymbol{\alpha}}$, in Section (4.3) we identify the semigroup of $B^{\boldsymbol{\alpha}}$ in $L^2(\mathbb{R})$ with respect to its invariant measure. In Section (4.4) we use the theory of Dirichlet forms to construct the process $\boldsymbol{X}$ associated to problem (4.4). Finally in Section (4.5) we consider a periodic layered medium and use the structure of $B^{\boldsymbol{\alpha}}$ to determine the asymptotic behavior of $\boldsymbol{X}$.

4.1.1 Notation

A diffusion process with sample space $\mathbb{R}^d$ is a four-tuple $X = (\Omega, \mathscr{F}, \{\mathbb{P}_x\}_{x\in\mathbb{R}^d}, \{X_t : t \geqslant 0\})$ where Ω is the Wiener space of continuous functions from $[0,\infty)$ to $\mathbb{R}^d$, $\mathscr{F}$ is the σ-algebra of subsets of Ω generated by finite-dimensional cylinders, and for each $x \in \mathbb{R}^d$, $\mathbb{P}_x^B$ is the Wiener measure on $(\Omega, \mathscr{F})$ such that $\mathbb{P}_x(\{\omega : \omega(0) = x\}) = 1$. Here, only regular diffusions are considered, that is, those that for every $x, y \in \mathbb{R}^d$, the $\mathbb{P}_x$ probability of reaching y in finite time is positive. Standard Brownian motion will be denoted by B or W, and for $\alpha \in (0,1)$, skew Brownian motion (i.e., with a single interface at zero) will be denoted by B^α.

The sigma algebra of Borel sets of $\mathbb{R}^d$ will be denoted by $\mathscr{B}$, and for $A \in \mathscr{B}$, $\mathbb{1}_A$ denotes the indicator function of A. For $A \in \mathscr{B}$, the following stopping times are considered: the time to hit A, H_A and the time to exit from A, E_A,

$$H_A := \inf\{t \geqslant 0 : B_t^{\boldsymbol{\alpha}} \in A\}, \quad E_A := \inf\{t \geqslant 0 : B_t^{\boldsymbol{\alpha}} \notin A\}, \quad A \in \mathscr{B}. \tag{4.5}$$

The occupation time of A up to time t is denoted by

$$O_A(t) := \int_0^t \mathbb{1}_A(B_s^{\boldsymbol{\alpha}})\,\mathrm{d}s, \quad A \in \mathscr{B},\ t \geqslant 0. \tag{4.6}$$

Whenever any of the random functionals in (4.5) and (4.6) is evaluated on a stochastic process other than $B^{\boldsymbol{\alpha}}$, say Z, a superscript will be used, e.g., $H_A^Z := \inf\{t \geqslant 0 : Z_t \in A\}$; in the case of skew Brownian motion B^α, the superscript α will be used instead of B^α to avoid double superindices. Finally, the local time of Brownian motion B will be denoted by $L = \{L(t,x) : t \geqslant 0, x \in \mathbb{R}\}$, with the following convention in the occupation times formula

$$2\int_A L(t,x)\,\mathrm{d}x = O_A^B(t), \quad A \in \mathscr{B}(\mathbb{R}),\ t \geqslant 0. \tag{4.7}$$

4.2 A canonical representation.

Consider a countable set of real numbers $S := \{x_k : k \in \mathbb{Z}\}$, with $x_0 = 0$ and $x_k < x_{k+1}$ for all k. Assume furthermore that S has no accumulation points. The intervals between interfaces will be denoted by $I_k := (x_k, x_{k+1})$. Define the function $\boldsymbol{\alpha}$ on S with

$$\boldsymbol{\alpha} : S \mapsto (0,1) \smallsetminus \{\tfrac{1}{2}\}, \quad \boldsymbol{\alpha}(x_k) = \alpha_k, \quad k \in \mathbb{Z}. \tag{4.8}$$

The set S will be called the set of interfaces, and we refer to α_k as the “skewness” of the interface x_k. Our aim is to construct a regular diffusion $B^{\boldsymbol{\alpha}} = \{B_t^{\boldsymbol{\alpha}} : t \geqslant 0\}$ with values on $\mathbb{R}$ and the following features:

- (i) for $x \in (x_k, x_{k+1})$, the distribution of $B^{\boldsymbol{\alpha}}$ starting at x and stopped at the exit time of (x_k, x_{k+1}) is that of a stopped Brownian motion, and
- (ii) starting at the interface x_k, and for any δ small enough, the probability of hitting $x_k + \delta$ before $x_k - \delta$ is α_k.

If $S = \{0\}$, $B^{\boldsymbol{\alpha}}$ is skew Brownian motion B^{α_0} as in Itô and McKean (1963); Walsh (1978). In (4.8), the skewness is not allowed to take the values of 0 or 1 to avoid reflecting boundaries, and the value $1/2$ is excluded so that no artificial interfaces are introduced.

The process $B^{\boldsymbol{\alpha}} = (\Omega, \mathscr{F}, \{\mathbb{P}_x\}_{x\in\mathbb{R}}, \{B_t^{\boldsymbol{\alpha}} : t \geqslant 0\})$ will be constructed as a regular diffusion with scale s and speed measure m, via a random time change of

Brownian motion (see for example Itô and McKean, 1974; Breiman, 1992; Revuz and Yor, 1991; Freedman, 1971).

The scale of $B^{\boldsymbol{\alpha}}$ is the unique, up to additive constants, continuous and strictly increasing function $s : \mathbb{R} \to \mathbb{R}$ such that

$$\mathbb{P}_x(H_b < H_a) = \mathbb{P}_x(E_{(a,b)} = H_b) = \frac{s(x) - s(a)}{s(b) - s(a)}, \quad a < b,\ x \in (a, b). \tag{4.9}$$

The speed measure of $B^{\boldsymbol{\alpha}}$ is the unique Radon measure m on $\mathbb{R}$ such that for any $c < x < d$

$$\mathbb{E}_x \left(E_{(c,d)}\right) = \int_c^d G_{c,d}(x, y)\ \mathrm{d}m(y), \tag{4.10}$$

where $G_{c,d}$ is defined on $[c, d]$ by,

$$G_{c,d}(x, y) = \begin{cases} \frac{(s(x)-s(c))(s(d)-s(y))}{s(d)-s(c)} & \text{if} \quad c \leqslant x \leqslant y \leqslant d, \\ \frac{(s(y)-s(c))(s(d)-s(x))}{s(d)-s(c)} & \text{if} \quad c \leqslant y \leqslant x \leqslant d. \end{cases} \tag{4.11}$$

Both m and s can be described as positive measures or continuous increasing functions. For ease of notation the symbols s and m will be used interchangeably in both cases. In particular, for an interval (a, b), whether $s((a, b))$ denotes the number $s(a) - s(b)$ or the interval $(s(a), s(b))$ should be clear from the context. Properties (i) and (ii) outlined above can now be recast in terms of s and m. First, since by (i), $B^{\boldsymbol{\alpha}}$ behaves like Brownian on the interior of any I_k, the densities of m and s must be piecewise constant. Let

$$m(\mathrm{d}x) = m'(x)\,\mathrm{d}x = m_k\,\mathrm{d}x, \quad s(\mathrm{d}x) = s'(x)\,\mathrm{d}x = s_k\,\mathrm{d}x, \quad x \in [x_k, x_{k+1}),\ k \in \mathbb{Z}. \tag{4.12}$$

Fix k and consider the process starting at x_k. Let $I_\delta := (x_k - \delta, x_k + \delta)$ with $\delta < \min\{|I_{k-1}|, |I_k|\}$, then by (ii),

$$\mathbb{P}_{x_k}(E_{I_\delta} = H_{x_k+\delta}) = \frac{s(x_k) - s(x_k - \delta)}{s(x_k + \delta) - s(x_k - \delta)} = \frac{s_{k-1}}{s_k + s_{k-1}} = \alpha_k. \tag{4.13}$$

On the other hand, by (i), the time it takes $B^{\boldsymbol{\alpha}}$ to exit I_δ from x_k must have the same law as the time it takes a reflected Brownian motion starting at 0 to reach δ, therefore we must have $\mathbb{E}_{x_k}(E_{I_\delta}) = \delta^2$. Using (4.11) yields,

$$\begin{aligned}\mathbb{E}_{x_k}\left(E_{I_\delta}\right) &= \frac{s_{k-1}s_k}{s_{k-1}+s_k}\left\{\int_{x_k}^{x_k+\delta}(x_k+\delta-y)m_k\,\mathrm{d}y + \int_{x_k-\delta}^{x_k}(y-x_k+\delta)m_{k-1}\,\mathrm{d}y\right\} \\ &= \frac{s_{k-1}s_k}{s_{k-1}+s_k}\frac{\delta^2}{2}\left(m_{k-1}+m_k\right) = \delta^2 \qquad (4.14)\end{aligned}$$

Equations (4.13) and (4.14) can be solved to obtain

$$m_k = \frac{2}{s_k}, \quad s_k = \frac{1-\alpha_k}{\alpha_k}s_{k-1}, \quad k \in \mathbb{Z}, \tag{4.15}$$

which by setting $s_0 = 1$ gives

$$s_k = \prod_{j=1}^{k}\frac{1-\alpha_j}{\alpha_j}, \quad s_{-k} = \prod_{j=-k+1}^{0}\frac{\alpha_j}{1-\alpha_j}, \quad k \geqslant 1. \tag{4.16}$$

We can now state the following theorem.

Theorem 4.2.1. *Consider the measures s and m defined by (4.16) and (4.15), and let B be a Brownian motion on $\mathbb{R}$ with local times $\{L(t,x) : t \geqslant 0, x \in \mathbb{R}\}$. Let $\tilde{m}$ be the measure on $(\mathbb{R}, \mathscr{B})$ with piecewise constant density*

$$\tilde{m}'(x) = \frac{m'(x)}{s'(x)} = \frac{2}{s_k^2}, \quad x \in s(I_k), \quad k \in \mathbb{Z}.$$

Define $\phi(r) := \int_{\mathbb{R}} L(r,x)\,\mathrm{d}\tilde{m}(x)$, $r \geqslant 0$, and denote its associated time change by $\tau := \phi^{-1}$, i.e., $\tau(t) = \inf\{s \geqslant 0 : \phi(s) = t\}$. Let $\hat{B} : \Omega \to \Omega$ be given by

$$\hat{B}_t = s^{-1}(B_{\tau(t)}), \quad t \geqslant 0, \tag{4.17}$$

and define

$$\mathbb{P}_x = \mathbb{P}^B_{s(x)} \circ \hat{B}^{-1}, \quad B^{\boldsymbol{\alpha}}_t = \hat{B}_t, \quad x \in \mathbb{R},\, t \geqslant 0. \tag{4.18}$$

Then $B^{\boldsymbol{\alpha}} := (\Omega, \mathscr{F}, \{\mathbb{P}_x\}_{x\in\mathbb{R}}, \{B^{\boldsymbol{\alpha}}_t : t \geqslant 0\})$ is a canonical model for a regular diffusion satisfying (4.13) and such that under $\mathbb{P}_x$, $x \in I_k$, the distribution of $B^{\boldsymbol{\alpha}}_{t\wedge E_{I_k}}$ is that of a Brownian motion started at x and stopped at the exit time of I_k.

Proof. Note that since S has no accumulation points, m, $\tilde{m}$ and s are Radon measures. The fact that $B^{\boldsymbol{\alpha}}$ is a regular diffusion with m and s as speed and scale measures follows from classical results (see Itô and McKean, 1974; Breiman, 1992). To establish the relationship between $B^{\boldsymbol{\alpha}}$ and Brownian motion, fix $k \in \mathbb{Z}$ and consider $x \in I_k$. For $r \leqslant E^B_{s(I_k)}$, the occupation times formula (4.7) gives $\phi(r) = \frac{r}{s_k^2}$. Also, since τ is an increasing function,

$$\tau(t \wedge E_{I_k}) = \tau(t) \wedge E^B_{s(I_k)} = s_k^2\, t \wedge E^B_{s(I_k)}.$$

The stopped process satisfies,

$$B^{\boldsymbol{\alpha}}_{t \wedge E_{I_k}} - x = \frac{1}{s_k}\left(B_{\tau(t \wedge E_{I_k})} - s(x)\right) = \frac{1}{s_k}\big(B_{s_k^2\, t \wedge E^B_{s(I_k)}} - s(x)\big).$$

The proof is finished by establishing that

$$\mathbb{P}^B_{s(x)}\big(B_{s_k^2\, t \wedge E^B_{s(I_k)}} \in s_k\, \mathrm{d}y\big) = \mathbb{P}^W_x\big(W_{t \wedge E^W_{I_k}} \in \mathrm{d}y\big), \quad y \in [x_k, x_{k+1}], \tag{4.19}$$

where W is standard Brownian motion with distribution $\{\mathbb{P}^W_x\}_{x \in \mathbb{R}}$. Consider first $y \in I_k$ and $r > 0$, then

$$\begin{aligned}\mathbb{P}^B_{s(x)}\big(B_{r \wedge E^B_{s(I_k)}} \in s_k\, \mathrm{d}y\big) &= \mathbb{P}^B_{s(x)}\big(B_r \in s_k\, \mathrm{d}y,\, r < E^B_{s(I_k)}\big) \\ &= \mathbb{P}^B_{s(x)}\big(B_r \in s_k\, \mathrm{d}y\big) - \mathbb{P}^B_{s(x)}\big(B_r \in s_k\, \mathrm{d}y,\, r \geqslant E^B_{s(I_k)}\big).\end{aligned}$$

Conditioning on the value of B at exiting $s(I_k)$ and using the strong Markov property gives,

$$\begin{aligned}&P^B_{s(x)}\big(B_{r \wedge E^B_{s(I_k)}} \in s_k\, \mathrm{d}y\big) = \mathbb{P}^B_{s(x)}\big(B_r \in s_k\, \mathrm{d}y\big) - \\ &\quad \sum_{j=k,k+1} \mathbb{P}^B_{s(x)}\big(E^B_{s(I_k)} = H^B_{s(x_j)}\big) \int_0^r \mathbb{P}^B_{s(x_j)}\big(B_{r-u} \in s_k\, \mathrm{d}y\big)\, \mathbb{P}_{s(x)}\big(H^B_{s(x_j)} \in \mathrm{d}u\big).\end{aligned} \tag{4.20}$$

Consider now $y = x_k$, then

$$\mathbb{P}^B_{s(x)}\big(B_{r \wedge E^B_{s(I_k)}} = s_k\, x_k\big) = \mathbb{P}^B_{s(x)}\big(E^B_{s(I_k)} < r,\, B_{E^B_{s(I_k)}} = s_k\, x_k\big). \tag{4.21}$$

The corresponding relation holds for $y = x_{k+1}$. Formulae for the probabilities on the right hand side of (4.20) and (4.21) are well known (see for example Borodin and Salminen, 2002); the substitution $r = s_k^2 t$ gives the probabilities on the right hand side of (4.19). □

It also follows that $B^{\boldsymbol{\alpha}}$ is a special case of the processes introduced in Le Gall (1983),

Proposition 4.2.2. *Multi-skew Brownian motion is a solution to*

$$X_t = X_0 + W_t + \sum_{k\in\mathbb{Z}}(2\alpha_k - 1)L^{\boldsymbol{\alpha}}(t, x_k) \tag{4.22}$$

where W is Brownian motion and $L^{\boldsymbol{\alpha}}(t,x)$, $t \geqslant 0$, $x \in \mathbb{R}$, is the symmetric local time of $B^{\boldsymbol{\alpha}}$.

Proof. Refer to the notation of Theorem (4.2.1). Using Tanaka's formula on $(B_t^{\boldsymbol{\alpha}} - x_k)^+$ and $(B_t^{\boldsymbol{\alpha}} - x_k)^-$ respectively (see Walsh, 1978) gives

$$L^{\boldsymbol{\alpha}}(t, x_k^+) = \frac{1}{s_k}L(\tau(t), s(x_k)), \quad L^{\boldsymbol{\alpha}}(t, x_k^-) = \frac{1}{s_{k-1}}L(\tau(t), s(x_k)), \quad k \in \mathbb{Z},\ t \geqslant 0. \tag{4.23}$$

On the other hand, Tanaka's formula on $s^{-1}(B_{\tau(t)})$ gives

$$\begin{aligned} B_t^{\boldsymbol{\alpha}} &= \int_0^{\tau(t)} \frac{1}{s'(B_s)}\,\mathrm{d}B_s + \frac{1}{2}\sum_{k\in\mathbb{Z}}\left(\frac{1}{s_k} - \frac{1}{s_{k-1}}\right)L(\tau(t), s(x_k)) \\ &= \int_0^{\tau(t)} \frac{1}{s'(B_s)}\,\mathrm{d}B_s + \frac{1}{2}\sum_{k\in\mathbb{Z}}\left(L^{\boldsymbol{\alpha}}(t, x_k^+) - L^{\boldsymbol{\alpha}}(t, x_k^-)\right). \end{aligned}$$

Combining (4.23) and (4.15) yields

$$2L^{\boldsymbol{\alpha}}(t, x_k) := L^{\boldsymbol{\alpha}}(t, x_k^+) + L^{\boldsymbol{\alpha}}(t, x_k^-) = \frac{1}{2\alpha_k - 1}\left(L^{\boldsymbol{\alpha}}(t, x_k^+) - L^{\boldsymbol{\alpha}}(t, x_k^-)\right). \tag{4.24}$$

The proof is finished by noting that the martingale $M_r := \int_0^r \frac{1}{s'(B_s)}\,\mathrm{d}B_s$, $r \geqslant 0$, has quadratic variation process given by $\langle M, M\rangle = \phi = \tau^{-1}$. Dubins representation theorem gives that $\{M_{\tau(t)} : t \geqslant 0\}$ is Brownian motion (Revuz and Yor, 1991, p. 170). □

4.2.1 The semigroup of $B^{\boldsymbol{\alpha}}$ in $C_b(\mathbb{R})$

The representation of $B^{\boldsymbol{\alpha}}$ as a regular diffusion endows its semigroup $T = \{T_t : t \geqslant 0\}$, $T_t f(x) = \mathbb{E}_x f(B_t^{\boldsymbol{\alpha}})$, $x \in \mathbb{R}$, with the Feller property, namely $T_t : C_b \to C_b$, where $C_b = C_b(\mathbb{R})$ denotes the Banach space of continuous bounded functions with the norm of uniform convergence. Moreover, the map $t \mapsto T_t f$ is continuous with respect to uniform convergence on compact subsets of $\mathbb{R}$, and is strongly continuous on C_0, the set of functions in C_b that vanish at infinity (Kallenberg, 2002, Chapter 19).

The resolvent $G = \{G_\lambda : \lambda > 0\}$ of T is defined pointwise by $G_\lambda f(x) := \int_0^\infty e^{-\lambda s} T_s f(x)\, \mathrm{d}s$, $x \in \mathbb{R}$, $f \in C_b$. The infinitesimal generator of T is $\mathcal{A} := \lambda - G_\lambda^{-1}$ on its domain $D_{\mathcal{A}} := \mathrm{Ran}(G_\lambda)$, this definition being independent of λ. Furthermore, $\mathcal{A}f = \lim_{t\to 0} \frac{1}{t}[T_t f - f]$, and $D_{\mathcal{A}}$ coincides with the subset of C_b where $\frac{1}{t}[T_t - I]$ converges boundedly and pointwise to an element of C_b (Freedman, 1971, Theorem 53).

The operator $\mathcal{A}$ can also be explicitly computed in terms of the measures m and s (see Freedman, 1971, Theorem 75). Its domain $D_{\mathcal{A}} \subseteq C_b$ coincides with the set of functions f of C_b such that the s-derivative $\frac{\mathrm{d}f}{\mathrm{d}s}(x) := \frac{1}{s'(x)} f'(x) = \frac{m'(x)}{2} f'(x)$ exists for all $x \in \mathbb{R}$, is right continuous, of locally bounded variation, and there is $g = \mathcal{A}f \in C_b$ such that

$$\frac{\mathrm{d}f}{\mathrm{d}s}(x) - \frac{\mathrm{d}f}{\mathrm{d}s}(y) = \int_x^y g(z)\, \mathrm{d}m(z), \quad x, y \in \mathbb{R}. \tag{4.25}$$

We write for short, $\mathcal{A}f = \frac{\mathrm{d}}{\mathrm{d}m}\frac{\mathrm{d}f}{\mathrm{d}s}$. Evaluating (4.25) first for points $x, y \in I_k$, and then for $x < x_k < y$, one arrives to,

$$\mathcal{A}f(x) = \frac{1}{2} f''(x), \quad f \in D_A,\ x \in \mathbb{R} \setminus S, \tag{4.26}$$

$$D_{\mathcal{A}} = \left\{ f \in C_b : f'' \text{ exits in } \mathbb{R} \setminus S, \text{ and } \alpha_k f'(x_k^+) = (1 - \alpha_k) f'(x_k^-),\ k \in \mathbb{Z} \right\}. \tag{4.27}$$

4.2.2 Recurrence and invariance.

By definition, the regularity of the diffusion $B^{\boldsymbol{\alpha}}$ implies that $\mathbb{P}_x(H_y < \infty) > 0$ for all $x, y \in \mathbb{R}$. The process $B^{\boldsymbol{\alpha}}$ is called recurrent if $\mathbb{P}_x(H_y < \infty) = 1$ for all $x, y \in \mathbb{R}$, and is called transient otherwise. In the recurrent case, $B^{\boldsymbol{\alpha}}$ is called positive recurrent if $\mathbb{P}_x(|B^{\boldsymbol{\alpha}}_t| \in K) \nrightarrow 0$ as $t \to \infty$ for any compact set K and $x \in \mathbb{R}$ (Kallenberg, 2002).

Recall that a positive measure μ on $\mathscr{B}$ is invariant for $B^{\boldsymbol{\alpha}}$ if $\int_{\mathbb{R}} T_t g \,\mathrm{d}\mu = \int_{\mathbb{R}} g \,\mathrm{d}\mu$ for all $t > 0$ and $\mathscr{B}$-measurable functions g. The following lemma is well known in the case of strongly continuous semigroups on C_b, and is a prerequisite for the derivations in Section (4.3). Here, T is continuous only with respect to uniform convergence on compact subsets of $\mathbb{R}$, however, the fact that $D_{\mathcal{A}} = \mathrm{Ran}(G_\lambda)$ makes the result still hold.

Lemma 4.2.3. *A Radon measure is invariant for the semigroup T on C_b if and only if $\int_{\mathbb{R}} \mathcal{A}f \,\mathrm{d}\mu = 0$ for all $f \in D_{\mathcal{A}}$. In particular, the speed measure m is invariant.*

Proof. Let μ denote an arbitrary Radon measure and let $g \in C_b$. For $\lambda > 0$, consider $f_\lambda := G_\lambda g \in D_{\mathcal{A}}$. Then

$$\begin{aligned}
\int_{\mathbb{R}} \mathcal{A}f_\lambda(x) \,\mathrm{d}\mu(x) &= \int_{\mathbb{R}} (\lambda - G_\lambda^{-1}) f_\lambda(x) \,\mathrm{d}\mu(x) = \int_{\mathbb{R}} (\lambda G_\lambda g(x) - g(x)) \,\mathrm{d}\mu(x) \\
&= \int_{\mathbb{R}} \int_0^\infty (\lambda e^{-\lambda t} T_t g(x) - g(x)) \,\mathrm{d}t \,\mathrm{d}\mu(x) \\
&= \int_0^\infty \lambda e^{-\lambda t} \int_{\mathbb{R}} (T_t g(x) - g(x)) \,\mathrm{d}\mu(x) \,\mathrm{d}t, \quad \lambda > 0.
\end{aligned}$$

The by the uniqueness of the Laplace transform, μ is invariant if and only if $\int_{\mathbb{R}} \mathcal{A}f_\lambda(x) \,\mathrm{d}\mu(x) = 0$ for all $\lambda > 0$, $x \in \mathbb{R}$. Writing $\mu = m$ and using (4.27), one therefore also obtains

$$\begin{aligned}\int_{\mathbb{R}} \mathcal{A}f(x)\, m(\,\mathrm{d}x) &= \sum_{k\in\mathbb{Z}} \int_{I_k} \tfrac{1}{2} f''(x)\, m_k \,\mathrm{d}x \\ &= \sum_{k\in\mathbb{Z}} \tfrac{1}{2}(m_{k-1} f'(x_k^-) - m_k f'(x_k^+)) = 0.\end{aligned}$$

In particular the speed measure m is invariant for T. □

The following theorem characterizes the conditions for recurrence, positive recurrence and existence of an invariant probability measure.

Theorem 4.2.4. *The process $B^{\boldsymbol{\alpha}}$ is recurrent if and only if $s(\mathbb{R}^-) = s(\mathbb{R}^+) = \infty$. In the recurrent case, the following statements are equivalent: (i) $B^{\boldsymbol{\alpha}}$ is positive recurrent, (ii) $m(\mathbb{R}) < \infty$, (iii) ${}^{m}\!/_{m(\mathbb{R})}$ is the unique invariant probability measure for T, (iv) as $t \to \infty$, the transition probabilities $\mathbb{P}_x(B_t^{\boldsymbol{\alpha}} \in \cdot)$ converge weakly to ${}^{m}\!/_{m(\mathbb{R})}$ for all x, and (v) $\mathbb{E}_x(H_y) < \infty$ for all $x, y \in \mathbb{R}$.*

Proof. Consider the discrete process given by the consecutive visits of $B^{\boldsymbol{\alpha}}$ to distinct interfaces, namely, let $\eta_0 = \inf\{t \geqslant 0 : B_t^{\boldsymbol{\alpha}} \in S\}$, $Z_0 = B_0^{\boldsymbol{\alpha}}$ and define recursively

$$\eta_{n+1} = \inf\{t > \eta_n : B_t^{\boldsymbol{\alpha}} \in S \smallsetminus \{Z_n\}\}, \quad Z_n = B_{\eta_n}^{\boldsymbol{\alpha}}, \quad n \geqslant 0.$$

Let $K(n) \in \mathbb{Z}$ be such that $Z_n = x_{K(n)}$, then

$$\eta_{n+1} = \eta_n + E_{(x_{K(n)-1}, x_{K(n)+1})}(B^{\boldsymbol{\alpha}} \circ \theta \eta_n)$$

where for $t \geqslant 0$, θ_t is the shift operator, $\theta_t(\omega) = \theta(t + \cdot)$, $\omega \in \Omega$. The strong Markov property of $B^{\boldsymbol{\alpha}}$ gives that the process $Z = \{Z_n : n \geqslant 1\}$ is a Markov chain with values on S and transition probabilities and $n \geqslant 1$,

$$\mathbb{P}_x(Z_{n+1} = x_j \big| Z_n = x_k) = \begin{cases} \beta_k & j = k+1, \\ \\ 1 - \beta_k & j = k-1. \end{cases}, \quad x \in \mathbb{R},\ n \geqslant 0, \tag{4.28}$$

where

$$\beta_k := \frac{|I_{k-1}|s_{k-1}}{|I_k|s_k + |I_{k-1}|s_{k-1}} = \frac{|I_{k-1}|\alpha_k}{|I_k|(1-\alpha_k) + |I_{k-1}|\alpha_k}, \quad k \in \mathbb{Z}. \tag{4.29}$$

Also, $B^{\boldsymbol{\alpha}}$ is recurrent if and only if Z is recurrent. The theory of discrete time birth-death process (see for example Bhattacharya and Waymire, 1990b) gives that Z is recurrent if and only if

$$\sum_{k=1}^{\infty}\prod_{j=1}^{k}\frac{1-\beta_j}{\beta_j} = \frac{1}{|I_0|}\sum_{k=1}^{\infty} s_k|I_k| = \infty \quad \text{and} \quad \sum_{k=-\infty}^{0}\prod_{j=k}^{0}\frac{\beta_j}{1-\beta_j} = \frac{1}{|I_0|}\sum_{k=-\infty}^{0} s_k|I_k| = \infty. \tag{4.30}$$

To prove the equivalence between statements (i) to (iii) apply Lemma 23.19 of Kallenberg (2002) to the process $s(B^{\boldsymbol{\alpha}})$. Theorem IV.4.7 of Mandl (1968) gives $(ii) \Leftrightarrow (iv)$. Finally the equivalence between (i) and (v) follows from $\mathbb{E}_x H_y = \int_y^\infty m(x,\infty)\,\mathrm{d}z$, $x, y \in \mathbb{R}$ (Bhattacharya and Waymire, 1990b, p. 422). □

The following corollary indicates the role that the skewness $\boldsymbol{\alpha}$ and the separation between interfaces play in the recurrence properties of $B^{\boldsymbol{\alpha}}$.

Corollary 4.2.5. *Let $\{\beta_k : k \in \mathbb{Z}\}$ be as in (4.29), then $B^{\boldsymbol{\alpha}}$ is recurrent if,*

$$\liminf_{k\to\infty} \beta_k < \frac{1}{2} \quad \textit{and} \quad \limsup_{k\to-\infty} \beta_k > \frac{1}{2} \tag{4.31}$$

If in addition,

$$\frac{\alpha_k}{1-\alpha_k} < \frac{|I_{k-1}|}{|I_k|} \quad \textit{and} \quad \frac{1-\alpha_{-k}}{\alpha_{-k}} < \frac{|I_{-k}|}{|I_{-k-1}|} \tag{4.32}$$

for all but finitely many $k \in \mathbb{Z}$, then $B^{\boldsymbol{\alpha}}$ is positive recurrent.

Proof. Apply the ratio test to the conditions in (4.30) and to $\sum_{j=0}^{\pm\infty} m_k|I_k| < \infty$. □

4.3 The semigroup of $B^{\boldsymbol{\alpha}}$ in $L^2(\mathbb{R}, m)$

Our goal is to next extend the semigroup T to a semigroup $\boldsymbol{T}$ in the space $L^2_m := L^2(\mathbb{R}, m)$ and characterize its infinitesimal generator as this will be useful for the analysis in the next section. Throughout, boldface will be used to denote operators corresponding to L^2_m-extensions. Define

$$\boldsymbol{T}_t u(x) = \mathbb{E}_x u(B^{\boldsymbol{\alpha}}_t) = \int_{\mathbb{R}} u(y)\, \mathbb{P}_x(B^{\boldsymbol{\alpha}}_t \in \mathrm{d}y), \quad x \in \mathbb{R},\ u \in L^2_m,\ t \geqslant 0. \tag{4.33}$$

Using the invariance of m and Jensen's inequality gives

$$\int_{\mathbb{R}} [\mathbb{E}_x u(B^{\boldsymbol{\alpha}}_t)]^2 \,\mathrm{d}m(x) \leqslant \int_{\mathbb{R}} \mathbb{E}_x u^2(B^{\boldsymbol{\alpha}}_t)\,\mathrm{d}m(x) = \int_{\mathbb{R}} u^2 \,\mathrm{d}m,$$

so equation (4.33) makes sense for $u \in L^2_m$.

Recall that the semigroup T is strongly continuous in C_0 with respect to uniform convergence on $\mathbb{R}$. Therefore $C_0 \cap L^2_m$ is a dense subset of L^2_m contained in the center of T, that is $C_0 \cap L^2_m \subset \{f \in L^2_m : T_t f \xrightarrow{m} f \text{ as } t \downarrow 0\}$, where "$\xrightarrow{m}$" denotes convergence in the m measure. As in Ma and Röckner (1991, section II.4), equation (4.33) defines a strongly continuous contraction semigroup $\boldsymbol{T} := \{\boldsymbol{T}_t : t \geqslant 0\}$ on L^2_m. The infinitesimal generator $\boldsymbol{A}$ of $\boldsymbol{T}$ is a densely defined and closed operator in L^2_m; its domain $D_{\boldsymbol{A}}$ is given by the set of functions $u \in L^2_m$ such that $\boldsymbol{A}u := \lim_{t\to 0} \frac{1}{t}(\boldsymbol{T}_t u - u)$ exists in L^2_m. The resolvent of $\boldsymbol{T}$ is defined by the family of strongly continuous contractions $\boldsymbol{G}_\lambda := (\lambda - \boldsymbol{A})^{-1} : L^2_m \to D_{\boldsymbol{A}}$, $\lambda > 0$. The restriction of any of the boldface operators to C_b coincide with their analogues in Section (4.2.1). The following is probably well know, but the proof is included for completeness.

Lemma 4.3.1. *A function $u \in L^2_m$ belongs to $D_{\boldsymbol{A}}$ if and only if there is a sequence $\{f_n : n \geqslant 0\}$ in $D_{\mathcal{A}}$ such that $f_n \xrightarrow{L^2_m} u$ and $\mathcal{A} f_n \xrightarrow{L^2_m} h$, in this case $h = \boldsymbol{A}u$.*

Proof. Let $u \in D_{\boldsymbol{A}}$ and fix $\lambda > 0$, then there is $v \in L^2_m$ with $\boldsymbol{G}_\lambda v = u$. Consider a sequence $\{g_n : n \geqslant 0\}$ in C_b converging in L^2_m to v, and let $f_n := G_\lambda g_n \in D_{\mathcal{A}}$.

Since $\lambda \boldsymbol{G}_\lambda$ is a contraction, then $f_n \xrightarrow{L^2_m} u$. Now, $\mathcal{A} f_n = g_n + \lambda f_n$ and therefore $\mathcal{A} f_n$ converges in L^2_m. Since $\boldsymbol{A}$ is a closed operator, $\mathcal{A} f_n \xrightarrow{L^2_m} \boldsymbol{A} u$. □

In what follows, for $i \geqslant 0$, ∂^i will denote the i-th generalized derivative, and $H^i_m := H^i(\mathbb{R}, m)$ the usual Sobolev space of order i. For $k \in \mathbb{Z}$, the following notation will also be used: $L^2_{m_k} := L^2(I_k, m)$ and $H^i_{m_k} := H^i(I_k, m)$. Note that since m' is piecewise constant, $L^2_{m_k}$ and $H^i_{m_k}$ coincide with the corresponding spaces on I_k with respect to Lebesgue measure for each k.

Theorem 4.3.2. *The infinitesimal generator of $B^{\boldsymbol{\alpha}}$ in L^2_m is given by*

$$\boldsymbol{A} u = \sum_{k \in \mathbb{Z}} \tfrac{1}{2} \partial^2 (u \cdot \mathbb{1}_{I_k}), \quad u \in D_{\boldsymbol{A}}, \tag{4.34}$$

$$D_{\boldsymbol{A}} = \{ u \in H^1_m : \boldsymbol{A} u \in L^2_m \text{ and } \alpha_k \, \partial u(x_k^+) = (1 - \alpha_k) \, \partial u(x_k^-) \text{ for all } k \in \mathbb{Z} \}. \tag{4.35}$$

Proof. For $f \in D_{\mathcal{A}}$ the interface conditions in (4.27) give $m_k f'(x_k^+) = m_{k-1} f'(x_k^-)$, $k \in \mathbb{Z}$, and therefore

$$(-\mathcal{A} f, f)_{L^2_m} = \tfrac{1}{2} (f', f')_{L^2_m}. \tag{4.36}$$

Let $u \in D_{\boldsymbol{A}}$ and $\{f_n : n \geqslant 0\}$ as in Lemma (4.3.1). By the continuity of $\mathcal{A}$, applying (4.36) to $f_n - f_{n+1} \in D_{\mathcal{A}}$, gives that $\{f'_n : n \geqslant 0\}$ is a Cauchy sequence in L^2_m. For any $k \in \mathbb{Z}$, $\{f'_n : n \geqslant 0\}$ is also Cauchy in $L^2_{m_k}$, and since each f_n is twice continuously differentiable on $\bar{I}_k$, one then has that $u \in H^2_{m_k}$, $f'_n \xrightarrow{L^2_{m_k}} \partial u$ and $\frac{1}{2} f''_n \xrightarrow{L^2_{m_k}} \frac{1}{2} \partial^2 u = \boldsymbol{A} u$ on I_k (Showalter, 1994). This establishes (4.34).

In order to calculate $D_{\boldsymbol{A}}$, consider the sequence $\{f_n : n \geqslant 0\}$ defined above, and choose a subsequence of it (denoted again by f_n) such that $f_n \xrightarrow{a.e.} f$ and $\mathcal{A} f_n \xrightarrow{a.e.} \boldsymbol{A} u$ on $\mathbb{R}$. Fix $k \in \mathbb{Z}$, then $f''_n \xrightarrow{a.e.} \partial^2 u$ and $f'_n \xrightarrow{L^2_{m_k}} \partial u$ on I_k. Moreover, if $x \in I_k$ is such that $f_n(x) \to u(x)$, then

$$u(x) - u(x_k) = \int_{x_k}^{x} \partial u(y) \, \mathrm{d}y = \lim_{n \to \infty} \int_{x_k}^{x} f'_n(y) \, \mathrm{d}y = \lim_{n \to \infty} [f_n(x) - f_n(x_k)].$$

Therefore $f_n(x_k) - u(x_k)$ as $n \to \infty$, and u is absolutely continuous on all of $\mathbb{R}$. The jump condition on ∂u will now be established in a similar fashion. Fix $k \in \mathbb{Z}$, and consider a subsequence of $\{f_n : n \geqslant 0\}$ such that $f'_{n_j} \xrightarrow{a.e} \partial u$ on I_k. Choose $x \in I_k$ such that $f'_{n_j}(x) \to \partial u(x)$. Since $\partial^2 u$ is integrable in I_k, ∂u can be extended continuously to $\bar{I}_k$, e.g. $\partial u(x_k^+) := \lim_{\epsilon \downarrow 0}(\partial u(x) - \int_{x_k+\epsilon}^{x} \partial^2 u \, \mathrm{d}y)$, and we may write,

$$\partial u(x) - \partial u(x_k^+) = \int_{x_k}^{x} \partial^2 u(y) \, \mathrm{d}y = \lim_{j\to\infty} \int_{x_k}^{x} f''_{n_j}(y) \, \mathrm{d}y = \lim_{j\to\infty} [f'_{n_j}(x) - f'_{n_j}(x_k^+)],$$

so $f'_{n_j}(x_k^+) \to \partial u(x_k^+)$. A further subsequence $\{f_{n_{j_i}} : j \geqslant 0\}$ can now be chosen so the derivatives converge a.e. to ∂u on I_{k-1}. Applying the same reasoning as for I_k one gets that for such a subsequence $f'_{n_{j_i}}(x_k^+) \to \partial u(x_k^+)$ and $f'_{n_{j_i}}(x_k^-) \to \partial u(x_k^-)$ as $i \to \infty$. This gives $m_k \, \partial u(x_k^+) = m_{k-1} \, \partial u(x_k^-)$. The function ∂u can now be defined on all of $\mathbb{R}$ and integration by parts yields

$$(\boldsymbol{A}u, v)_{L^2_m} = \sum_{k\in\mathbb{Z}} (\tfrac{1}{2}\partial^2 u, v)_{L^2_{m_k}} = -\tfrac{1}{2}(\partial u, \partial v)_{L^2_m}, \quad u, v \in D_{\boldsymbol{A}}. \tag{4.37}$$

Applying (4.37) to u and $f_n - u$ gives $u \in H^1_m$ and $f_n \xrightarrow{H^1_m} u$.

If $\tilde{D}_{\boldsymbol{A}}$ denotes the set on the righthand side of (4.35), it has been proven so far that $D_{\boldsymbol{A}} \subseteq \tilde{D}_{\boldsymbol{A}}$. To prove the other inclusion one may make use of the one-to-one correspondence between infinitesimal generators of contraction semigroups and bilinear coercive forms. Consider the bilinear form on L^2_m defined by $\boldsymbol{A}$,

$$\mathcal{E}(u, v) := (-\boldsymbol{A}u, v)_{L^2_m} = \tfrac{1}{2}(\partial u, \partial v)_{L^2_m}, \quad u, v \in D_{\boldsymbol{A}}. \tag{4.38}$$

Since m assigns positive measure to every open set of $\mathbb{R}$, the form $\mathcal{E}(\cdot,\cdot)$ can be extended to a coercive closed form (also denoted by $\mathcal{E}$) with domain $D_{\mathcal{E}}$ and such that equation (4.38) holds for all $u \in D_{\boldsymbol{A}}$ and $v \in D_{\mathcal{E}}$ (Ma and Röckner, 1991, p 43). The domain $D_{\mathcal{E}}$ is given by the completion of $D_{\boldsymbol{A}}$ with respect to $\|\cdot\|_{H^1_m}$, and $\mathcal{E}$ on $D_{\mathcal{E}}$ is the unique bilinear extension of $\mathcal{E}$ on (4.38) that is continuous with respect to $\|\cdot\|_{H^1_m}$. To see that $D_{\mathcal{E}} = H^1_m$, assume there is $v \in H^1_m$ such that $(u, v)_{H^1_m} = 0$

for all $u \in D_{\boldsymbol{A}}$, then integration by parts gives

$$0 = (u, v)_{L^2_m} + (\partial u, \partial v)_{L^2_m} = 2(\tfrac{1}{2}u - \boldsymbol{A}u, v)_{L^2_m}, \quad \text{for all } u \in D_{\boldsymbol{A}}.$$

Since $(\frac{1}{2} - \boldsymbol{A}) = \boldsymbol{G}^{-1}_{1/2}$ is onto L^2_m, $v \equiv 0$. The domain of $\boldsymbol{A}$ is characterized in terms of $\mathcal{E}$ as

$$D_{\boldsymbol{A}} = \{u \in H^1_m : v \mapsto \mathcal{E}(u, v) \text{ is continuous w.r.t. } \|\cdot\|_{L^2_m} \text{ on } H^1_m\}. \tag{4.39}$$

Let $u \in \tilde{D}_{\boldsymbol{A}}$ and $v \in H^1_m$. Integration by parts can be carried out to obtain

$$\begin{aligned} |\mathcal{E}(u, v)| &= |(\partial u, \partial v)_{L^2_m}| \leqslant \sum_{k \in Z} |(-\partial^2 u, v)_{L^2_{m_k}}| \\ &\leqslant \sum_{k \in Z} \|\partial^2 u\|_{L^2_{m_k}} \|v\|_{L^2_{m_k}} \leqslant \|\boldsymbol{A}u\|_{L^2_m} \|v\|_{L^2_m}. \end{aligned}$$

Since $\boldsymbol{A}u \in L^2_m$, and by virtue of (4.39), $u \in D_{\boldsymbol{A}}$. ☐

Remark 4.3.3. A characterization of $\boldsymbol{A}$ on the Sobolev spaces with respect to Lebesgue measure is also possible. Note that from the proof of Theorem (4.3.2) if $u \in D_{\boldsymbol{A}}$, then $u\, m' \in L^2(\mathbb{R})$, u is absolutely continuous and its generalized derivative satisfies $m'\partial u \in L^2(\mathbb{R})$. Also, for any $x, y \in \mathbb{R}$,

$$\int_y^x \boldsymbol{A}u\, m(\,\mathrm{d}z) = \tfrac{1}{2}m'(x^-)\,\partial u(x^-) - \tfrac{1}{2}m'(y^+)\,\partial u(y^+),$$

which says that $m'\partial u$ is absolutely continuous and $\partial(m'\partial u) \in L^2(\mathbb{R})$. Therefore $u \in D_{\boldsymbol{A}}$ if and only if $m'\partial u \in H^1(\mathbb{R})$. Furthermore

$$\boldsymbol{A}u = \frac{1}{2m'}\,\partial(m'\,\partial u) = \frac{1}{m'}\,\partial\left(\frac{1}{s'}\,\partial u\right), \quad u \in D_{\boldsymbol{A}}. \tag{4.40}$$

4.4 Advection-diffusion in layered media

Consider a countable set of interfaces $\{z_k : k \in \mathbb{Z}\}$ with no accumulation points, and a sequence of positive numbers $\{D_k : k \in \mathbb{Z}\}$. Denote points in $\mathbb{R}^2$ by

$\boldsymbol{x} = (x, y)$ and let $J_k := (z_k, z_{k+1})$, $k \in \mathbb{Z}$. Our aim is to now relate multi-skew Brownian motion to the advection-diffusion equation in $\mathbb{R}^2$ with coefficients that are constant on sets of the form $J_k \times \mathbb{R}$. These sets will be referred to as "layers".

Suppose $\boldsymbol{D}$ is a two-dimensional diffusion coefficient that depends only on the x coordinate and has the form

$$\boldsymbol{D}(\boldsymbol{x}) = \begin{bmatrix} D_x(x) & 0 \\ 0 & D_y(x) \end{bmatrix}, \quad D_x(x) = \sum_{k\in\mathbb{Z}} D_k \mathbb{1}_{J_k}(x), \tag{4.41}$$

with D_x and D_y bounded away from zero on compact sets of $\mathbb{R}$, and bounded away from infinity everywhere. Furthermore, suppose $\boldsymbol{U}$ is a two-dimensional vector field of the form

$$\boldsymbol{U}(\boldsymbol{x}) = (0, U(x)) \tag{4.42}$$

such that ${}^{U}\!/\!\sqrt{D_y}$ is measurable and bounded away from infinity.

Suppose that $c(\boldsymbol{x}, t)$ satisfies Kolmogorov's forward equation,

$$\partial_t c = \nabla\cdot(\tfrac{1}{2}\boldsymbol{D}\,\nabla c) - \nabla\cdot(c\,\boldsymbol{U}), \tag{4.43}$$

where spatial derivatives are to be understood in the weak sense. Specifically, we look for $c \in C^0([0,\infty), H^1(\mathbb{R}^2)) \cap C^1([0,\infty), L^2(\mathbb{R}^2))$ such that for $t \geqslant 0$, and all u in the class of infinitely differentiable functions with compact support $C_c^\infty(\mathbb{R}^2)$,

$$\partial_t(u, c(t,\cdot))_{L^2(\mathbb{R}^2)} = -\boldsymbol{\mathcal{E}}(u, c(t,\cdot)), \tag{4.44}$$

where $\boldsymbol{\mathcal{E}}$ is the bilinear form naturally associated with (4.43),

$$\begin{aligned} \boldsymbol{\mathcal{E}}(u,v) &= -(u, \nabla\cdot(\tfrac{1}{2}\boldsymbol{D}\,\nabla v) - \nabla\cdot(v\,\boldsymbol{U}))_{L^2(\mathbb{R}^2)} \\ &= \int_{\mathbb{R}^2} \tfrac{1}{2}\boldsymbol{D}\nabla u\cdot\nabla v\,\mathrm{d}\boldsymbol{x} + \int_{\mathbb{R}} U \int_{\mathbb{R}} u\,\partial_y v\,\mathrm{d}y\,\mathrm{d}x, \quad u, v \in C_c^\infty(\mathbb{R}^2). \end{aligned} \tag{4.45}$$

The task is to now establish that $\boldsymbol{\mathcal{E}}(\cdot,\cdot)$ is a regular Dirichlet form on $L^2(\mathbb{R}^2)$ associated to a diffusion process in the sense of Ma and Röckner (1991). Note first that (4.42) gives $\boldsymbol{\mathcal{E}}(u,u) = \frac{1}{2}(\|\sqrt{D_x}\,\partial_x u\|^2_{L^2(\mathbb{R}^2)} + \|\sqrt{D_y}\,\partial_y u\|^2_{L^2(\mathbb{R}^2)})$, $u \in C_c^\infty(\mathbb{R}^2)$. Also, by Cauchy-Schwartz inequality, $\boldsymbol{\mathcal{E}}(\cdot,\cdot)$ satisfies the weak sector condition,

$$\begin{aligned} |\boldsymbol{\mathcal{E}}(u,v)| &\leqslant \boldsymbol{\mathcal{E}}(u,u)^{\frac{1}{2}}\,\boldsymbol{\mathcal{E}}(v,v)^{\frac{1}{2}} + \left\|\tfrac{U}{\sqrt{D_y}}\right\|_\infty \|\sqrt{D_y}\,\partial_y u\|_{L^2(\mathbb{R}^2)}\,\|v\|_{L^2(\mathbb{R}^2)} \\ &\leqslant C\left[\boldsymbol{\mathcal{E}}(u,u) + (u,u)_{L^2(\mathbb{R}^2)}\right]^{\frac{1}{2}}\left[\boldsymbol{\mathcal{E}}(v,v) + (v,v)_{L^2(\mathbb{R}^2)}\right]^{\frac{1}{2}} \end{aligned} \tag{4.46}$$

for $u, v \in C_c^\infty$ and some positive constant C. The closability of $\boldsymbol{\mathcal{E}}(\cdot,\cdot)$ and its contraction properties are established in the following lemma.

Lemma 4.4.1. *The form $\boldsymbol{\mathcal{E}}(\cdot,\cdot)$ in (4.45) extends uniquely to a regular and local Dirichlet form (also denoted by $\boldsymbol{\mathcal{E}}$) on $L^2(\mathbb{R}^2)$ with domain $D_{\boldsymbol{\mathcal{E}}} = L^2(\mathbb{R}^2) \cap H^1(\mathbb{R}^2, \boldsymbol{D})$, where $H^1(\mathbb{R}^2, \boldsymbol{D})$ denotes the Sobolev space of order one with respect to the measure $\mathrm{d}\boldsymbol{D}(\boldsymbol{x}) := D_x D_y\,\mathrm{d}\boldsymbol{x}$.*

Proof. Let $\{u_n : n \geqslant 0\} \subset C_c^\infty(\mathbb{R}^2)$ be a Cauchy sequence with respect to $\boldsymbol{\mathcal{E}}(\cdot,\cdot)$ such that $u_n \to 0$ in $L^2(\mathbb{R}^2)$. Therefore $\{\sqrt{D_x}\,\partial_x u_n : n \geqslant 0\}$ is a Cauchy sequence and $\partial_x u_n \to f_x$ for some f_x in $L^2(\mathbb{R}^2, D_x)$. Let $K \subset \mathbb{R}^2$ compact, and choose $c_K > 0$ be such that $D_x(x) > c_K$ for all $\boldsymbol{x} \in K$, then for any $u \in L^2(\mathbb{R}^2, D_x)$ Cauchy-Schwartz inequality gives

$$\int_K |u|\,\mathrm{d}\boldsymbol{x} = \int_K |u|\frac{1}{D_x}\,\mathrm{d}D_x \leqslant \frac{|K|}{c_K}\|u\|_{L^2(\mathbb{R}^2, D_x)},$$

and then $L^2(\mathbb{R}^2, D_x) \subseteq L^1_{loc}(\mathbb{R}^2)$. Therefore $\partial_x u_n \to f_x$ in $L^1_{loc}(\mathbb{R}^2)$. Let $v \in C_c^\infty(\mathbb{R}^2)$ and denote by K_v its support, then

$$\int_{\mathbb{R}^2} f_x\,v\,\mathrm{d}\boldsymbol{x} = \lim_{n\to\infty}\int_{K_v} \partial_x u_n\,v\,\mathrm{d}\boldsymbol{x} = -\lim_{n\to\infty}\int_{K_v} f_x\,\partial_x v\,\mathrm{d}\boldsymbol{x} = 0,$$

and so $f_x = 0$. An identical argument shows that $\partial_y u_n \to 0$ in $L^2(\mathbb{R}^2, D_y)$ and therefore $\boldsymbol{\mathcal{E}}(u_n, u_n) \to 0$, and $\boldsymbol{\mathcal{E}}(\cdot,\cdot)$ is closable. Since (4.46) holds, $\boldsymbol{\mathcal{E}}(\cdot,\cdot)$ can be uniquely extended to $D_{\boldsymbol{\mathcal{E}}}$, the completion of $C_c^\infty(\mathbb{R}^2)$ with respect to the norm $(\boldsymbol{\mathcal{E}}(\cdot,\cdot) + (\cdot,\cdot)_{L^2(\mathbb{R}^2)})^{\frac{1}{2}}$ (Ma and Röckner, 1991, Section I.3). This gives $D_{\boldsymbol{\mathcal{E}}} = L^2(\mathbb{R}^2) \cap H^1(\mathbb{R}^2, \boldsymbol{D})$. The contraction properties that make $(\boldsymbol{\mathcal{E}}, D_{\boldsymbol{\mathcal{E}}})$ a Dirichlet form follow from Ma and Röckner (1991, Section II.2.d). Also, $(\boldsymbol{\mathcal{E}}, D_{\boldsymbol{\mathcal{E}}})$ is regular, since $C_c^\infty(\mathbb{R}^2)$ is dense in $D_{\boldsymbol{\mathcal{E}}}$ with respect to the norms of $H^1(\mathbb{R}^2, \boldsymbol{D})$ and $L^\infty(\mathbb{R}^2)$. Finally $(\boldsymbol{\mathcal{E}}, D_{\boldsymbol{\mathcal{E}}})$ is local, since $\boldsymbol{\mathcal{E}}(u,v) = 0$ for any pair u and v with disjoint support. $\square$

By Ma and Röckner (1991, Theorem V.1.11), there exists a diffusion process $\boldsymbol{X} = \{\boldsymbol{X}_t : t \geqslant 0\}$ on $\mathbb{R}^2$ associated to $(\boldsymbol{\mathcal{E}}, D_{\boldsymbol{\mathcal{E}}})$. Namely, if $\boldsymbol{T}^{\boldsymbol{X}} = \{\boldsymbol{T}_t^{\boldsymbol{X}} : t \geqslant 0\}$ is the $L^2(\mathbb{R}^2)$-semigroup of $\boldsymbol{X}$ and $\boldsymbol{A}^{\boldsymbol{X}} : D_{\boldsymbol{A}^{\boldsymbol{X}}} \to L^2(\mathbb{R}^2)$ is its infinitesimal generator, then $\boldsymbol{\mathcal{E}}(u,v) = -(\boldsymbol{A}^{\boldsymbol{X}}u, v)_{L^2(\mathbb{R}^2)}$ for all $u \in D_{\boldsymbol{A}^{\boldsymbol{X}}}$, $v \in D_{\boldsymbol{\mathcal{E}}}$. Integration by parts in (4.45) gives

$$\boldsymbol{A}^{\boldsymbol{X}}u = \nabla\cdot(\tfrac{1}{2}\boldsymbol{D}\nabla u) + U\,\partial_y u, \quad u \in D_{\boldsymbol{A}^{\boldsymbol{X}}} = \{u \in D_{\boldsymbol{\mathcal{E}}} : \boldsymbol{D}\nabla u \in H^1(\mathbb{R}^2)\}. \tag{4.47}$$

The following results characterizes the process $\boldsymbol{X}$.

Theorem 4.4.2. *Let $\psi : \mathbb{R} \to \mathbb{R}$ be the piecewise continuous linear function with*

$$\psi(0) = 0,\ \partial_x\psi(x) = \sqrt{D_k}, \quad x \in I_k,\ k \in \mathbb{Z}, \tag{4.48}$$

and denote its inverse by $\varphi = \psi^{-1}$. Let $S = \{x_k = \varphi(z_k) : k \in \mathbb{Z}\}$ and consider the multi-skew Brownian motion $B^{\boldsymbol{\alpha}} = \{B_t^{\boldsymbol{\alpha}} : t \geqslant 0\}$ with interfaces in S and skewness $\boldsymbol{\alpha} = \{\alpha_k : k \in \mathbb{Z}\}$ given by

$$\alpha_k = \frac{\sqrt{D_k}}{\sqrt{D_k} + \sqrt{D_{k-1}}}, \quad k \in \mathbb{Z}. \tag{4.49}$$

Let $W = \{W_t : t \geqslant 0\}$ be a standard Brownian motion independent of $B^{\boldsymbol{\alpha}}$. Then the diffusion process $\boldsymbol{X}$ associated with the Dirichlet form $\boldsymbol{\mathcal{E}}$ in (4.45) has the form $\boldsymbol{X} = (X, Y) = \{(X_t, Y_t) : t \geqslant 0\}$, where

$$X_t = \psi(B_t^{\boldsymbol{\alpha}}), \quad t \geqslant 0 \tag{4.50}$$

and Y is the Itô process given by

$$\mathrm{d}Y_t = U(X_t)\,\mathrm{d}t + \sqrt{D_y(X_t)}\,\mathrm{d}W_t. \tag{4.51}$$

Proof. Use Theorem (4.2.1) to construct a multi-skew Brownian motion $(\Omega, \mathscr{F}, \{\mathbb{P}_x\}_{x\in\mathbb{R}}, B^{\boldsymbol{\alpha}})$ as in the statement of the theorem. By (4.15) one may choose the scale and speed measures of $B^{\boldsymbol{\alpha}}$ to be $m_k = \sqrt{D_k}$, $s_k = 2/\sqrt{D_k}$, $x \in I_k$. Since ψ is a one-to-one continuous function, $X = \psi(B^{\boldsymbol{\alpha}})$ is a regular diffusion with semigroup given by $\boldsymbol{T}^X_t u = \boldsymbol{T}_t(u \circ \psi)$, $t \geqslant 0$, $u \in L^2(\mathbb{R})$. The choice of ψ and m makes $\|u\|_{L^2(\mathbb{R})} = \|u \circ \psi\|_{L^2_m}$ and $\|\boldsymbol{T}^X_t u\|_{L^2(\mathbb{R})} = \|\boldsymbol{T}_t(u \circ \psi)\|_{L^2_m}$, therefore the semigroup $\boldsymbol{T}^X$ of X is indeed defined on $L^2(\mathbb{R})$. Let $(\boldsymbol{A}, D_{\boldsymbol{A}})$ be the generator of $B^{\boldsymbol{\alpha}}$ in L^2_m as in Theorem (4.3.2) and $(\boldsymbol{A}^X, D_{\boldsymbol{A}^X})$ be the generator of X on $L^2(\mathbb{R})$, then $D_{\boldsymbol{A}^X} = \{u \in L^2(\mathbb{R}) : u \circ \psi \in D_{\boldsymbol{A}}\}$. Now, the chain rule gives $\|u \circ \psi\|^2_{H^1_m} = \|u\|^2_{L^2(\mathbb{R})} + 2\|\partial_x u\|^2_{L^2(\mathbb{R}, 1/2 D_x)}$, and the choice of $\boldsymbol{\alpha}$ makes the jump condition $\alpha_k \partial_x (u \circ \psi)(x_k^+) = (1 - \alpha_k)\partial_x(u \circ \psi)(x_k^-)$ equivalent to the continuity of $D_x \partial_x u$ at z_k. Finally,

$$\boldsymbol{A}^X u(x) = \sum_{k\in\mathbb{Z}} \tfrac{1}{2}\partial_x^2((u \circ \psi) \cdot \mathbb{1}_{I_k})(\varphi(x)) = \sum_{k\in\mathbb{Z}} \tfrac{1}{2} D_k\, \partial_x^2 u(x) \cdot \mathbb{1}_{J_k}(x) = \partial_x(\tfrac{1}{2} D_x \partial_x u)(x), \tag{4.52}$$

with domain

$$D_{\boldsymbol{A}^X} = \{u \in L^2(\mathbb{R}) \cap H^1(\mathbb{R}, D_x) : D_x \partial_x u \in H^1(\mathbb{R})\}. \tag{4.53}$$

The characterization in (4.52, 4.53) gives that X is the diffusion process associated with the Dirichlet form $(\mathcal{E}^X, D_{\mathcal{E}^X})$ given by

$$\mathcal{E}^X(u, v) = \int_{\mathbb{R}} \tfrac{1}{2} D_x\, \partial_x u\, \partial_x v \,\mathrm{d}x, \quad D_{\mathcal{E}^X} = L^2(\mathbb{R}) \cap H_1(\mathbb{R}, D_x). \tag{4.54}$$

Let W be standard Brownian motion independent of $B^{\boldsymbol{\alpha}}$, and let $\{\mathbb{P}_{\boldsymbol{x}}\}_{\boldsymbol{x}\in\mathbb{R}^2}$ be the family of probability measures generated by the process $(B^{\boldsymbol{\alpha}}, W)$ on the two dimensional Wiener space $(\boldsymbol{\Omega}, \boldsymbol{\mathcal{F}})$. The proof is finished by establishing that $\boldsymbol{X} := (X, Y)$, with X constructed above and Y defined as in (4.51), solves the martingale problem for the operator $\boldsymbol{A}^{\boldsymbol{X}}$ in (4.47) under $\mathbb{P}_{\boldsymbol{x}}$ for all $\boldsymbol{x} \in \mathbb{R}^2$. This is proven in Ramirez et al. (2006, Lemma 2.3) for the case of D_x, D_y bounded away from zero. A localization argument, i.e., Stroock and Varadhan (1979, Theorem 6.6.1), guarantees that this argument can be carried on without change to the case of $\boldsymbol{D}$ in (4.41). $\square$

Remark 4.4.3. In general, the construction of a diffusion from a local Dirichlet form must be done on the one-point compactification of the sample space, as to include the possibility of explosion of the process in finite time. In the case of $\boldsymbol{X}$, the decomposition $\boldsymbol{X} = (X, Y)$ allows one to a-posteriori rule out this possibility. To see this, first note that Feller's criteria for explosion of regular diffusions gives that $\{\infty\}$ is inaccessible for X (see Kallenberg, 2002, Theorem 23.12). One the other hand, $\mathbb{P}_{\boldsymbol{x}}$-a.s.

$$|Y_t - Y_0| \leqslant \|U\|_{L^\infty(\mathbb{R})} t + \sqrt{\|D\|_{L^\infty(\mathbb{R})}}\, |W_t|, \quad t \geqslant 0,$$

and the process in the right hand side does not explode in finite time.

Remark 4.4.4. The condition of no accumulation points on the interfaces $\{z_k : k \in \mathbb{Z}\}$ can be relaxed. In particular, if $z_k \uparrow b$ as $k \to \infty$ and $z_k \downarrow a$ as $k \to -\infty$ for some $a < b$, the construction $\boldsymbol{X} = \psi(B_t^{\boldsymbol{\alpha}})$ can be carried on $(a, b) \times \mathbb{R}$, under the condition $|z_{k+1} - z_k| > \delta\sqrt{2D_k}$ for some $\delta > 0$, so the interfaces $\{x_k : k \in \mathbb{Z}\}$ have no accumulation point.

Note that even in the case of a finite state space described in Remark (4.4.4), the process X cannot have an invariant probability measure. To see this, note that its generator $\boldsymbol{A}^X$ is a self-adjoint operator, and the unique solution to $\boldsymbol{A}^X v = 0$ is the piecewise function with $\partial_x v = \frac{1}{D_k}$ on J_k, $k \in \mathbb{Z}$. On the other hand, since $|J_k| > \delta\sqrt{2D_k}$ must hold, the invariant measure for X will be finite if and only if $\delta \sum_{k=0}^{\pm\infty} \frac{1}{\sqrt{D_k}} < \sum_{k=0}^{\pm\infty} \frac{|J_k|}{D_k} < \infty$, which violates the boundedness of D_x. In the case of finite state space and finite number of layers, ergodicity is possible when reflecting boundaries are introduced, and in particular, a central limit theorem (i.e., the Taylor-Aris formula for effective dispersion) for the two dimensional process $\boldsymbol{X}$ can be obtained (see Ramirez et al., 2006).

4.5 Example: a geometry with alternating layers.

We now consider a periodic arrangement of layers with alternating widths, and exploit the symmetries of the medium to establish some properties of the associated diffusion process. As in Section (4.4), consider interfaces $\{z_k : k \in \mathbb{Z}\}$ and let $J_k = (z_{k+1} - z_k)$. Let $z_0 = 0$ and assume $l_1 := z_{2k} - z_{2k-1}$, $l_2 := z_{2k+1} - z_{2k}$ for all $k \in \mathbb{Z}$. Let M_1 and M_2 denote the union of all odd and all even layers respectively,

$$M_1 := \bigcup_{k\in\mathbb{Z}} J_{2k+1} \quad M_2 := \bigcup_{k\in\mathbb{Z}} J_{2k},$$

For $\boldsymbol{D}$ and $\boldsymbol{U}$ defined in (4.41) and (4.42), assume there are $D_2 > D_1 > 0$ and $U_2 > U_1 > 0$ with (see Figure 4.1)

$$D_x(\boldsymbol{x}) = D_y(\boldsymbol{x}) = D_1 \mathbb{1}_{M_1}(x) + D_2 \mathbb{1}_{M_2}(x), \quad U(\boldsymbol{x}) = U_1 \mathbb{1}_{M_1}(x) + U_2 \mathbb{1}_{M_2}(x), \quad \boldsymbol{x} \in \mathbb{R}^2. \tag{4.55}$$

Let $(\boldsymbol{\Omega}, \boldsymbol{\mathcal{F}}, \{\mathbb{P}_{\boldsymbol{x}}\}_{\boldsymbol{x}\in\mathbb{R}^2}, \boldsymbol{X})$ be the diffusion constructed in Theorem (4.4.2) with $\boldsymbol{U}$ and $\boldsymbol{D}$ given by (4.55). Therefore,

$$\boldsymbol{X}_t = (X_t, Y_t), \quad X_t = \psi(B_t^{\boldsymbol{\alpha}}), \quad \mathrm{d}Y_t = U(X_t)\,\mathrm{d}t + \sqrt{D_y(X_t)}\,\mathrm{d}W_t, \quad t \geqslant 0, \tag{4.56}$$

where ψ is given in equation (4.48), W is a standard Brownian motion independent of X, and $B^{\boldsymbol{\alpha}}$ is a multi-skew Brownian motion with interfaces $S = \{x_k = \varphi(z_k) : k \in Z\}$, $\varphi := \psi^{-1}$, and skewness $\boldsymbol{\alpha}$ with values

$$\alpha_{2k} = \frac{\sqrt{D_2}}{\sqrt{D_2} + \sqrt{D_1}} := \alpha, \quad \alpha_{2k-1} = \frac{\sqrt{D_1}}{\sqrt{D_2} + \sqrt{D_1}} = 1 - \alpha, \quad k \in \mathbb{Z}.$$

By Theorem (4.2.1), the process $B^{\boldsymbol{\alpha}}$ is given by a scaling of standard Brownian motion B under a random time change. The speed and scale measures of $B^{\boldsymbol{\alpha}}$ have densities with values $m_i = \sqrt{D_i}$, $s_i = {}^2\!/\!\sqrt{D_i}$ on $\varphi(M_i)$, $i = 1, 2$. Below we state the main result of this section.

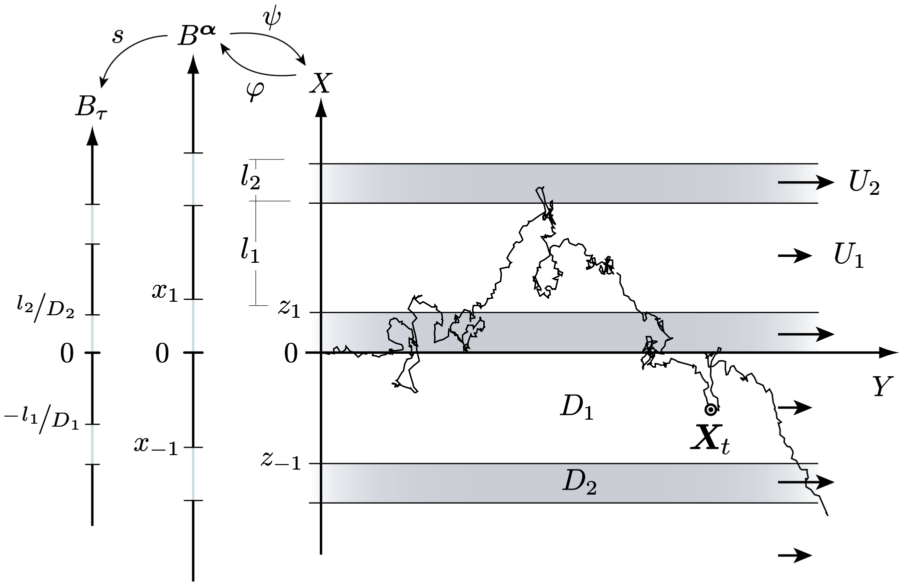

Figure 4.1: Advection-diffusion in a periodic layered media and the process $X = \psi(B^{\boldsymbol{\alpha}})$

Theorem 4.5.1. *Let* $\boldsymbol{X} = (X, Y)$ *be as in (4.56), then (i)*

$$\lim_{t\to\infty} \frac{1}{t}\, \mathbb{E}_0 X_t = 0, \quad \lim_{t\to\infty} \frac{1}{t}\, \mathbb{E}_0 X_t^2 = \frac{D_2 D_1 (l_2 + l_1)}{l_2 D_1 + l_1 D_2}. \tag{4.57}$$

(ii) Y *satisfies the following central limit theorem: As* $n \to \infty$*, the distribution of* $\{{}^1/\!\sqrt{n}\, Y_{\lfloor nt \rfloor} : t \geqslant 0\}$ *converges weakly to the Wiener measure with "effective" drift and diffusion coefficient given by*

$$U_{\mathit{eff}} = \frac{U_2 l_2 + U_1 l_1}{l_2 + l_1}, \quad D_{\mathit{eff}} = \frac{D_2 l_2 + D_1 l_1}{l_2 + l_1} + \frac{l_1^2 l_2^2 (U_2 - U_1)^2}{3(l_1 + l_2)^2} \left(\frac{l_1}{D_1} + \frac{l_2}{D_2} \right). \tag{4.58}$$

For ease of exposition, the proof will be given in two parts. First we consider equation (4.57). The central limit theorem in *(ii)* will be proved near the end of this section.

Proof of part (i) of Theorem (4.5.1). Consider the discrete process tracking the visits of X to the interfaces as in the proof of Theorem (4.2.4). Let $X_0 = Z_0 = 0$,

$\eta_0 = 0$ and define recursively

$$\eta_{n+1} = \inf\big\{t > \eta_n : X_t \in \{z_k : k \in \mathbb{Z}\} \smallsetminus \{Z_n\}\big\}, \quad Z_n = X_{\eta_n}, \quad n \geqslant 0. \tag{4.59}$$

The symmetry of the arrangement of layers makes $\{\eta_{n+1} - \eta_n : n \geqslant 0\}$ a sequence of i.i.d. positive random variables with the same distribution as $E^X_{(-l_1,l_2)}$ under $\mathbb{P}_0$. The process Z is a Markov chain with values on $\{z_k : k \in \mathbb{Z}\}$ and transition probabilities determined by the scale measure of B^α. Moreover, the increments $\{Z_{2(n+1)} - Z_{2n} : n \geqslant 0\}$ form a sequence of i.i.d. random variables with

$$Z_{2(n+1)} - Z_{2n} = \begin{cases} 0 & \text{w.p. } \beta^2 + (1-\beta)^2, \\ l_1 + l_2 & \text{w.p. } \beta(1-\beta), \\ -l_1 - l_2 & \text{w.p. } \beta(1-\beta), \end{cases} \quad , \quad \beta := \frac{l_1 D_2}{l_2 D_1 + l_1 D_2}. \tag{4.60}$$

Consider the renewal process $\{N(t) : t \geqslant 0\}$ given by

$$N(t) = \sup\{n \geqslant 0 : \eta_{2n} < t\}. \tag{4.61}$$

One then has the following decomposition

$$X_t = \sum_{n=1}^{N(t)} (Z_{2n} - Z_{2(n-1)}) + (X_t - X_{\eta_{2N(t)}}), \quad t \geqslant 0. \tag{4.62}$$

Since $\mathbb{E}_0(Z_{2n} - Z_{2(n-1)}) = 0$ for all n, and the process Z is independent of N, the strong law of large numbers can be used to calculate the asymptotic variance of X,

$$\lim_{t\to\infty} \frac{\mathbb{E}_0 X_t^2}{t} = \mathbb{E}_0(Z_2 - Z_0)^2 \left[\lim_{t\to\infty} \frac{\mathbb{E}_0 N(t)}{t}\right] = \frac{\mathbb{E}_0(Z_2 - Z_0)^2}{2\,\mathbb{E}_0(E^X_{(-l_1,l_2)})} = \frac{D_2 D_1 (l_2 + l_1)}{l_2 D_1 + l_1 D_2}. \tag{4.63}$$

$\square$

We now turn our attention to the transversal process Y and its asymptotic behavior described in (4.58). Is evident that Y is determined by the time the process X spends on M_1 and M_2 respectively. To this effect we prove first the following slightly general but elementary result.

Proposition 4.5.2. *Let (a,b) be an interval, $-\infty \leqslant a < b \leqslant \infty$, and assume A_1 are A_2 disjoint sets with $(a,b) = A_1 \cup A_2$. Consider the measure $\tilde{m}$ with density $\tilde{m}' = m_1 \mathbb{1}_{A_1} + m_2 \mathbb{1}_{A_2}$, with $m_1 > m_2 > 0$ and $\tilde{m}(\{a\}) = \tilde{m}(\{b\}) = 0$. Let B be Brownian motion reflecting at the finite endpoints of (a,b) (if any), and denote by L its local time family. Define $\phi(r) := \int_a^b L(x,r)\,\mathrm{d}\tilde{m}(x)$ and $\tau = \phi^{-1}$. Consider the process $\tilde{X}_t = B_{\tau(t)}$, $t \geqslant 0$, then $\mathbb{P}_x$-a.s. for any $x \in (a,b)$,*

$$O^{\tilde{X}}_{A_1}(t) = \frac{1}{m_1 - m_2}\left(m_1 t - \frac{m_1 m_2}{2}\tau(t)\right), \quad O^{\tilde{X}}_{A_2}(t) = \frac{1}{m_1 - m_2}\left(\frac{m_1 m_2}{2}\tau(t) - m_2 t\right). \tag{4.64}$$

Proof. The process $\tilde{X}$ is a regular diffusion in natural scale with speed measure $\tilde{m}$ (Breiman, 1992, p. 373). Moreover by the occupation times formula (4.7), $\phi(r) = \frac{m_1}{2} O^B_{A_1}(t) + \frac{m_2}{2} O^B_{A_2}(t)$. Perform a change of variables to write

$$O^{\tilde{X}}_{A_i}(t) = \int_0^t \mathbb{1}_{A_i}(B_{\tau(u)})\,\mathrm{d}u = \int_0^{\tau(t)} \mathbb{1}_{A_i}(B_u)\,\phi'(u)\,\mathrm{d}u = \frac{m_i}{2} O^B_{A_i}(\tau(t)), \quad i = 1, 2. \tag{4.65}$$

Therefore, the following system of equations holds true with probability one for all $t \geqslant 0$,

$$\frac{2}{m_1} O^{\tilde{X}}_{A_1}(t) + \frac{2}{m_2} O^{\tilde{X}}_{A_2}(t) = \tau(t), \quad O^{\tilde{X}}_{A_1}(t) + O^{\tilde{X}}_{A_2}(t) = t. \tag{4.66}$$

Solving gives (4.64). ☐

Decompose the stochastic integral in (4.56) as

$$\begin{aligned} Y_t &= U_1 O^X_{M_1}(t) + U_2 O^X_{M_2}(t) + \sqrt{D_1} \int_0^t \mathbb{1}_{M_1}(X_s)\,\mathrm{d}W_s + \sqrt{D_2} \int_0^t \mathbb{1}_{M_2}(X_s)\,\mathrm{d}W_s \\ &:= Y^U(t) + \sqrt{D_1}\, Y^{D_1}(t) + \sqrt{D_2}\, Y^{D_2}(t). \end{aligned} \tag{4.67}$$

The martingales Y^{D_1} and Y^{D_2} satisfy

$$\langle Y^{D_1} \rangle = O^X_{M_1}, \quad \langle Y^{D_2} \rangle = O^X_{M_2}, \quad \langle Y^{D_1}, Y^{D_2} \rangle = 0,$$

where $\langle\cdot\rangle$, and $\langle\cdot,\cdot\rangle$ denote the quadratic and cross variation processes respectively. By Knight's theorem (see Revuz and Yor, 1991, p. 172), there exist two independent Brownian motions $W^{(1)}$ and $W^{(2)}$ such that

$$\big(W^{(1)}(t), W^{(2)}(t)\big) = \big(Y^{D_1}(\tau^{(1)}(t)), Y^{D_2}(\tau^{(2)}(t))\big)\,, \quad t \geqslant 0,$$

where $\tau^{(2)}$ and $\tau^{(2)}$ denote the time changes associated with the additive functionals $O^X_{M_2}$ and $O^X_{M_1}$ respectively. One can therefore write Y in terms of occupation times for X as,

$$Y_t = U_1 O^X_{M_1}(t) + U_2 O^X_{M_2}(t) + \sqrt{D_1}\; W^{(1)}(O^X_{M_1}(t)) + \sqrt{D_2}\; W^{(2)}(O^X_{M_2}(t)). \tag{4.68}$$

Recall that the process $s(B^{\boldsymbol{\alpha}})$ is on natural scale and has speed measure taking values ${}^{m_i}\!/_{s_i} = {}^{D_i}\!/_{2}$ on $s(\varphi(M_i))$, $i = 1, 2$. Therefore, there exists a Brownian motion B, such that

$$X_t = \psi(B^{\boldsymbol{\alpha}}_t) = \psi \circ s^{-1}(B_{\tau(t)}), \quad t \geqslant 0, \tag{4.69}$$

with τ being the time change associated with

$$\phi(r) = \tfrac{1}{4} D_1 O^B_{s(\varphi(M_1))}(r) + \tfrac{1}{4} D_2 O^B_{s(\varphi(M_2))}(r), \quad r \geqslant 0.$$

Denote with tilde the image of sets under $s \circ \varphi$, namely $\tilde{A} := s(\varphi(A))$, $A \subseteq \mathbb{R}$. Proposition (4.5.2) gives then

$$O^X_{M_2}(t) = O^{B_\tau}_{\tilde{M}_2}(t) = \tfrac{1}{4} D_2 O^B_{\tilde{M}_2}(\tau(t)) = \frac{D_2 t - \frac{1}{4} D_2 D_1\, \tau(t)}{D_2 - D_1}, \quad t \geqslant 0, \tag{4.70}$$

and similarly for $O^X_{M_1}$.

The asymptotic behavior of Y will follow from (4.70) and the results in Ramirez et al. (2006) applied to a process $\bar{\boldsymbol{X}} = (\bar{X}, \bar{Y})$ related to $\boldsymbol{X}$, where now $\bar{X}$ is ergodic. Denote $\tilde{l}_1 := {}^{2l_1}\!/_{D_1}$, $\tilde{l}_2 := {}^{2l_2}\!/_{D_2}$.

Lemma 4.5.3. *Let B be Brownian motion on $\mathbb{R}$ and consider the map*

$$\sigma(x) := \tfrac{1}{2}\tilde{l}_2 - \left| \Big[(x + \tfrac{1}{2}\tilde{l}_1) \mod (\tilde{l}_1 + \tilde{l}_2) \Big] - \tfrac{1}{2}(\tilde{l}_1 + \tilde{l}_2) \right|, \quad x \in \mathbb{R}. \tag{4.71}$$

Then $\bar{B} := \{\sigma(B_t),\ t \geqslant 0\}$ *is reflected Brownian motion on* $({}^{-\tilde{l}_1}\!/_2, {}^{\tilde{l}_2}\!/_2)$*. Moreover, the map* σ *preserves occupation times, namely*

$$O^{\bar{B}}_{(0,\frac{1}{2}\tilde{l}_2)}(t) = O^{B}_{\tilde{M}_2}(t), \quad O^{\bar{B}}_{(-\frac{1}{2}\tilde{l}_1,0)}(t) = O^{B}_{\tilde{M}_1}(t), \quad t \geqslant 0. \tag{4.72}$$

Proof. That $\bar{B}$ is reflected Brownian motion follows from explicitly calculating its family of transition probability densities (see Bhattacharya and Waymire, 1990b, p. 400). Finally, note that if $x \in \tilde{C}$, then $x \in (k(\tilde{l}_1 + \tilde{l}_2), k(\tilde{l}_1 + \tilde{l}_2) + \tilde{l}_{M_2})$ for some $k \in \mathbb{Z}$, and therefore $\sigma(x) \in (0, {}^{\tilde{l}_2}\!/_2)$. Similarly for $x \in \tilde{M}_1$. $\square$

Proof of part (ii) of Theorem (4.5.1). Consider a skew diffusion $\bar{X}$ in $\bar{J} := ({}^{-l_1}\!/_2, {}^{l_2}\!/_2)$ with instantaneous reflection at the endpoints and diffusion coefficient given by ${}^1\!/_2 D_1 \mathbb{1}_{(-l_1/2,0)} + {}^1\!/_2 D_2 \mathbb{1}_{(0,l_2/2)}$ (Ramirez et al., 2006). Then $\bar{X}$ can be constructed as a scaling of $\bar{B}$ under a random time change (Breiman, 1992, p. 373). Let $\bar{m}$, $\bar{s}$ and $\bar{\psi}$ be given by the restrictions of m, s and ψ to $s^{-1}(\bar{J})$, with $\bar{m}(\{{}^{\tilde{l}_2}\!/_2\}) = \bar{m}(\{-{}^{\tilde{l}_1}\!/_2\}) = 0$. As usual, let $\bar{\phi} := \frac{1}{4} D_1 O^{\bar{B}}_{(-l_1/2,0)} + \frac{1}{4} D_2 O^{\bar{B}}_{(0,l_2/2)}$ and $\bar{\tau} := \bar{\phi}^{-1}$, then $\bar{X} = \bar{\psi} \circ \bar{s}^{-1}(\bar{B}_{\bar{\tau}})$. By (4.72), $\phi(r) = \bar{\phi}(r)$ for all r and therefore $\tau = \bar{\tau}$. Since proposition (4.65) applied to $\bar{X}$ gives an identical equation to (4.70) for the bar processes, we have

$$O^{X}_{M_2}(t) = O^{\bar{X}}_{(0,l_2/2)}(t), \quad O^{X}_{M_1}(t) = O^{\bar{X}}_{(-l_1/2,0)}(t), \quad t \geqslant 0. \tag{4.73}$$

Finally, construct a two-dimensional process $\bar{\boldsymbol{X}} = (\bar{X}, \bar{Y})$ on $\bar{J} \times \mathbb{R}$, with

$$\mathrm{d}\bar{Y}_t = U(\bar{X}_t)\,\mathrm{d}t + \sqrt{D_y(\bar{X}_t)}\,\mathrm{d}W_t, \quad t \geqslant 0.$$

As in (4.68), a decomposition of $\bar{Y}$ in terms of the occupation times $({}^{-l_1}\!/_2, 0)$ and $(0, {}^{l_2}\!/_2)$ by $\bar{X}$ is possible. Equation (4.73) gives then that $Y \overset{d}{=} \bar{Y}$ under $\mathbb{P}_0$. The result follows by applying Ramirez et al. (2006, corollary 2.2) to the process $\bar{\boldsymbol{X}}$. $\square$

Some further information about the pre-asymptotic behavior of Y (in particular, of Y^U in (4.67)) can be obtained using the discrete process Z in (4.59) (see also

Proposition (4.5.2)). Note first that the distribution of the time a particle spends in M_1 between consecutive visits to the interfaces has density

$$\mathbb{P}_{Z_n}\big(O^X_{M_1}(\eta_{n+1})-O^X_{M_1}(\eta_n)\in \mathrm{d}s\big)=\mathbb{P}_{z_k}\big(O^X_{M_1}(E^X_{(z_{k-1},z_{k+1})})\in \mathrm{d}s\big),\quad s>0, n\geqslant 0, k\in\mathbb{Z},$$

and similarly for the set M_2. Fix $k=0$, and make $J := J_{-1}\cup J_0 = (-l_1, l_2)$, $\tilde{J}=s(\varphi(J))$. Let B the Brownian motion in (4.69), since $E^X_J=\phi\big(E^B_{\tilde{J}}\big)$ $\mathbb{P}_x$-a.s. for any $x\in J$, then equation (4.65) gives

$$O^X_{M_2}(E^X_J)=O^{B_\tau}_{\tilde{J}_0}\big(E^{B_\tau}_{\tilde{J}}\big)=\tfrac{1}{4}D_2 O^B_{\tilde{J}_0}\big(E^B_{\tilde{J}}\big), \tag{4.74}$$

and similarly for $O^X_{M_1}(E^X_J)$. For $i=1,2$, let $\{T^{(i)}_j : j\geqslant 1\}$ be a sequence of i.i.d. random variables distributed as $O^X_{M_i}(E^X_J)$ under $\mathbb{P}_0$. Therefore we have the following equalities in $\mathbb{P}_0$ distribution

$$\begin{aligned} Y^U_{\eta_n} &\overset{d}{=} \sum_{j=1}^{n} U_2T^{(2)}_j+U_1T^{(1)}_j \quad n\geqslant 1, && (4.75)\\ U_2T^{(2)}_j+U_1T^{(1)}_j &\overset{d}{=} \int_0^{E^B_{\tilde{J}}} \tfrac{1}{4}U_1D_1\,\mathbb{1}_{\tilde{J}_{-1}}(B_s)+\tfrac{1}{4}U_2D_2\,\mathbb{1}_{\tilde{J}_0}(B_s)\,\mathrm{d}s, \quad j\geqslant 1. && (4.76)\end{aligned}$$

The moment generating function for the additive functional in (4.76) can be calculated using the Feynman-Kac formula to get

$$\mathbb{E}_0(e^{-\lambda Y^U_{\eta_n}})=\left[\frac{\sinh(\sqrt{\lambda l_1 \mathrm{P}_1})\sqrt{D_2U_2}+\sinh(\sqrt{\lambda l_2\mathrm{P}_2})\sqrt{D_1U_1}}{\cosh(\sqrt{\lambda l_2\mathrm{P}_2})\sinh(\sqrt{\lambda l_1\mathrm{P}_1})\sqrt{D_2U_2}+\cosh(\sqrt{\lambda l_1\mathrm{P}_1})\sinh(\sqrt{\lambda l_2\mathrm{P}_2})\sqrt{D_1U_1}}\right]^n \tag{4.77}$$

where $\mathrm{P}_i := {}^{2l_iU_i}/_{D_i}$, $i=1,2$.

Remark 4.5.4. As suggested by the notation above and in Section (4.4), $c(t,\boldsymbol{x})$ in (4.43) is a model for the concentration of a solute undergoing diffusion-advection in a medium with diffusion tensor $\frac{1}{2}\boldsymbol{D}$, immersed in a fluid moving with velocity (advection) $\boldsymbol{U}$. The process $\boldsymbol{X}$ is then a model for the motion of individual particles. The physical motivation for the results above come from seeking understanding of the effect that sharp discontinuities in $\boldsymbol{D}$ and $\boldsymbol{U}$ have on the motion of particles. For instance, the example described by (4.55), is an idealization of a medium composed mainly of a matrix where transport is slow and mostly due to diffusion, dissected by fissures or cracks where fast advective transport dominates. That is, $\mathrm{P}_2 \gg \mathrm{P}_1$ where the dimensionless $\mathrm{P}_i := {}^{2l_iU_i}/_{D_i}$, $i = 1, 2$ is called the Péclet number in physical applications. In such a case, for large t, $Y^U(t) \gg \sqrt{D_i}\, Y^{D_i}(t)$ for $i = 1, 2$, and equation (4.77) gives then an approximation to the moment generating function of Y in terms of the important physical properties of the medium.

As a final application of proposition (4.5.2) we give a straightforward proof of an "arcsine" law for skew Brownian motion. This result was obtained in Barlow et al. (1989) using techniques from the theory of excursions applied in the context of Brownian motion in graphs with a single vertex (of which skew Brownian motion is a special case).

Corollary 4.5.5. *Assume $\alpha > \frac{1}{2}$ and let $(\Omega, \mathscr{F}, \{\mathbb{P}_x\}_{x\in\mathbb{R}}, B^\alpha)$ be skew Brownian motion, then*

$$\mathbb{P}_0\big(O^{\alpha}_{(-\infty,0)}(t) \in \mathrm{d}u\big) = \frac{\alpha(1-\alpha)t}{(1-\alpha)^2(t-u)+\alpha^2 u}\, \frac{\mathrm{d}u}{\pi\sqrt{u}\sqrt{t-u}}, \qquad u \in (0, t). \tag{4.78}$$

Moreover, $\mathbb{E}_0 O^{\alpha}_{(-\infty,0)}(t) = (1-\alpha)t$ and $\mathbb{E}_0 O^{\alpha}_{[0,\infty)}(t) = \alpha t$.

Proof. In the notation of (4.5.2), let $A_1 = [0, \infty)$ and $A_2 = (-\infty, 0)$. Then $\phi(r)$ has the arcsine distribution on $({}^{m_2 r}/_2, {}^{m_1 r}/_2)$, and one can obtain the distribution of τ by writing $\mathbb{P}_0(\tau(t) \in \mathrm{d}r) = \frac{\mathrm{d}}{\mathrm{d}r}\mathbb{P}_0(\tau(t) \leqslant r) = \frac{\mathrm{d}}{\mathrm{d}r}\mathbb{P}_0(t \leqslant \phi(r))$,

$$\mathbb{P}_0(\tau(t) \in \mathrm{d}r) = \frac{2t}{\pi\sqrt{m_1 m_2}}\, \frac{\mathrm{d}r}{r\sqrt{r - \frac{2t}{m_1}}\sqrt{\frac{2t}{m_2} - r}}, \qquad r \in \left(\tfrac{2t}{m_1}, \tfrac{2t}{m_2}\right). \tag{4.79}$$

Finally, apply the linear transformation in (4.64) to get

$$\mathbb{P}_0\big(O^{\tilde{X}}_{(-\infty,0)}(t) \in \mathrm{d}u\big) = \frac{\sqrt{m_1 m_2}\, t}{m_2(t-u)+m_1 u}\, \frac{\mathrm{d}u}{\pi\sqrt{u}\sqrt{t-u}}, \qquad u \in (0, t). \tag{4.80}$$

The result for skew Brownian motion, follows by making $m_1 = 2\alpha^2$, $m_2 = 2(1-\alpha)^2$.

□

5 GENERAL CONCLUSION

This thesis studied a collection of stochastic processes and their associated partial differential equations (PDEs) arising from models of diffusion and fluid flow. Numerical methods for one-dimensional diffusion equation with a potential, and viscous Burgers equation are considered in Part (2). Part (3) establishes a homogenization result for the advection-diffusion equation on a cylinder under mild conditions on the diffusion coefficient and flow velocity. Finally, Part (4) studies a stochastic process associated with the one-dimensional diffusion equation in the case where the diffusion coefficient is piecewise constant with a countable set of discontinuities. In each instance, the properties of the stochastic process are used to study properties of the PDE, and vice versa.

During the process of preparation of this work many interesting questions were raised and a lot of them remain unsolved. Below, I elaborate on some of the more important open problems and avenues of research that I believe might be worthwhile following.

In Chorin and Hald (2005), analytical methods are used to obtain a stationary solution u to the viscous Burgers equation (2.22) on $\mathbb{R}$ and its Fourier transform $\hat{u}(k)$, $k \in \mathbb{R}$. More significantly, the authors consider the energy spectrum $E(k) := \hat{u}(k)\overline{\hat{u}(k)}$ (the bar denoting complex conjugate) and show that $E(k) = C(\nu)k^{-2+\gamma(\nu)}$, where γ is a positive correction term that vanishes as ν tends to 0. The significance of this result is that it establishes in closed form, one of the classical spectral scaling laws for the energy dissipation in boundary layers. On the other hand, one may use this result to establish the appropriate "physical" probability distribution on the wave numbers required to finish the probabilistic representation of equation (2.27). In that case, the stochastic representation of Burgers equation given in Part (2) might shed light on the physics of energy cascade phenomena in fluid mechanics.

In the general subject of diffusion in heterogenous media, a next natural step beyond the problem solved in Part (3) is to determine the stochastic process associated with the diffusion-advection equation for a diffusion coefficient discontinuous along general surfaces. The existence of such a process can be proven using the Dirichlet forms approach as in Section (4.4). The effect of higher dimensions on the stochastic process has been addressed in Mastrangelo and Mouloud (1990); Portenko (1998) considering hyperplanes of discontinuity. A process analogous to skew Brownian motion in 2-dimensions with an interface formed by the intersection of two lines at an angle is described in Aryasova and Portenko (2003), the case of a circular interface is treated in Portenko (2005) and Decamps et al. (2006). On the other hand, analytic expressions for the velocity field of irrotational flow in a medium with conductivity fields discontinuous along different closed surfaces are available (see Eames and Bush, 1999). An important open problem, especially in the context of flow in porous media, would be to identify the connection between a Brownian motion with skewness at a surface and the advection-diffusion equation in a medium with "intrusions", that is, regions where the conductivity and the diffusion coefficient change with respect to constant background values.

With respect to multi-skew Brownian motion, the most blatant omission in the treatment given in Part (4) is ruling out the possibility of accumulation points in the set of interfaces. If this is allowed, the construction of the process could be done either by specifying its infinitesimal generator, or through a stochastic integral of the form (4.1). Depending on the behavior of the skewness values, however, there might be points where the densities of the speed and scale measures converge to zero or infinity, and thus creating singular points for the diffusion. A mathematical characterization of such behavior would be desirable.

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