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Analytic expressions of the solutions of advection-diffusion problems in 1D with discontinuous coefficients

Antoine Lejay,* Lionel Lenôtre,† Géraldine Pichot‡

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Abstract

In this article, we provide a method to compute analytic expressions of the resolvent kernel of differential operators of the diffusion type with discontinuous coefficients in one dimension. Then we apply it when the coefficients are piecewise constant. We also perform the Laplace inversion of the resolvent kernel to obtain expressions of the transition density functions or fundamental solutions. We show how these explicit formula are useful to simulate advection-diffusion problems using particle tracking techniques.

Keywords: advection diffusion problems; resolvent kernels; transition density functions; discontinuous coefficients; particle tracking techniques

1 Introduction

We consider linear second-order parabolic operators $\mathcal{A}_{x,(a,\rho,b)}^B$ with domain $\text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B)$ such as:

$$\mathcal{A}_{x,(a,\rho,b)}^B f(x) := \frac{1}{2}\rho(x)\partial_x(a(x)\partial_x f(x)) + b(x)\partial_x f(x),$$

with a and b possibly discontinuous. The coefficients a and b may be discontinuous at different points and/or may have several points of discontinuities.

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We are interested in deriving analytic expressions of the resolvent kernels (or of its Laplace inversion, the so-called transition density functions) of such operators and to use these analytic expressions in the context of particle tracking methods [13, 14, 43]. These analytic expressions may also provide other very interesting results as asymptotics in long time [49] and short time [10], various quantities such as option prices in finance [46], solution of inverse problems [28] or understanding of the underlying equations and their spectral properties [25, 26].

Due to the discontinuities of a and/or b , the derivation of analytic expressions of the resolvent kernel of $(\mathcal{A}_{x,(a,\rho,b)}^B, \text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B))$ requires special methods. Commonly, these analytic expressions are derived using probabilistic methods or arguments [2, 6, 17, 23, 58]. However, the derivation is quite heavy and sometimes cumbersome. Other approaches, described in [25, 26], in the same spirit of the method proposed in this paper, consider only the case $b = 0$.

Our first contribution consists in proposing a general computation method which provides explicit, closed form formula of the resolvent kernel when both a and b are discontinuous; extending the previous results we cited right above. It also generalizes the so-called *method of images* which was only usable when the symmetries in the coefficients allow it [60]. The method we propose is more universal and systematic than the existing ones with probabilistic arguments which tends to treat the problems case by case. In the situation where a and b are piecewise constant, we show how to end up, through a simple change of variable, to the study of a Skew Brownian motion [39] with drift (called the drifted Skew Brownian motion).

Then we are interested in using the analytic expression of the resolvent kernel of $\mathcal{A}_{x,(a,\rho,b)}^B$ in the context of solving advection-diffusion problems with a particle tracking technique. We consider the classical advection-diffusion operator:

$$\mathcal{L}_x^B f(t, x) := \frac{1}{2} \partial_x (a(x) \partial_x f(x)) + b(x) \partial_x f(x),$$

with domain $\text{Dom}(\mathcal{L}_x^B)$. On purpose, we take the same coefficient a and b as the ones in the expression of $\mathcal{A}_{x,(a,\rho,b)}^B$.

The coefficient a is classically called the diffusivity coefficient and the coefficient b the drift. The operator $(\mathcal{L}_x^B, \text{Dom}(\mathcal{L}_x^B))$ is encountered in many applications: in (with only a few references) geophysics for soil [12, 29, 32, 52, 57], air [56] and ocean [54]; astrophysics [61]; molecular dynamics [8]; population ecology [9, 36]; finance [11, 24, 59]. The discontinuities come generally from the medium, which contains permeable or semi-permeable barriers. For example, in thermodynamics or electronics, the materials are built with layers possessing different conductivity in order to reach some effective behavior. Similarly, in population ecology, different intertwined habitats has to be dealt with while studying the concentration of insects' population.

When a and b are discontinuous, the Gaussian approximation is no longer valid [27, 32] and special particle tracking schemes have to be designed. In the literature, most of the already proposed schemes take $b = 0$ [5, 16, 17, 29, 40, 43, 47, 53, 57]. In [15, 42] (random walk based methods) — which are not sensitive with regard to the values of the drifts — as well as in [13, 17] (*exact simulation techniques*), either a or b is discontinuous but not both.

Our second contribution consists in emphasizing the connection between the two operators $\mathcal{A}_{x,(a,1,b)}^B$ and \mathcal{L}_x^B . In fact, when the coefficients a and b are the same, the two operators \mathcal{L}_x^B and $\mathcal{A}_{x,(a,1,b)}^B$ ($\rho = 1$) differ only because they are defined with different ambient spaces. We demonstrate rigorously that it is possible to compute the resolvent kernel of \mathcal{L}_x^B with the one of $\mathcal{A}_{x,(a,1,b)}^B$. The resolvent of $\mathcal{A}_{x,(a,1,b)}^B$ is itself obtained using the computation method presented in the first part of our paper. Therefore, in our approach, a and b may be discontinuous and possibly

at different points of discontinuities. Additionally, we show that computing the resolvent kernel of $\mathcal{A}_{x,(a,1,b)}^B$ in the case of one interface of discontinuity in an infinite domain is sufficient to design a general particle tracking algorithm in the general case of advection-diffusion problems with multiple interfaces of discontinuities. This last result is obtained by using the definition of *interface layers* around the discontinuities as proposed in [44] together with the Markov property of the stochastic process associated to \mathcal{L}_x^B .

Outline. In Section 2, we recall a few results regarding second-order differential operators of the diffusion type and their resolvent equations whose solutions are the Green functions: their factorized forms and their minimal pairs in particular. In Section 3, we provide our computation method which provide analytic closed form expression of the resolvent kernel (Green function). In Section 4, we treat in full detail the situation where the diffusivity and the advective term (or drift) are piecewise constant. We show how it reduces, through a simple change of variable, to the study of the drifted Skew Brownian motion. Using inverse Laplace transforms, we derive some explicit expressions for the transition density function (or the fundamental solution) for some particular situations. In Sections 5 and 6, we show that this general methodology is useful for solving advection-diffusion problems with particle tracking techniques. Section 5 details the case of one interface of discontinuity and Section 6 proposes a general algorithm to handle the case of multiple interfaces.

2 Operators and their resolvents

In this section, we present the second-order differential operators we consider as well as some of its main properties that will be used subsequently in Section 3. More precisely, we consider a large-class of operators which depends on 3 functions and whose ambient space of the space of bounded, continuous functions.

For some constants $0 < c \leq C$, we define

$$\mathfrak{c} := \{a : \mathbb{R} \rightarrow \mathbb{R}_+ \text{ measurable} \mid c \leq a(x) \leq C, \forall x \in \mathbb{R}\}, \quad (2.1)$$

$$\mathfrak{b} := \{b : \mathbb{R} \rightarrow \mathbb{R} \text{ measurable} \mid |b(x)| \leq C, \forall x \in \mathbb{R}\} \quad (2.2)$$

$$\text{and } \mathfrak{M} := \{(a, \rho, b) : \mathbb{R} \rightarrow \mathbb{R}^3 \mid a, \rho \in \mathfrak{c}, b \in \mathfrak{b}\}.$$

We denote by $\mathcal{C}(I, J)$ the space of continuous functions from $I \subset \mathbb{R}$ to a state space J . Denote by \mathcal{C}_0 the class of continuous functions vanishing at infinities equipped with the uniform norm $\|\cdot\|_\infty$. It is indeed a Banach space.

To each $(a, \rho, b) \in \mathfrak{M}$, we associate the second-order differential operator whose existence is asserted by Proposition 2.1 below:

$$\begin{aligned} \mathcal{A}_{x,(a,\rho,b)}^B f(x) &:= \frac{1}{2} \rho(x) \partial_x (a(x) \partial_x f(x)) + b(x) \partial_x f(x), \\ \text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B) &= \{f \in \mathcal{C}_0 \mid \mathcal{A}_{x,(a,\rho,b)}^B f \in \mathcal{C}_0\}. \end{aligned}$$

2.1 Factorized forms

Following the approach of W. Feller [22], we look at a *factorized form* of $\mathcal{A}_{x,(a,\rho,b)}^B$. This factorized form is particularly suitable for providing an explicit expression of resolvent kernel.

Definition 2.1. For a function $f \in \mathcal{C}_0$, the differentiability of f at x with respect to a continuous and increasing function $G : \mathbb{R} \rightarrow \mathbb{R}$ is defined as

$$D_x^G f(x) = \lim_{y \searrow x} \frac{f(y) - f(x)}{G(y) - G(x)}$$

when the limit exists.

Remark 2.1. When $G(x) = x$, the differentiability is just the classical differentiability. Hence, we write ∂_x in spite of $D_x^{G: x \rightarrow x}$.

Proposition 2.1. Let $(a, \rho, b) \in \mathfrak{M}$. The differential operator $(\mathcal{A}_{x,(a,\rho,b)}^B, \text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B))$ is well defined and can be factorized as:

$$\mathcal{A}_{x,(a,\rho,b)}^B = \frac{1}{2} D_x^M D_x^S,$$

where S is the scale function, M is the speed measure with

$$S(x) = \int_0^x \frac{\kappa(y)}{a(y)} dy \text{ and } M(x) = \int_0^x \frac{1}{\rho(y)\kappa(y)} dy, \quad (2.3)$$

$$s(x) = \frac{\kappa(x)}{a(x)}, \quad m(x) = \frac{1}{\kappa(x)\rho(x)}, \quad h(x) = \int_0^x \frac{2b(y)}{a(y)\rho(y)} dy \text{ and } \kappa(x) = e^{-h(x)}. \quad (2.4)$$

Remark 2.2. Using Definition 2.1,

$$D_x^S f(x) = s(x)^{-1} \partial_x f(x) \text{ and } D_x^M f(x) = m(x)^{-1} \partial_x f(x).$$

Proof. For the above functions S and M , let us define $\Omega := \frac{1}{2} D_x^M D_x^S$ with domain

$$\text{Dom}(\Omega) := \{f \in \mathcal{C}_0 \mid \Omega f \in \mathcal{C}_0\}, \quad (2.5)$$

$$= \{f \in \mathcal{C}_0 \mid \forall \lambda > 0, \exists w \in \mathcal{C}_0 \text{ s.t. } (\lambda - \Omega)f = w\}. \quad (2.6)$$

The existence of $(\Omega, \text{Dom}(\Omega))$ as well as the equivalence between (2.5) and (2.6) follows from classical results of W. Feller [18–21].

Now let Φ be a continuous, increasing function with $\Phi(0) = 0$ and $f \in \mathcal{C}_0$ be such that $f \circ \Phi \in \text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B)$ (which we assume to be not empty in a first time). Then,

$$\begin{aligned} \mathcal{A}_{x,(a,\rho,b)}^B(f \circ \Phi)(x) &= \left(\frac{\rho(x)}{2} a(x) \Phi''(x) + b(x) \Phi'(x) \right) \partial_z f(\Phi(x)) \\ &\quad + \frac{\rho(x)}{2} \Phi'(x) \partial_x (a(x) (\Phi')^{-1}(x) \partial_x f(\Phi(x))). \end{aligned}$$

In the meanwhile, choosing $\Phi(x)$ such that $\Phi(0) = 0$ and $\Phi'(x) = \kappa(x) = \exp(-h(x))$ where h and κ given by (2.4) ensures that

$$\frac{\rho(x)}{2} a(x) \Phi''(x) + b(x) \Phi'(x) = 0$$

and

$$\begin{aligned} \mathcal{A}_{x,(a,\rho,b)}^B(f \circ \Phi)(x) &= \frac{\rho(x)}{2} \Phi'(x) \partial_x \left(a(x) \left(\frac{1}{\Phi'(x)} \partial_x (f \circ \Phi)(x) \right) \right) \\ &= \frac{1}{2} m(x)^{-1} \partial_x (s(x)^{-1} \partial_x (f \circ \Phi)(x)) = \frac{1}{2} D_x^M D_x^S (f \circ \Phi)(x) = \Omega(f \circ \Phi)(x). \end{aligned}$$

Hence, $f \circ \Phi \in \text{Dom}(\Omega)$ and then $(\Omega, \text{Dom}(\Omega))$ extends $(\mathcal{A}_{x,(a,\rho,b)}^B, \text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B))$.

Finally, performing the same reasoning by starting with Ω instead of $\mathcal{A}_{x,(a,\rho,b)}^B$ shows the equality between the two operators. Moreover, it proves that $\text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B) \neq \emptyset$ since $\text{Dom}(\Omega) \neq \emptyset$. The operator $(\mathcal{A}_{x,(a,\rho,b)}^B, \text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B))$ is therefore well defined. \square

In dimension 1, solving $\mathcal{A}_{x,(a,\rho,b)}^B f = g$ with $g \in \mathcal{C}_0$ is equivalent to solve a Sturm-Liouville problem. A first application of using the factorized form is then to give some continuity properties of f and $D_x^S f$.

Lemma 2.1. *Let $f \in \text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B)$ with $(a, \rho, b) \in \mathfrak{M}$. Then f is continuous, differentiable and $D_x^S f$ is itself continuous.*

Proof. From the definition of the domain of $\mathcal{A}_{x,(a,\rho,b)}^B$ (see (2.5)), the problem $(\lambda - \mathcal{A}_{x,(a,\rho,b)}^B)f(x) = w(x)$ is a Sturm-Liouville problem that may be transformed into solving a first-order differential equation in $(f, D_x^S f)$, which are then necessarily (absolutely) continuous. \square

We now recall the definition of the resolvent kernel, which we aim at computing here.

Definition 2.2 (Resolvent kernel). *The resolvent kernel of $\mathcal{A}_{x,(a,\rho,b)}^B$ is a function $(\lambda, x, y) \in \mathbb{R}_+ \times \mathbb{R} \times \mathbb{R} \mapsto \mathfrak{r}_{\mathcal{A}_{x,(a,\rho,b)}^B}(\lambda; x, y)$ such that the family $(G_\lambda)_{\lambda>0}$ of linear operators defined by*

$$G_\lambda f(x) := \int_{\mathbb{R}} \mathfrak{r}_{\mathcal{A}_{x,(a,\rho,b)}^B}(\lambda; x, y) f(y) dy, \quad \forall f \in \mathcal{C}_0 \quad (2.7)$$

is the resolvent of $(\mathcal{A}_{x,(a,\rho,b)}^B, \text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B))$. This means that $G_\lambda = (\lambda - \mathcal{A}_{x,(a,\rho,b)}^B)^{-1}$ in \mathcal{C}_0 . Formally,

$$(\lambda - \mathcal{A}_{x,(a,\rho,b)}^B) \mathfrak{r}_{\mathcal{A}_{x,(a,\rho,b)}^B}(\lambda; x, y) = \delta_y(x).$$

2.2 Minimal pair and their continuity

With the factorized form of the operator comes two particular families of functions. These functions play a central role to compute the resolvent kernel.

Proposition 2.2 ([21, Theorem 6.1]). *There exist two families $\{\phi(\lambda; \cdot)\}_{\lambda>0}$ and $\{\psi(\lambda; \cdot)\}_{\lambda>0}$ of continuous, positive functions from \mathbb{R} to \mathbb{R} such that*

$$\begin{aligned} (\lambda - \mathcal{A}_{x,(a,\rho,b)}^B)u(\lambda; x) &= 0, \quad \forall x \in \mathbb{R}, \lambda > 0, \text{ for } u = \phi \text{ or } \psi, \\ \phi(\lambda; 0) &= \psi(\lambda; 0) = 1, \quad \phi \text{ is decreasing from } +\infty \text{ to } 0, \\ \psi &\text{ is valued increasing from } 0 \text{ to } +\infty. \end{aligned}$$

The pair (ϕ, ψ) is called the minimal pair.

Being unbounded, $\phi(\lambda; \cdot)$ and $\psi(\lambda; \cdot)$ do not belong to $\text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B)$. The proof of the next lemma is similar to the one of Lemma 2.1.

Lemma 2.2. *For each $\lambda > 0$, the functions $\phi(\lambda; \cdot)$, $\psi(\lambda; \cdot)$, $D_x^S \phi(\lambda; \cdot)$ and $D_x^S \psi(\lambda; \cdot)$ are continuous on \mathbb{R} .*

3 Resolvent kernel of knotted operators

Using the notations of (2.1)-(2.2), we set

$$\mathfrak{C} := \mathfrak{c} \cap \mathcal{C}(\mathbb{R}, \mathbb{R}) \text{ and } \mathfrak{B} := \mathfrak{b} \cap \mathcal{C}(\mathbb{R}, \mathbb{R})$$

as well as

$$\mathfrak{H} := \{(a, \rho, b) : \mathbb{R} \rightarrow \mathbb{R}^3 \mid a, \rho \in \mathfrak{C}, b \in \mathfrak{B}\} \subset \mathfrak{M}.$$

Notation 3.1. For two functions ξ_- and ξ_+ from \mathbb{R} to \mathbb{R}^d ($d \geq 1$), we define their *knotted* as

$$\begin{aligned} \xi_- \bowtie \xi_+ &: \mathbb{R} \longrightarrow \mathbb{R}^d, \\ x &\longmapsto \xi_-(x)\mathbb{1}_{x < 0} + \xi_+(x)\mathbb{1}_{x \geq 0}. \end{aligned}$$

For a space \mathfrak{F} of continuous functions from \mathbb{R} to \mathbb{R}^d , we write

$$\mathfrak{F}^{\bowtie} := \{f_- \bowtie f_+ \mid f_-, f_+ \in \mathfrak{F}\}.$$

The problem of *knotted* operators consists in finding suitable conditions at the interface when “gluing” the diffusion processes they generate (See *e.g.* [37]). In our case, we have a natural interpretation of the transmission condition but we are interested in finding analytic expressions.

Remark 3.1. We choose to *knot* functions at 0 for convenience of the presentation. Actually, everything we propose in this paper does not require a and b to be *knotted* at the same point nor to have only one single point of *knotted*.

We now restrict our attention to coefficients which are obtained by knotting simpler ones.

Hypothesis 3.1. We consider two families $(a_{\pm}, \rho_{\pm}, b_{\pm})$ in \mathfrak{H} from which we define

$$(a, \rho, b) = (a_-, \rho_-, b_-) \bowtie (a_+, \rho_+, b_+) \in \mathfrak{H}^{\bowtie}.$$

Notation 3.2. To $(a_{\pm}, \rho_{\pm}, b_{\pm}) \in \mathfrak{H}$ we associate the corresponding operators $\mathcal{A}_{x, (a_{\pm}, \rho_{\pm}, b_{\pm})}^B$, scales functions S_{\pm} , speed measures M_{\pm} with density m_{\pm} , the minimal pairs (ϕ_{\pm}, ψ_{\pm}) , and so on.

Remark 3.2. With (2.4) and (2.3), the scale measure S and the density m of speed measure M of $\mathcal{A}_{x, (a, \rho, b)}^B$ satisfy $S = S_- \bowtie S_+$ and $m = m_- \bowtie m_+$.

Notation 3.3. We define

$$g(\lambda; x, y) := \frac{\mathfrak{r}_{\mathcal{A}_{x, (a, \rho, b)}^B}(\lambda; x, y)}{m(y)} \text{ for } (\lambda, x, y) \in \mathbb{R}_+ \times \mathbb{R} \times \mathbb{R}. \quad (3.1)$$

As it will be seen below in (3.7), this kernel $g(\lambda; x, y)$ is symmetric in (x, y) .

We now give a characterization of the resolvent kernel from which we deduce our analytic conditions. Let us recall the formal expression in Definition 2.2. With Lemma 2.1, continuity conditions are imposed at 0, which are translated in (3.3)-(3.4) below. The effect of the Dirac mass in Definition 2.2 is rewritten as a condition on the jump of a flow: See (3.6) below. Condition (3.2) can be solved locally using the minimal pairs as they form a local basis for solutions.

Proposition 3.1. Let $(a, \rho, b) \in \mathfrak{H}^{\boxtimes}$ as in Hypothesis 3.1. The kernel $g(\lambda; x, y)$ given by (3.7) associated to $(\mathcal{A}_{x,(a,\rho,b)}^B, \text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B))$ solves:

$$(\lambda - \mathcal{A}_{x,(a,\rho,b)}^B)g(\lambda; x, y) = 0, \quad x, y \in \mathbb{R}, \quad x \notin \{y, 0\}, \quad (3.2)$$

$$g(\lambda; 0-, y) = g(\lambda; 0+, y), \quad y \neq 0, \quad (3.3)$$

$$g(\lambda; y-, y) = g(\lambda; y+, y), \quad y \neq 0, \quad (3.4)$$

$$D_x^{S-}g(\lambda; 0-, y) = D_x^{S+}g(\lambda; 0+, y), \quad y \neq 0, \quad (3.5)$$

$$\begin{cases} D_x^{S-}g(\lambda; y-, y) - D_x^{S-}g(\lambda; y+, y) = 2, & \text{if } y < 0, \\ D_x^{S+}g(\lambda; y-, y) - D_x^{S+}g(\lambda; y+, y) = 2, & \text{if } y > 0. \end{cases} \quad (3.6)$$

Notation 3.4. We define the *Wronskian* of two suitable functions f and g as $\text{Wr}[f, g](x) := f(x)D_x^Sg(x) - g(x)D_x^Sf(x)$.

Proof. From [21, §7, p. 475] or [30], using the minimal pair (ϕ, ψ) of $\mathcal{A}_{x,(a,\rho,b)}^B$, $g(\lambda; x, y)$ may be written as:

$$g(\lambda; x, y) = \frac{2}{W} \begin{cases} \psi(\lambda; x)\phi(\lambda; y) & \text{if } x < y, \\ \phi(\lambda; x)\psi(\lambda; y) & \text{if } x \geq y \end{cases} \quad (3.7)$$

with $W = \text{Wr}[\phi(\lambda; \cdot), \psi(\lambda; \cdot)](x)$ (this function is constant in x). Eq. (3.2) follows from (3.7). From Lemma 2.2, $u(\lambda; \cdot)$ and $D^S u(\lambda; \cdot)$ are continuous for $u = \phi, \psi$. Thus $x \mapsto g(\lambda; x, y)$ is continuous, which leads to (3.3). In addition, $x \mapsto D_x^Sg(\lambda; x, y)$ is continuous when $x \neq 0$. As $S = S_- \boxtimes S_+$, this leads to (3.5).

Let us assume that $y > 0$. When $x \geq y$, $D_x^{S+}g(\lambda; y + h, y) = \frac{2}{W}D_x^{S+}\phi(\lambda; y + h)\psi(\lambda; y)$. Using the expression of W , for $h > 0$,

$$\psi(\lambda; y + h)D_x^{S+}\phi(\lambda; y + h) = -W + \phi(\lambda; y + h)D_x^{S+}\psi(\lambda; y + h).$$

Thus,

$$D_x^{S+}g(\lambda; y + h, y) = \frac{2}{W} (-W + \phi(\lambda; y + h)D_x^{S+}\psi(\lambda; y + h)) \frac{\psi(\lambda; y)}{\psi(\lambda; y + h)}. \quad (3.8)$$

Similarly, when $x < y$, $D_x^{S+}g(\lambda; y - h, y) = \frac{2}{W}D_x^{S+}\psi(\lambda; y - h)\phi(\lambda; y)$. Using the expression of W , for a $h > 0$ yields

$$D_x^{S+}g(\lambda; y - h, y) = \frac{2}{W} (W + \psi(\lambda; y - h)D_x^{S+}\phi(\lambda; y - h)) \frac{\phi(\lambda; y)}{\phi(\lambda; y - h)}. \quad (3.9)$$

Summing the two expressions (3.8) and (3.9) and using the continuity of $\phi, \psi, D_x^{S+}\psi$ and $D_x^{S+}\phi$ at y yields (3.6) for the case $y > 0$ as $h \rightarrow 0$.

For the case $y < 0$, use the same arguments with the operator D_x^{S-} . □

Hypothesis 3.2. For $(a, \rho, b) = (a_-, \rho_-, b_-) \boxtimes (a_+, \rho_+, b_+)$ as in Hypothesis 3.1, we assume that the minimal pairs (ϕ_{\pm}, ψ_{\pm}) associated to $(a_{\pm}, \rho_{\pm}, b_{\pm})$ are known.

This is the case when the coefficients $(a_{\pm}, \rho_{\pm}, b_{\pm})$ are constant as well as for many other cases [7]. The piecewise constant case is treated in full details in Section 4.

Notation 3.5. We consider two suitable continuous functions u and v . The Wronskian (negative side) of u and v is defined by

$$\begin{aligned}\text{WrN}[u, v](x) &:= u(x)D_x^{S^-}v(x) - v(x)D_x^{S^-}u(x), \quad x < 0, \\ \text{WrP}[u, v](x) &:= u(x)D_x^{S^+}v(x) - v(x)D_x^{S^+}u(x), \quad x \geq 0, \\ \text{WrSNP}[u, v](0) &:= u(0)D_x^{S^+}v(0) - v(0)D_x^{S^-}u(0), \\ \text{and } \text{WrSPN}[u, v](0) &:= u(0)D_x^{S^-}v(0) - v(0)D_x^{S^+}u(0).\end{aligned}$$

Theorem 3.1. *Assume Hypothesis 3.2.*

Let $g(\lambda; x, y)$ be the kernel associated to $(\mathcal{A}_{x,(a,\rho,b)}^B, \text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B))$ through (3.1). Then

$$g(\lambda; x, y) := \begin{cases} g_{y \geq 0}(\lambda; x, y) & \text{if } y \geq 0, \\ g_{y < 0}(\lambda; x, y) & \text{if } y < 0, \end{cases} \quad (3.10)$$

where for $y \geq 0$

$$\begin{aligned}g_{y \geq 0}(\lambda; x, y) &= c_1^+ \phi_+(\lambda; y) \psi_-(\lambda; x) \mathbb{1}_{x \leq 0} \\ &\quad + (c_2^+ \phi_+(\lambda; y) \phi_+(\lambda; x) + c_3^+ \phi_+(\lambda; y) \psi_+(\lambda; x)) \mathbb{1}_{x \in]0, y[} \\ &\quad + (c_2^+ \phi_+(\lambda; y) \phi_+(\lambda; x) + c_3^+ \psi_+(\lambda; y) \phi_+(\lambda; x)) \mathbb{1}_{x \geq y} \quad (3.11)\end{aligned}$$

with

$$\begin{aligned}c_1^+ &:= \frac{-2}{\Theta^+} \text{WrP}[\psi_+, \phi_+](\lambda; 0), & c_2^+ &:= \frac{-2}{\Theta^+} \text{WrSPN}[\psi_+, \psi_-](\lambda; 0), \\ c_3^+ &:= \frac{2}{\Theta^+} \text{WrSPN}[\phi_+, \psi_-](\lambda; 0) \quad \text{and } \Theta^+ &:= \text{WrP}[\phi_+, \psi_+](y) \text{WrSPN}[\phi_+, \psi_-](\lambda; 0) > 0\end{aligned}$$

while for $y < 0$,

$$\begin{aligned}g_{y < 0}(\lambda; x, y) &:= c_1^- \psi_-(\lambda; y) \phi_+(\lambda; x) \mathbb{1}_{x \geq 0} \\ &\quad + (c_2^- \psi_-(\lambda; y) \psi_-(\lambda; x) + c_3^- \psi_-(\lambda; y) \phi_-(\lambda; x)) \mathbb{1}_{x \in]y, 0[} \\ &\quad + (c_2^- \psi_-(\lambda; y) \psi_-(\lambda; x) + c_3^- \phi_-(\lambda; y) \psi_-(\lambda; x)) \mathbb{1}_{x \leq y} \quad (3.12)\end{aligned}$$

with

$$\begin{aligned}c_1^- &:= \frac{2}{\Theta^-} \text{WrN}[\phi_-, \psi_-](\lambda; 0), & c_2^- &:= \frac{2}{\Theta^-} \text{WrSNP}[\phi_-, \phi_+](\lambda; 0), \\ c_3^- &:= \frac{2}{\Theta^-} \text{WrSPN}[\phi_+, \psi_-](\lambda; 0) \quad \text{and } \Theta^- &:= \text{WrN}[\phi_-, \psi_-](y) \text{WrSPN}[\phi_+, \psi_-](\lambda; 0) > 0.\end{aligned}$$

The coefficients Θ^+ (resp. Θ^-) do not depend on y as $\text{WrP}[\phi_+, \psi_+]$ (resp. $\text{WrN}[\phi_-, \psi_-]$) is constant in x .

Remark 3.3. As it is evident from the proof, multiple interfaces as well as boundary conditions may be considered by a similar approach.

Proof. As the dimension is one, solving a second-order differential equation is equivalent to solve a first-order system. For $x \geq 0$, we have already found two independent solutions $\phi_+(\lambda; \cdot)$ and $\psi_+(\lambda; \cdot)$.

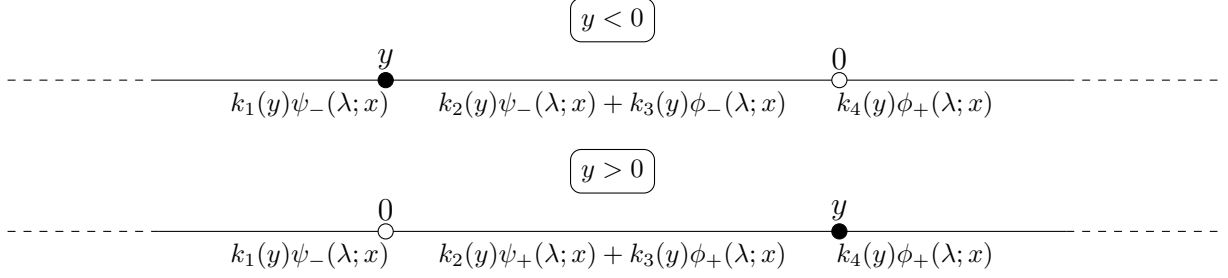


Figure 1: Splitting the state space to define superpositions.

Any solution to $\mathcal{A}_{x,(a_+, \rho_+, b_+)}^B f(x) = \lambda f(x)$ on $J \subset [0, +\infty[$ is thus locally a superposition of $\phi_+(\lambda; \cdot)$ and $\psi_+(\lambda; \cdot)$. A similar superposition can be considered for $x < 0$ with two independent solutions $\phi_-(\lambda; \cdot)$ and $\psi_-(\lambda; \cdot)$.

We have the following picture: To take (3.2)-(3.3) into account, the space is split into the intervals $]-\infty, 0 \wedge y]$, $]0 \wedge y, 0 \vee y[$ and $[0 \vee y, +\infty[$ (See Figure 1).

Case $y \geq 0$. Let us set:

$$\begin{aligned} k_1^+(y) &= c_1^+ \phi_+(\lambda; y), & k_2^+(y) &= c_2^+ \phi_+(\lambda; y), \\ k_3^+(y) &= c_3^+ \phi_+(\lambda; y) & \text{and } k_4^+(y) &= c_2^+ \phi_+(\lambda; y) + c_3^+ \psi_+(\lambda; y). \end{aligned}$$

We look for the resolvent kernel under the form (3.11). Our choice ensures from that as $x \rightarrow \infty$, $g(\lambda; x, y)$ decreases to 0. If there are other boundary conditions, then the functions ϕ_- and ψ_+ may be introduced as well on the set $\{x \leq 0\}$ or $\{x \geq y\}$.

The interface conditions at 0 and y are linear ones. Conditions (3.5), (3.3) and (3.6) lead us to solve

$$N_{y \geq 0}(\lambda, y) \mathbf{k}^+(y) = \mathbf{f} \text{ with } \mathbf{f} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 2 \end{bmatrix}, \mathbf{k}^+(y) = \begin{bmatrix} k_1^+(y) \\ k_2^+(y) \\ k_3^+(y) \\ k_4^+(y) \end{bmatrix}$$

and

$$N_{y \geq 0}(\lambda, y) = \begin{bmatrix} \psi_-(\lambda; 0) & -\phi_+(\lambda; 0) & -\psi_+(\lambda; 0) & 0 \\ D_x^{S^-} \psi_-(\lambda; 0) & -D_x^{S^+} \phi_+(\lambda; 0) & D_x^{S^+} \psi_+(\lambda; 0) & 0 \\ 0 & \phi_+(\lambda; y) & \psi_+(\lambda; y) & -\phi_+(\lambda; y) \\ 0 & D_x^{S^+} \phi_+(\lambda; y) & D_x^{S^+} \psi_+(\lambda; y) & -D_x^{S^+} \phi_+(\lambda; y) \end{bmatrix}.$$

Case $y < 0$. Let us set:

$$\begin{aligned} k_1^-(y) &= c_3^- \phi_-(\lambda; y) + c_2^- \psi_-(\lambda; y), & k_2^-(y) &= c_3^- \psi_-(\lambda; y), \\ k_3^-(y) &= c_2^- \psi_-(\lambda; y), & k_4^-(y) &= c_1^- \psi_-(\lambda; y). \end{aligned}$$

We look for the resolvent kernel under the form (3.12). Conditions (3.5), (3.3) and (3.6) lead us to solve

$$N_{y < 0}(\lambda, y) \mathbf{k}^-(y) = \mathbf{f} \text{ with } \mathbf{f} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 2 \end{bmatrix}, \mathbf{k}^-(y) = \begin{bmatrix} k_1^-(y) \\ k_2^-(y) \\ k_3^-(y) \\ k_4^-(y) \end{bmatrix}$$

and

$$N_{y<0}(\lambda, y) = \begin{bmatrix} 0 & \phi_-(\lambda; 0) & \psi_-(\lambda; 0) & -\phi_+(\lambda; 0) \\ 0 & D_x^{S-}\phi_-(\lambda; 0) & D_x^{S-}\psi_-(\lambda; 0) & -D_x^{S+}\phi_+(\lambda; 0) \\ \psi_-(\lambda; y) & -\phi_-(\lambda; y) & -\psi_-(\lambda; y) & 0 \\ D_x^{S-}\psi_-(\lambda; y) & -D_x^{S-}\phi_-(\lambda; y) & -D_x^{S-}\psi_-(\lambda; y) & 0 \end{bmatrix}.$$

The general formula follows from algebraic manipulations. \square

Remark 3.4. The distribution of many random variables (hitting time, occupation time) related to a diffusion may be recovered from the minimal pairs (ϕ, ψ) (see e.g. [50]). One finds also the minimal pair (ϕ, ψ) of $\mathcal{A}_{x,(a,\rho,b)}^B$ through (3.7). Since $\phi(\lambda; 0) = \psi(\lambda; 0) = \phi_{\pm}(0) = \psi_{\pm}(0) = 1$, the Wronskian W between ϕ and ψ is given by

$$g(\lambda; 0, 0) = \frac{2}{W} = c_1^+ = c_1^- = \frac{2}{\text{WrSPN}[\phi_+, \psi_-](\lambda; 0)} \text{ so that } W = \text{WrSPN}[\phi_+, \psi_-](\lambda; 0).$$

It is immediate that $g(\lambda; 0, y)/g(\lambda; 0, 0) = \phi(\lambda; y)\mathbb{1}_{y \geq 0} + \psi(\lambda; y)\mathbb{1}_{y < 0}$ and thereby

$$\psi(\lambda; y) = \psi_-(y) \text{ if } y \leq 0 \text{ and } \phi(\lambda; y) = \phi_+(y) \text{ if } y \geq 0.$$

Moreover,

$$\psi(\lambda; y) = \frac{W}{2} \frac{g(\lambda; x, y)}{\phi(\lambda; x)} = \frac{W}{2} \frac{g(\lambda; x, y)}{\phi_+(x)} \text{ for } 0 \leq y < x$$

Thus, $\psi(\lambda; y)$ is recovered from the last coefficient in (3.11) and the condition $\psi(\lambda; 0) = 1$, so that

$$\psi(\lambda; y) = \frac{c_2^+ \phi_+(\lambda; y) + \psi_+(\lambda; y)c_3^+}{c_1^+} \text{ for } y \geq 0.$$

Similarly,

$$\phi(\lambda; y) = \frac{c_3^- \phi_-(\lambda; y) + c_2^- \psi_-(\lambda; y)}{c_1^-} \text{ for } y < 0.$$

It can be easily verified by a direct computation that $c_3^{\pm} + c_2^{\pm} = c_1^{\pm}$.

4 Particular case of piecewise constant coefficients

In this section, we give a closed form expression of the resolvent kernel $r(\lambda; x, y)$ as well as a closed form expression of the transition function $q(t, x, y)$ when the coefficients are piecewise constants.

4.1 Reduction to the drifted Skew Brownian motion

We actually reduce the number of involved variables problem by performing a simple change of variable. Although everything here can be done in the context of Partial Differential Equations, we illustrate this change of variable by their relations on stochastic processes.

Proposition 4.1 ([19, 30, 48]). *When $(a, \rho, b) \in \mathfrak{M}$, the operator $(\mathcal{A}_{x,(a,\rho,b)}^B, \text{Dom}(\mathcal{A}_{x,(a,\rho,b)}^B))$ is the infinitesimal generator of a Feller process X .*

Feller processes associated to knotted operators with coefficients in \mathfrak{H}^\boxtimes can be expressed in term of solutions to Stochastic Differential Equations with Local Time, an aspect which we do not develop here (See *e.g.* [14, 15, 38, 39] among many other references).

We now restrict ourselves to piecewise constant coefficients.

Notation 4.1. We define

$$\mathfrak{K} := \{f : \mathbb{R} \rightarrow \mathbb{R} \mid f \text{ is constant}\}$$

$$\text{and } \mathfrak{P} := \{(a, \rho, b) \mid a, \rho \in \mathfrak{K} \cap \mathfrak{C} \text{ and } b \in \mathfrak{K} \cap \mathfrak{B}\} \subset \mathfrak{H}.$$

We then identify constants and functions in \mathfrak{K} .

We recall Notation 3.1.

Definition 4.1 (Drifted Skew Brownian motion). *For some constants $\beta \in (0, 1)$ and $\gamma_-, \gamma_+ \in \mathbb{R}$, we define*

$$\begin{aligned} (a_-, \rho_-, b_-) &:= (1 - \beta, (1 - \beta)^{-1}, \gamma_-) \in \mathfrak{P}, \\ (a_+, \rho_+, b_+) &:= (\beta, \beta^{-1}, \gamma_+) \in \mathfrak{P} \end{aligned}$$

as well as

$$\text{DSBM}(\beta, \gamma_+, \gamma_-) := (a_-, \rho_-, b_-) \boxtimes (a_+, \rho_+, b_+) \in \mathfrak{P}^\boxtimes.$$

The process Y associated to $(\mathcal{A}_{x, \text{DSBM}(\beta, \gamma_+, \gamma_-)}^B, \text{Dom}(\mathcal{A}_{x, \text{DSBM}(\beta, \gamma_+, \gamma_-)}^B))$ is called a drifted Skew Brownian motion (DSBM). It is a Skew Brownian motion if $\gamma_- = \gamma_+ = 0$ [39]. It is a Brownian motion with piecewise constant drift when $\beta = 1/2$ and a Brownian motion when in addition $\gamma_- = \gamma_+ = 0$.

The next result follows from straightforward computations.

Lemma 4.1. *Let X be the stochastic process associated to the operator $\mathcal{A}_{x, (a, \rho, b)}^B$ with piecewise constant coefficients $(a, \rho, b) \in \mathfrak{P}^\boxtimes$. For $\kappa_-, \kappa_+ > 0$ we set $G(x) := \kappa(x) \cdot x$ be a piecewise linear change of variable with $\kappa := \kappa_- \boxtimes \kappa_+ \in \mathfrak{K}^\boxtimes$. Then $Y = G(X)$ is associated to the operator $\mathcal{A}_{x, (a\kappa, \rho\kappa, b\kappa)}^B$ with $(a\kappa, \rho\kappa, b\kappa) \in \mathfrak{P}^\boxtimes$.*

Proposition 4.2 (Reduction to a drifted Skew Brownian motion). *Let X be the stochastic process associated to the operator $\mathcal{A}_{x, (a, \rho, b)}^B$ with piecewise constant coefficients $(a, \rho, b) \in \mathfrak{P}^\boxtimes$.*

Consider the piecewise linear change of variable $G(x) = \frac{1}{\sqrt{a(x)\rho(x)}}x$. The process $Y = G(X)$ is a DSBM with coefficients

$$(a_Y, \rho_Y, \gamma) = \left(\frac{a}{\sqrt{a\rho}}, \frac{\rho}{\sqrt{a\rho}}, \frac{b}{\sqrt{a\rho}} \right) = \text{DSBM}(\beta, \gamma_+, \gamma_-)$$

with

$$\beta = \frac{\sqrt{a_+}/\sqrt{\rho_+}}{\sqrt{a_+}/\sqrt{\rho_+} + \sqrt{a_-}/\sqrt{\rho_-}}, \quad \gamma_+ = \frac{b_+}{\sqrt{a_+\rho_+}} \text{ and } \gamma_- = \frac{b_-}{\sqrt{a_-\rho_-}}.$$

The resolvent kernel $\mathfrak{r}_{\mathcal{A}_{x, (a, \rho, b)}^B}$ of X associated to $(a, \rho, b) \in \mathfrak{H}$ is given by

$$\mathfrak{r}_{\mathcal{A}_{x, (a, \rho, b)}^B}(\lambda; x, y) = \frac{\mathfrak{r}_{\text{DSBM}(\beta, \gamma_+, \gamma_-)}(\lambda; G(x), G(y))}{\sqrt{a(y)\rho(y)}} \quad (4.1)$$

where $\mathfrak{r}_{\text{DSBM}(\beta, \gamma_+, \gamma_-)}$ is the resolvent kernel of the DSBM. A similar relation holds for the density.

Proof. The identification of (a_Y, ρ_Y, γ) follows from Lemma 4.1. The process Y is characterized by its scale function and its speed measure. Multiplying the scale function by a constant $c > 0$ and dividing the speed measure by the same constant $c < 0$ give rise to the same process. Choosing $c = (\sqrt{a_+}/\sqrt{\rho_+} + \sqrt{a_-}/\sqrt{\rho_-})^{-1}$ leads to identify the process Y as the one associated to DSBM $(\beta, \gamma_+, \gamma_-)$. \square

The advantage of using G is that the number of parameters defining $(a, \rho, b) \in \mathfrak{P}^\infty$, which is 6, is reduced to only 3: $(\beta, \gamma_+, \gamma_-)$. Besides, the parameter β has an explicit interpretation in term of stochastic process as the parameter of a Skew Brownian motion [39, 42]. We use the special form of the drifted Skew Brownian motion to get explicit expressions for the densities and the resolvent kernel of X from the ones of $Y = G(X)$.

4.2 Explicit computations of the resolvent kernel of the DSBM

The coefficients of the DSBM are piecewise constant ones. The results of Section 3 can therefore be used. According to Proposition 4.2, it is enough to compute $\mathfrak{r}_{\text{DSBM}(\beta, \gamma_+, \gamma_-)}$ to get an expression for the resolvent kernel $\mathfrak{r}_{\mathcal{A}_{x, (a, \rho, b)}^B}$ with $(a, \rho, b) \in \mathfrak{P}^\infty$.

The speed measure m of the process Y associated to $\mathcal{A}_{x, \text{DSBM}(\beta, \gamma_+, \gamma_-)}^B$ is

$$m(x) = \begin{cases} m_+(x) := \beta e^{2\gamma_+ x} & \text{if } x \geq 0, \\ m_-(x) := (1 - \beta) e^{2\gamma_- x} & \text{if } x < 0. \end{cases}$$

and its scale function S is $S(x) = \int_0^x s(y) dy$ with $s(x) = 1/m(x)$. According to Proposition 5.3,

$$\mathfrak{r}_{\text{DSBM}(\beta, \gamma_+, \gamma_-)}(\lambda, x, y) = g(\lambda, x, y)m(y), \quad (4.2)$$

where $g(\lambda, x, y)$ is given by Theorem 3.1 in which the minimal pairs $(\phi_\pm(\lambda; \cdot), \psi_\pm(\lambda; \cdot))$ are

$$\begin{aligned} \psi_\pm(\lambda; x) &= \exp\left(\left(-\gamma_\pm + \sqrt{\gamma_\pm^2 + 2\lambda}\right)x\right) \text{ for } x \in \mathbb{R} \\ \text{and } \phi_\pm(\lambda; x) &= \exp\left(\left(-\gamma_\pm - \sqrt{\gamma_\pm^2 + 2\lambda}\right)x\right) \text{ for } x \in \mathbb{R}. \end{aligned}$$

It is here noteworthy that these minimal pairs do not depend on β .

The next proposition is an application of Theorem 3.1 and (4.2) after some algebraic manipulation. Its formulation requires the following bunch of notations

Notation 4.2. We set

$$\lambda_+ := \gamma_+^2 + 2\lambda > 0, \quad \lambda_- := \gamma_-^2 + 2\lambda > 0 \text{ and } \mu := \beta\gamma_+ - (1 - \beta)\gamma_-.$$

and define the constants

$$\begin{aligned} \Theta &:= \mu + \beta\sqrt{\lambda_+} + (1 - \beta)\sqrt{\lambda_-}, \\ \Theta_+ &:= -\mu + \beta\sqrt{\lambda_+} - (1 - \beta)\sqrt{\lambda_-} \text{ and } \Theta_- := -\mu - \beta\sqrt{\lambda_+} + (1 - \beta)\sqrt{\lambda_-}. \end{aligned}$$

Proposition 4.3. *With the above notations on Θ , Θ_+ , Θ_- , λ_+ and λ_- , for any $\lambda > 0$, $x, y \in \mathbb{R}$,*

$$\mathfrak{r}_{\text{DSBM}(\beta, \gamma_+, \gamma_-)}(\lambda; x, y) = \frac{1}{\Theta} \times \begin{cases} 2\beta \exp(\gamma_+ y - \sqrt{\lambda_+} y - \gamma_- x + \sqrt{\lambda_-} x) \\ \quad \text{if } x \leq 0 \leq y, \\ \lambda_+^{-1/2} \exp(\gamma_+(y-x)) \times \left[\Theta \exp(-\sqrt{\lambda_+}(y-x)) + \Theta_+ \exp(-\sqrt{\lambda_+}(x+y)) \right] \\ \quad \text{if } 0 < x \leq y, \\ \lambda_+^{-1/2} \exp(-\gamma_+(x-y)) \times \left[\Theta \exp(-\sqrt{\lambda_+}(x-y)) + \Theta_+ \exp(-\sqrt{\lambda_+}(x+y)) \right] \\ \quad \text{if } 0 < y \leq x, \\ 2(1-\beta) \exp(\gamma_- y - \gamma_+ x + \sqrt{\lambda_-} y - \sqrt{\lambda_+} x) \\ \quad \text{if } y < 0 \leq x, \\ \lambda_-^{-1/2} \exp(-\gamma_-(x-y)) \times \left[\Theta \exp(-\sqrt{\lambda_-}(x-y)) + \Theta_- \exp(\sqrt{\lambda_-}(y+x)) \right] \\ \quad \text{if } y \leq x < 0, \\ \lambda_-^{-1/2} \exp(\gamma_-(y-x)) \times \left[\Theta \exp(-\sqrt{\lambda_-}(y-x)) + \Theta_- \exp(\sqrt{\lambda_-}(y+x)) \right] \\ \quad \text{if } x \leq y < 0. \end{cases} \quad (4.3)$$

4.3 Some explicit expressions for the transition density function

The transition density function may be recovered from the Laplace inversion of the resolvent kernel [48]. Here we propose various explicit expressions of the transition density function $\mathfrak{q}_{\text{DSBM}(\beta, \gamma_+, \gamma_-)}$ whenever we manage to derive the Laplace inversions of $\mathfrak{r}_{\text{DSBM}(\beta, \gamma_+, \gamma_-)}$.

Notation 4.3. We define

$$\text{sgn}(y) := \mathbb{1}_{y \geq 0} - \mathbb{1}_{y < 0},$$

$$\text{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x e^{-v^2} dv \text{ and } \text{erfc}(x) := 1 - \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_x^{+\infty} e^{-v^2} dv.$$

4.3.1 General considerations on Laplace inversion

The density results from a Laplace inversion of the resolvent kernel, when possible. The general case seems to be difficult to deal with as it involves a denominator of type $a + \sqrt{c + 2\lambda} + \sqrt{d + 2\lambda}$ for some constants a, c, d . We did not find any expression for this in the literature. Yet we can see from the expression of Θ_+ , Θ_- and Θ that some cases lead to simplifications.

4.3.2 The situations in which $\lambda_+ = \lambda_-$

We first consider the situation in which $\lambda_+ = \lambda_-$. It may happen when $\beta_+ = \beta_- = 0$ (Skew Brownian motion), $\gamma_+ = \gamma_- \neq 0$ (Skew Brownian motion with a constant drift), or $\gamma_+ = -\gamma_-$ (Skew Brownian motion with a bang-bang drift).

In this case,

$$\Theta = \mu + \sqrt{\lambda_+}, \quad \Theta_+ = -\mu + (2\beta - 1)\sqrt{\lambda_+} \text{ and } \Theta_- = -\mu + \sqrt{\lambda_+}.$$

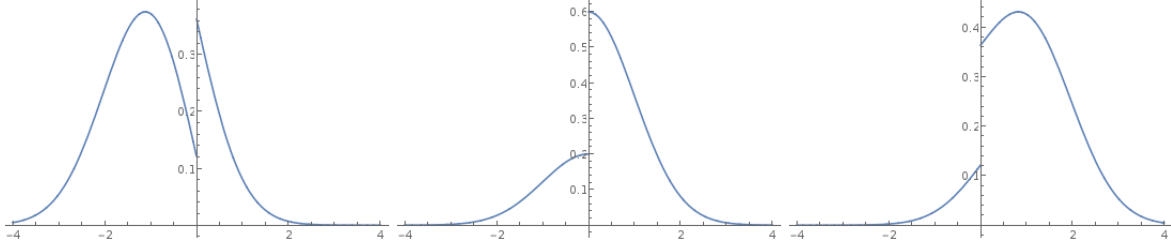


Figure 2: The density $\mathfrak{q}_{\text{DSBM}(\beta,0,0)}(t, x, y)$ of the SBM for $\beta = \frac{3}{4}$ at time $t = 1$ for the initial positions: $x = -1$, $x = 0$ and $x = 1$ (from left to right).

Let us recall some classical formula on inverse Laplace.

Lemma 4.2 (See [1]). For $k \geq 0$, $c > 0$, $\mu \in \mathbb{R}$,

$$\mathcal{L}^{-1}\left(\frac{1}{\sqrt{\lambda}} e^{-k\sqrt{\lambda}}\right) = \frac{1}{\sqrt{\pi t}} e^{-\frac{k^2}{4t}}, \quad (4.4)$$

$$\mathcal{L}^{-1}(f(c\lambda + d)) = \frac{1}{c} e^{-\frac{d}{c}t} \mathcal{L}^{-1}(f)\left(\frac{t}{c}\right), \quad (4.5)$$

$$\mathcal{L}^{-1}\left(\frac{e^{-k\sqrt{\lambda}}}{\mu + \sqrt{\lambda}}\right) = \frac{1}{\sqrt{\pi t}} e^{-\frac{k^2}{4t}} - \mu e^{\mu k} e^{\mu^2 t} \operatorname{erfc}\left(\mu\sqrt{t} + \frac{k}{2\sqrt{t}}\right). \quad (4.6)$$

In addition, when $\mu \neq 0$,

$$\frac{\mu}{\sqrt{\lambda_+}(\mu + \sqrt{\lambda_+})} = \frac{1}{\sqrt{\lambda_+}} + \frac{-1}{\mu + \sqrt{\lambda_+}}$$

so that

$$\frac{1}{\sqrt{\lambda_+}} \frac{\Theta_+}{\Theta} = \frac{2\beta}{\mu + \sqrt{\lambda_+}} - \frac{1}{\sqrt{\lambda_+}} \quad \text{and} \quad \frac{1}{\sqrt{\lambda_+}} \frac{\Theta_-}{\Theta} = \frac{2}{\mu + \sqrt{\lambda_+}} - \frac{1}{\sqrt{\lambda_+}}.$$

The formula of Lemma 4.2 are sufficient to compute termwise the inverse Laplace transforms of the resolvent kernel when $\lambda_+ = \lambda_-$.

4.3.3 The Skew Brownian Motion

The SBM of parameter $\beta \in (0, 1)$ is given by the choice of the coefficients $\text{DSBM}(\beta, 0, 0)$. Hence, $\lambda_+ = \lambda_-$ and $\mu = 0$. Thus, after an application of (4.4)-(4.5) to (5.13) as well as some rewriting,

$$\mathfrak{q}_{\text{DSBM}(\beta,0,0)}(t, x, y) = \frac{1}{\sqrt{2\pi t}} e^{-\frac{(y-x)^2}{2t}} + \operatorname{sgn}(y)(2\beta - 1) \frac{1}{\sqrt{2\pi t}} e^{-\frac{(|y|+|x|)^2}{2t}}.$$

This density was obtained in [58] through a probabilistic argument. Some plots are given in Figure 2.

4.3.4 The Skew Brownian Motion with a constant drift

The density of the SBM with a constant drift, which corresponds to the coefficient $\text{DSBM}(\beta, \gamma, \gamma)$ for some $\gamma \neq 0$ was computed in [2, 3, 17, 24] with different probabilistic arguments.

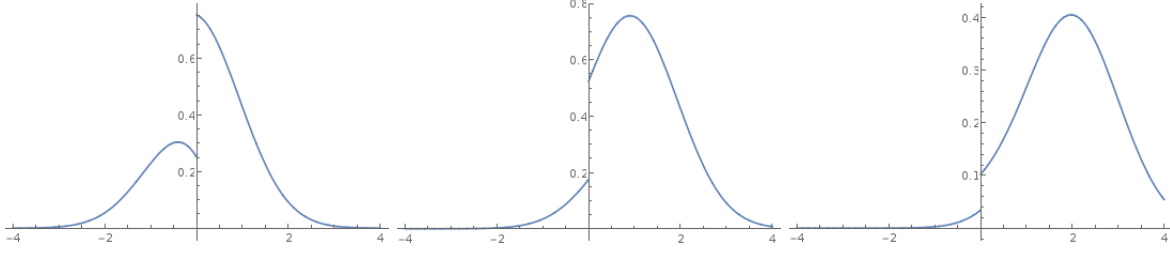


Figure 3: The density $\mathfrak{q}_{\text{DSBM}(\beta, \gamma, \gamma)}(t, x, y)$ of the SBM for $\beta = \frac{3}{4}$ with a constant drift $\gamma = 2$ at time $t = 1$ for the initial positions: $x = -1$, $x = 0$ and $x = 1$ (from left to right).

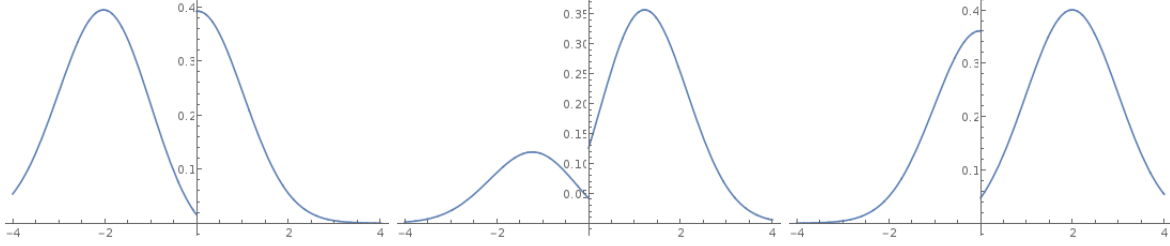


Figure 4: The density $\mathfrak{q}_{\text{DSBM}(\beta, \gamma, -\gamma)}(t, x, y)$ of the SBM for $\beta = \frac{3}{4}$ with a Bang bang drift $\gamma = 2$ at time $t = 1$ for the initial positions $x = -1$, $x = 0$ and $x = 1$ (from left to right).

In this case, $\lambda_+ = \lambda_- = \sqrt{\gamma^2 + 2\lambda}$ and $\mu = (2\beta - 1)\gamma$. With the formula of Lemma 4.2 (see Figure 3),

$$\begin{aligned} \mathfrak{q}_{\text{DSBM}(\beta, \gamma, \gamma)}(t, x, y) &= \frac{1}{\sqrt{2\pi t}} e^{-\frac{\gamma t - (y-x)^2}{2t}} + \text{sgn}(y)(2\beta - 1) \frac{1}{\sqrt{2\pi t}} e^{-\frac{(|y|+|x|)^2}{2t}} e^{-\gamma^2 \frac{t}{2}} e^{\gamma(y-x)} \\ &\quad + \text{sgn}(y)(\mathbb{1}_{y < 0} - \beta)\gamma(2\beta - 1) e^{\gamma(2\beta-1)(|y|+|x|)} e^{\gamma(y-x)} e^{2\gamma^2\beta(\beta-1)t} \\ &\quad \times \text{erfc} \left(\gamma(2\beta - 1) \sqrt{\frac{t}{2}} + \frac{|y| + |x|}{\sqrt{2t}} \right). \end{aligned}$$

We recover the density obtained in [2, 17] up to a conversion of erfc to its probabilistic counterpart.

4.3.5 The Bang-Bang Skew Brownian Motion

The Bang-Bang SBM is the diffusion corresponding to the choice of the coefficients $\text{DSBM}(\beta, \gamma, -\gamma)$ for some $\gamma \neq 0$. This process was introduced in [23]. It may also be called a *Skew Brownian motion with dry friction* [6].

In this case, $\lambda_+ = \lambda_- = \sqrt{\gamma^2 + 2\lambda}$ and $\mu = \gamma$. Again with Lemma 4.2 (see Figure 4)

$$\begin{aligned} \mathfrak{q}_{\text{DSBM}(\beta, \gamma, -\gamma)}(t, x, y) &= \frac{1}{\sqrt{2\pi t}} e^{-\frac{(\gamma t - \text{sgn}(y)(y-x))^2}{2t}} + \text{sgn}(y)(2\beta - 1) \frac{1}{\sqrt{2\pi t}} e^{-\frac{(|y|+|x|)^2}{2t}} e^{-\gamma^2 \frac{t}{2}} e^{\gamma(|y|-|x|)} \\ &\quad + \text{sgn}(y)(\mathbb{1}_{y < 0} - \beta)\gamma e^{2\gamma|y|} \text{erfc} \left(\gamma \sqrt{\frac{t}{2}} + \frac{|y| + |x|}{\sqrt{2t}} \right). \end{aligned}$$

This is the expression given in [23] up to a conversion of erfc into its probabilistic counterpart. It is also the one given in [6].

4.3.6 The constant Péclet case ($\mu = 0$)

We consider that $\gamma_- \neq \gamma_+$ and $\beta \neq 0$. Another situation in which a simplification occurs is when $\mu = \beta\gamma_+ - (1 - \beta)\gamma_- = 0$, which means that

$$\gamma_- = \kappa\gamma_+ \text{ with } \kappa = \frac{\beta}{1 - \beta} \text{ or equivalently } \mu = 0 \text{ when } \beta \neq \frac{1}{2}. \quad (4.7)$$

Remark 4.1. This assumption on γ_+ and γ_- is natural. Then Y is obtained through the transformation of Proposition 4.2 from a process X with piecewise constant coefficients (a, ρ, b) , then (4.7) is satisfied when

$$\frac{b_+}{\rho_+} = \frac{b_-}{\rho_-}.$$

When $a = 1$, the ratio b/ρ is called the *Péclet number*. It is a dimensionless quantity which plays a very important role in fluid mechanics by characterizing the effect of the convection against the diffusion and vice versa.

We give the density starting from 0. Actually, for $x < 0 < y$, the strong Markov property implies that

$$\mathfrak{q}_{\text{DSBM}(\beta, \gamma_+, \gamma_-)}(t, x, y) = \int_0^t \mathfrak{q}_{\text{DSBM}(\beta, \gamma_+, \gamma_-)}(t - s, 0, y) q_-(x, s) ds$$

where $q_-(x, s)$ is the density of the hitting time of 0 for the Brownian motion with drift γ_- . The Laplace transform of $q_-(x, s)$ is nothing more than $\psi_1(x)$. A similar computation holds for $y < 0 < x$.

Proposition 4.4. For any $t \geq 0$ and $\text{DSBM}(\beta, \gamma, \kappa\gamma)$, with $\gamma(y) = ((\kappa\gamma) \boxtimes \gamma)(y)$,

$$\begin{aligned} \mathfrak{q}_{\text{DSBM}(\beta, \gamma, \kappa\gamma)}(t, 0, y) &= \frac{2(\mathbb{1}_{y < 0} - \beta)^2}{(2\beta - 1)\sqrt{2\pi t}} e^{-\frac{(\gamma(y)^2 t - y)^2}{2t}} \\ &+ \frac{\gamma(y)(\mathbb{1}_{y < 0} - \beta)^2}{2(2\beta - 1)} \left(\operatorname{erfc}\left(\frac{y}{\sqrt{2t}} - \gamma(y)\sqrt{\frac{t}{2}}\right) - e^{2\gamma(y)y} \operatorname{erfc}\left(\frac{y}{\sqrt{2t}} + \gamma(y)\sqrt{\frac{t}{2}}\right) \right) \\ &- \frac{\beta(1 - \beta)e^{\gamma(y)y}}{2(2\beta - 1)\pi} \int_0^t e^{-\frac{\gamma(y)^2 \tau}{2}} \int_0^{\gamma^2(-x) - \gamma^2(x)} \sin(y\sqrt{r}) \sqrt{\gamma^2(-x) - \gamma^2(x) - r} e^{-\frac{r\tau}{2}} dr d\tau \\ &+ \frac{\beta(1 - \beta)e^{\gamma(y)y}}{2(2\beta - 1)\pi} \int_0^t e^{-\frac{\gamma(-y)^2 \tau}{2}} \int_0^{+\infty} \cos(y\sqrt{r + \gamma^2(-x) - \gamma^2(x)}) \sqrt{r} e^{-\frac{r\tau}{2}} dr d\tau. \end{aligned}$$

Proof. When (4.7) holds,

$$\frac{1}{\Theta} = \frac{\beta\sqrt{\lambda_+} - (1 - \beta)\sqrt{\lambda_-}}{\beta^2\lambda_+ - (1 - \beta)^2\lambda_-} = \frac{\beta\sqrt{\lambda_+} - (1 - \beta)\sqrt{\lambda_-}}{2\lambda(2\beta - 1)}. \quad (4.8)$$

In addition,

$$\Theta_+ = (2\beta - 1)\Theta \text{ and } \Theta_- = \Theta.$$

Each line in the right-hand side of (4.3) is easily inverted using (4.4) excepted when $y < 0 \leq x$ and $x \leq 0 < y$.

To simplify the formula, we consider starting at $x = 0$. With (4.8),

$$\begin{aligned} \mathfrak{r}_{\text{DSBM}(\beta, \kappa\gamma_+, \gamma_+)}(\lambda, 0, y) \\ = \frac{\beta\sqrt{\lambda_+} - (1-\beta)\sqrt{\lambda_-}}{(2\beta-1)\lambda} \left(\beta e^{(\gamma_+ - \sqrt{\lambda_+})y} \mathbb{1}_{y \geq 0} + (1-\beta) e^{(\gamma_- + \sqrt{\lambda_-})y} \mathbb{1}_{y < 0} \right). \end{aligned}$$

We focus on the term for $y > 0$, the other term being treated by symmetry. With (4.5), we could use λ_+ instead of λ as the parameter for the Laplace transform. Since $2\lambda = \lambda_+ - \gamma_+^2$,

$$\frac{\sqrt{\lambda_+}}{\lambda_+ - \gamma_+^2} e^{-\sqrt{\lambda_+}y} = \frac{\gamma_+}{(\lambda_+ - \gamma_+^2)\sqrt{\lambda_+}} e^{-\sqrt{\lambda_+}y} + \frac{1}{\sqrt{\lambda_+}} e^{-\sqrt{\lambda_+}y}.$$

Hence, the inverse Laplace of the first term in the right-hand side of the above expression can be computed with Lemma B.1, given in Appendix B, while the second term is inverted using (4.4).

Let us write $\nu = \gamma_-^2 - \gamma_+^2 = \gamma_+^2(2\beta - 1)/(1 - \beta)^2$. Thus, $\lambda_- = \lambda_+ + \nu$. Hence,

$$\frac{\sqrt{\lambda_-}}{\lambda} e^{-\sqrt{\lambda_-}y} = \frac{2\sqrt{\lambda_+ + \nu}}{\lambda_+ - \gamma_+^2} e^{-\sqrt{\lambda_+}y}.$$

Using the convolutional property of the Laplace transform and since $\mathcal{L}^{-1}(1/(a + \lambda))(t) = \exp(-at)$, we get that

$$\mathcal{L}^{-1} \left(\frac{2\sqrt{\lambda_+ + \nu}}{\lambda_+ - \gamma_+^2} e^{-\sqrt{\lambda_+}y} \right) = \frac{1}{2} \int_0^t e^{-\frac{\gamma_+^2}{2}\tau} \mathcal{L}^{-1} \left(\sqrt{\lambda_+ + \nu} e^{-\sqrt{\lambda_+}y} \right) (\tau) d\tau.$$

We conclude using Lemma B.2, given in Appendix B.

The case $y < 0$ is treated similarly. The final formula is obtained by gathering all the terms. \square

Such closed form formula open the door to numerical simulation using a class of Monte Carlo methods called *particles tracking techniques* [53, 62] as shown in the two following Sections.

5 Particle tracking techniques to solve advection-diffusion problems with one discontinuity

In this section, we show that the methodology derived in the Sections 3 and 4 is useful for solving advection-diffusion problems with particle tracking techniques. We consider here an infinite one dimensional porous medium with one discontinuity. Subsection 5.1 recall the forward formulation of advection-diffusion problems with one discontinuity. Subsection 5.2 emphasizes that the dynamic of the particles in particle tracking techniques is governed by the backward formulation. Then it shows that the *probability transition function* of the particles can be obtained by the Laplace inversion of the resolvent kernel $\mathfrak{r}_{\mathcal{A}_{x,(a,1,b)}^B}$ given in Proposition 4.2 (with $\rho = 1$ in (4.1)).

5.1 Problem settings: the forward formulation

Without loss of generality, let us consider a single interface at the point $y = 0$ between two layers possessing different diffusion/advective coefficients.

Let us consider a solute evolving in an infinite one dimensional porous medium described by a diffusivity $a = a_- \bowtie a_+ \in \mathfrak{C}^\infty$ and an advective force $b = b_- \bowtie b_+ \in \mathfrak{B}^\infty$.

The concentration $u(t, \cdot)$ at time t is given by the solution of the advection-diffusion equation:

$$\partial_t u(t, y) - \mathcal{L}_y^F u(t, y) = 0, \quad t > 0, \quad y \neq 0, \quad (5.1)$$

$$u(t, \cdot) \xrightarrow[t \rightarrow 0]{\text{weakly}} \nu, \quad (5.2)$$

$$a_-(0-) \partial_y u(t, 0-) - b_-(0-) u(t, 0-) = a_+(0+) \partial_y u(t, 0+) - b_+(0+) u(t, 0+), \quad (5.3)$$

$$u(t, 0-) = u(t, 0+), \quad (5.4)$$

where

$$\mathcal{L}_y^F u(t, y) = \begin{cases} \mathcal{L}_{-,y}^F u(t, y) = \frac{1}{2} \partial_y (a_-(y) \partial_y u(t, y)) - \partial_y (b_-(y) u(t, y)) & \text{if } y < 0, \\ \mathcal{L}_{+,y}^F u(t, y) = \frac{1}{2} \partial_y (a_+(y) \partial_y u(t, y)) - \partial_y (b_+(y) u(t, y)) & \text{if } y > 0. \end{cases} \quad (5.5)$$

Remark 5.1. When $\text{div}(b_\pm(y)) = 0$ at a point $y \neq 0$ (the fluid is incompressible around y), then $\partial_y (b_\pm(y) u(t, y)) = b_\pm(y) \partial_y u(t, y)$.

Remark 5.2. The conditions (5.3)-(5.4) ensure the mass conservation and the continuity of the density $u(t, y)$ at the interface. They have a natural interpretation in term of modeling [32].

The differential operator \mathcal{L}_y^F appears as the *knotting* of $\mathcal{L}_{-,y}^F$ and $\mathcal{L}_{+,y}^F$. Yet (5.5) is not sufficient to define an effective functional operator as its domain, that is the space of functions on which it acts, is not specified. In particular, the behavior at 0 shall be given [37].

Let $L^2(\mathbb{R})$ be the space of square summable functions equipped with the usual norm $\|\cdot\|_2$ and $H^1(\mathbb{R})$ be the Sobolev space of functions in $L^2(\mathbb{R})$ admitting a weak derivative in $L^2(\mathbb{R})$. When the initial mass repartition ν has a density n with respect to the Lebesgue measure which belongs to $L^2(\mathbb{R})$, the advection-diffusion equation (5.1)-(5.4) has to be understood in its variational form. Therefore, its solution $u(t, x)$ is sought in the intersection of $L^2([0, T]; H^1(\mathbb{R}))$ and $\mathcal{C}([0, T]; L^2(\mathbb{R}))$ and we are naturally lead to let \mathcal{L}_y^F act on $L^2(\mathbb{R})$. Its domain $\text{Dom}(\mathcal{L}_y^F)$ is thus defined as

$$\text{Dom}(\mathcal{L}_y^F) := \{u \in H^1(\mathbb{R}) \mid \mathcal{L}_y^F u \in L^2(\mathbb{R})\}.$$

Remark 5.3. If $u \in H^1(\mathbb{R})$ and $\mathcal{L}_y^F u \in L^2(\mathbb{R})$, then it is easily seen that $y \mapsto a(y) \partial_y u(y) + b(y) u(y)$ belongs to $H^1(\mathbb{R})$. As there exists a continuous version (the one we implicitly use) of a function in $H^1(\mathbb{R})$, $u(y)$ and $a(y) \partial_y u(y)$ are really defined for $y = 0-$ (resp. $y = 0+$) by continuity. Hence, the definition of $\text{Dom}(\mathcal{L}_y^F)$ directly implies the transmission conditions $[u]_0 = 0$ and $[a \partial_y u + b u]_0 = 0$, where $[f]_0 = f(0+) - f(0-)$ for a function f . Meanwhile, for a solution u to (5.1)-(5.2) with $u(t, \cdot) \in \text{Dom}(\mathcal{L}_x^F)$, for any $t > 0$, this naturally leads to the conditions (5.3)-(5.4).

Remark 5.4. The problem (5.1)-(5.4) can be understood as a *transmission problem* (or *diffraction problem*) which is an alternative to the weak formulation. Roughly speaking, the solution is classical away from 0 with some interface conditions at 0 [33–35].

The formulation (5.1)-(5.4) is the one used in physics. It gives the density of particles at the position y starting from a source density ν . When the initial distribution is a Dirac mass, this is a *Fokker-Planck* or a *Kolmogorov forward* equation.

5.2 Principle of particle tracking techniques

We propose to consider a particle tracking technique to solve (5.1)-(5.4). According to this technique, the concentration of the solute at time t can be derived from the positions of a plume of particles which are initially distributed with a probability measure ν . It has a natural interpretation: each particle carries some part of the mass of the solute. For that purpose, we display a stochastic process X such that $u(t, \cdot)$ is the density of $X(t)$ when the particles are initially distributed according to the measure ν . The existence of such a process, even in presence of discontinuous coefficients, follows from [55].

The solution $u(t, y)$ to (5.1)-(5.4) is given by

$$u(t, y) = \int_{\mathbb{R}} \nu(dx) q(t, x, y), \quad (5.6)$$

where kernel q is also called the *fundamental solution*. It is the *probability transition function* that governs the dynamic of the particles. Indeed, since the problem is time-homogeneous, $y \mapsto q(t, x, y)$ is the density of $X(s+t)$ given $X(s) = x$, for any $s, t \geq 0$. Hence, knowing $q(t, x, y)$ allows one to set-up a particle tracking scheme.

5.3 Dynamic of the particles and the backward formulation

The stochastic process we have to exhibit is actually the one so that

$$\lim_{t \rightarrow 0} \frac{\mathbf{E}_x[f(X(t))] - f(x)}{t} = \mathcal{L}_x^B f(x), \quad \forall f \in \text{Dom}(\mathcal{L}_x^B),$$

where \mathbf{E}_x is the expectation of X given $X(0) = x$ and \mathcal{L}_x^B is the backward operator, also called the *infinitesimal generator* of X . So the dynamic is read from the *backward operator* defined below.

5.3.1 The backward formulation

For suitable functions $\mathbf{v} : \mathbb{R}_+ \times \mathbb{R} \rightarrow \mathbb{R}$, we introduce the operator

$$\mathcal{L}_y^B \mathbf{v}(t, y) := \begin{cases} \mathcal{L}_{-,y}^B \mathbf{v}(t, y) = \frac{1}{2} \partial_y(a_-(y) \partial_y \mathbf{v}(t, y)) + b_-(y) \partial_y \mathbf{v}(t, y) & \text{if } y < 0, \\ \mathcal{L}_{+,y}^B \mathbf{v}(t, y) = \frac{1}{2} \partial_y(a_+(y) \partial_y \mathbf{v}(t, y)) + b_+(y) \partial_y \mathbf{v}(t, y) & \text{if } y > 0. \end{cases} \quad (5.7)$$

We could deal with the equation

$$\partial_t \mathbf{v}(t, y) - \mathcal{L}_y^B \mathbf{v}(t, y) = 0, \quad t > 0, \quad y \neq 0, \quad (5.8)$$

$$\mathbf{v}(t, y) \xrightarrow[t \rightarrow 0]{} f(y) \in L^2(\mathbb{R}), \quad (5.9)$$

$$a_-(t, 0-) \partial_y \mathbf{v}(t, 0-) = a_+(t, 0+) \partial_y \mathbf{v}(t, 0+), \quad (5.10)$$

$$\mathbf{v}(t, 0-) = \mathbf{v}(t, 0+). \quad (5.11)$$

As above, we define

$$\text{Dom}(\mathcal{L}_y^B) := \{\mathbf{v} \in H^1(\mathbb{R}) \mid \mathcal{L}_y^B \mathbf{v} \in L^2(\mathbb{R})\}.$$

Since $\mathcal{L}_y^B \mathbf{v} \in L^2(\mathbb{R})$ for $\mathbf{v} \in \text{Dom}(\mathcal{L}_y^B)$, $a(y)\partial_y \mathbf{v}(y) \in H^1(\mathbb{R})$. Using the same argument as in Remark 5.3, $\text{Dom}(\mathcal{L}_y^B)$ is well defined. Besides, for a variational solution \mathbf{v} to (5.8)-(5.9) with $\mathbf{v}(t, \cdot) \in \text{Dom}(\mathcal{L}_y^B)$, the condition (5.10)-(5.11) are implicitly satisfied for the proper choice of the version of $a\nabla \mathbf{v}(t, \cdot)$ which is continuous over \mathbb{R} (and so is $\mathbf{v}(t, \cdot)$). This is why no interface conditions appear in the definition of the domain of \mathcal{L}_y^B .

Here it is noteworthy to look at the reverse sign of the advective term as well as the difference in the interface conditions of the forward and backward formulations. In fact, no advective term is involved in the interface conditions for the backward formulation. See Annexe A for more details.

The solution $\mathbf{v}(t, y)$ to (5.8)-(5.11) is given by

$$\mathbf{v}(t, x) = \int_{\mathbb{R}} \mathbf{q}(t, x, y) f(y) dy. \quad (5.12)$$

Hence, the same kernel \mathbf{q} allows to consider both the forward and the backward equations (see 5.6 and 5.12).

5.3.2 The probability transition function \mathbf{q}

Let us consider the family indexed by x of solutions to (5.1)-(5.4) where the initial condition $\nu = \delta_x$, the Dirac mass at x . We denote by $\mathbf{q}(t, x, y) = \mathbf{u}(t, y)$ the elements of this family.

Proposition 5.1 ([4] or [55, Theorem II.3.8]). *There exists a transition density function $\mathbf{q}(t, x, y)$, $t > 0$, $x, y \in \mathbb{R}$ such that (\mathcal{L}_x^B applies on the x -variable, while \mathcal{L}_y^F applies on the y -variable):*

$$\begin{aligned} \partial_t \mathbf{q}(t, x, y) &= \mathcal{L}_x^B \mathbf{q}(t, x, y), \quad \forall t > 0, x, y \neq 0, \\ \partial_t \mathbf{q}(t, x, y) &= \mathcal{L}_y^F \mathbf{q}(t, x, y), \quad \forall t > 0, x, y \neq 0, \\ \mathbf{q}(t, x, y) &\xrightarrow[t \rightarrow 0]{\text{weakly}} \delta_y(x) \text{ and } \mathbf{q}(t, x, y) \xrightarrow[t \rightarrow 0]{\text{weakly}} \delta_x(y), \\ \forall t > 0, y \neq 0, x &\mapsto \mathbf{q}(t, x, y) \text{ satisfies (5.10)-(5.11),} \\ \forall t > 0, x \neq 0, y &\mapsto \mathbf{q}(t, x, y) \text{ satisfies (5.3)-(5.4).} \end{aligned}$$

In addition, the kernel $(t, x, y) \mapsto \mathbf{q}(t, x, y)$ satisfies the Chapman-Kolmogorov equation $\mathbf{q}(t + s, x, y) = \int_{\mathbb{R}} \mathbf{q}(t, x, z) \mathbf{q}(s, z, y) dz$ for any $s, t \geq 0$ and any $(x, y) \in \mathbb{R}^2$.

With suitable bounds on \mathbf{q} , it may be proved that a stochastic process X whose infinitesimal generator is \mathcal{L}_x^B exists. The resolvent kernel $\mathbf{r}(\lambda; x, y)$ of \mathcal{L}_x^B is defined as [48]:

$$\mathbf{r}(\lambda; x, y) = \int_0^{+\infty} e^{-\lambda s} \mathbf{q}(s, x, y) ds, \quad x, y \in \mathbb{R}, \lambda > 0.$$

So \mathbf{q} may be recovered through the Laplace inversion of the resolvent kernel $\mathbf{r}(\lambda; x, y)$. Consequently, we are only going to focus in the next subsection on the resolvent kernel of \mathcal{L}_x^B .

5.3.3 The resolvent kernel of \mathcal{L}_x^B

The *resolvent* of \mathcal{L}_x^B is the family of linear operator $(R_\lambda)_{\lambda>0}$ with $R_\lambda = (\lambda - \mathcal{L}_x^B)^{-1}$. It satisfies

$$R_\lambda f(x) := \int_{\mathbb{R}} \mathfrak{r}(\lambda; x, y) f(y) dy, \quad f \in L^2(\mathbb{R}). \quad (5.13)$$

Following formal application of the Laplace transform to (5.8)-(5.11), $x \mapsto \mathfrak{r}(\lambda; x, y)$ solves for any $y \in \mathbb{R}$,

$$(\lambda - \mathcal{L}_x^B) \mathfrak{r}(\lambda; x, y) = \delta_y(x). \quad (5.14)$$

Let us consider $(a, b) \in \mathfrak{C}^{\boxtimes} \times \mathfrak{B}^{\boxtimes}$, so that $(a, 1, b) \in \mathfrak{H}^{\boxtimes}$ satisfies Hypothesis 3.1.

The difference between the operators \mathcal{L}_x^B and $\mathcal{A}_{x,(a,1,b)}^B$ (with $\rho = 1$) lies in the fact that they are defined with different ambient spaces. However, we have the following connection.

Lemma 5.1. *Let $(a, 1, b) \in \mathfrak{H}^{\boxtimes}$. There exists a set D which is dense in both $\text{Dom}(\mathcal{L}_x^B)$ equipped with graph norm $f \mapsto \|f\|_{L^2(\mathbb{R})} + \|\mathcal{L}_x^B f\|_{L^2(\mathbb{R})}$ and $\text{Dom}(\mathcal{A}_{x,(a,1,b)}^B)$ also equipped with the graph norm $f \mapsto \|f\|_\infty + \|\mathcal{A}_{x,(a,1,b)}^B f\|_\infty$ such that $\mathcal{L}_x^B f = \mathcal{A}_{x,(a,1,b)}^B f$ for any $f \in D$.*

Proof. Let us define for some $\lambda > 0$

$$D := (\lambda - \mathcal{A}_{x,(a,1,b)}^B)^{-1}(\mathcal{C}_0 \cap L^2(\mathbb{R}))$$

so that $D \subset \text{Dom}(\mathcal{A}_{x,(a,1,b)}^B)$ by Proposition 2.1. The subset D does not depend on λ . Since $\mathcal{C}_0 \cap L^2(\mathbb{R})$ is dense in \mathcal{C}_0 , D is dense for the graph norm in $\text{Dom}(\mathcal{A}_{x,(a,1,b)}^B)$.

For f in D , there exists $k \in \mathcal{C}_0 \cap L^2(\mathbb{R})$ such that $(\lambda - \mathcal{A}_{x,(a,1,b)}^B) f = k$ for some $\lambda > 0$.

Let ϕ be a smooth function with compact support. An integration by parts leads to

$$\begin{aligned} \int_{\mathbb{R}} k(x) \phi(x) dx &= \int_{\mathbb{R}} \lambda f(x) \phi(x) dx - \int_{\mathbb{R}} \mathcal{A}_{x,(a,1,\rho)}^B f(x) \phi(x) dx \\ &= \int_{\mathbb{R}} \lambda f(x) \phi(x) dx + \int_{\mathbb{R}} a(x) \partial_x f(x) \partial_x \phi(x) dx + \int_{\mathbb{R}} b(x) \partial_x f(x) \phi(x) dx. \end{aligned}$$

Classical results show that f belongs to $H^1(\mathbb{R})$. This means that f is also a weak solution $(\lambda - \mathcal{L}_x^B) f = g$. Hence, it belongs to $\text{Dom}(\mathcal{L}_x^B)$. Since, $\mathcal{C}_0 \cap L^2(\mathbb{R})$ is dense in $L^2(\mathbb{R})$, it follows that D is also dense in $\text{Dom}(\mathcal{L}_x^B)$. \square

The next proposition shows that $\mathfrak{r}(\lambda; x, y)$ and consequently $\mathfrak{q}(t, x, y)$ satisfy (5.3)-(5.4) with respect to the variable y (forward equation) as well as (5.10)-(5.11) with respect to the variable x (backward equation).

Proposition 5.2. *Let $(a, 1, b) \in \mathfrak{H}^{\boxtimes}$. Let f be continuous and differentiable so that $D_x^S f$ is also continuous (such as $x \mapsto g(\lambda; x, y)$). Then $[a \partial_x f]_0 = 0$ and $[a \partial_x (fm) - b fm]_0 = 0$.*

Proof. Let $\kappa(x) = \exp(-h(x))$. With our definition of $h(x)$, $\kappa(0) = 1$ so that for $f \in \mathcal{C}_{*0}^1 \supset \text{Dom}(\mathcal{A}_{x,(a,1,b)}^B)$, for $\epsilon > 0$

$$D_x^S f(\pm\epsilon) = \frac{a(\pm\epsilon)}{\kappa(\pm\epsilon)} \partial_x f(\epsilon) \xrightarrow{\epsilon \rightarrow 0} a(0\pm) \partial_x f(0\pm).$$

Hence, $[D_x^S f]_0 = [a\partial_x f]_0$.

For m given in Proposition 2.1, $D_x^S m(x) = -b(x)/\kappa(x)^2$. Let f is such that $[f]_0 = [D_x^S f]_0 = 0$. Hence for $x \neq 0$,

$$D_x^S(fm)(x) = D_x^S f(x)m(x) + f(x)D_x^S m(x) \text{ so that } [D_x^S(fm)]_0 = [a\partial_x f - bf]_0.$$

This proves the result. □

The main result of the section is the following one. With Lemma 5.1 above, comparing (5.13) with (2.7) links the resolvent kernel $\mathfrak{r}(\lambda; x, y)$ of \mathcal{L}_x^B with ones of $\mathcal{A}_{x,(a,1,b)}^B$.

Proposition 5.3. *Let $(a, 1, b) \in \mathfrak{H}^{\text{pd}}$. The resolvent kernel $\mathfrak{r}(\lambda; x, y)$ of \mathcal{L}_x^B solution to the problem (5.14) is*

$$\mathfrak{r}(\lambda, x, y) = \mathfrak{r}_{\mathcal{A}_{x,(a,1,b)}^B}(\lambda; x, y).$$

Remark 5.5. When a and b are piecewise constant, $\mathfrak{r}_{\mathcal{A}_{x,(a,1,b)}^B}$ is given by (4.1), with $\rho = 1$, in Proposition 4.2.

6 Application to advection-diffusion problem with multiple interfaces

In Section 5, we have presented the methodology in the context of an infinite domain and a sole interface. Now we would like to handle multiple interfaces. For example, in the underground [62], interfaces may come from the high heterogeneity of the media (inclusions of rocks of different natures, fissures, ...) yielding discontinuities in the diffusivity and the advective term.

There are two possible methodologies. As said in Remark 3.3, the first one could consist in re-computing explicit expressions for the transition density function q according to given interfaces and boundary conditions. The expressions therefore changed if the number of interfaces or boundary conditions are changed. The other approach, chosen here and *e.g.* in [44], is based on an important point: the dynamic of the process X depends *mostly* on its immediate surrounding. From a practical point of view, an appropriate choice of parameters reduces the impact of other interfaces or boundary that are far enough from the current position of the particle (with respect to the time scale at which the algorithm is applied).

With this approach, the idea is first to define different zones as proposed in [44]:

- a *continuity zone* far enough from the discontinuities to guarantee with a high level of confidence no crossing of the interfaces,
- *interface layers*, around the discontinuities,

and to combine its respective algorithm, given below (one per zone).

Remark 6.1. In bounded domains with prescribed boundary conditions, boundary layers could be considered as well (see for example in [44]).

6.1 Algorithm in the continuity zone (far from the discontinuities)

In the *continuity zone*, one can respectively associate to $\mathcal{L}_{-,y}^B$ and $\mathcal{L}_{+,y}^B$ (defined on the free space) the stochastic processes X_- and X_+ , whose positions at time $t + \Delta t$ when $X_{\pm}(t) = x_{\pm}$ are

$$X_-(t + \Delta t) = x_- + \sqrt{a_-(x_-)}(W_{t+\Delta t} - W_t) + b_-(x_-) \Delta t, \quad (6.1)$$

$$X_+(t + \Delta t) = x_+ + \sqrt{a_+(x_+)}(W_{t+\Delta t} - W_t) + b_+(x_+) \Delta t. \quad (6.2)$$

Here W is as usual a Brownian motion.

As the process X is Markov, the distribution of $X(t + \Delta t)$ given $X(t)$ is the same as the one of $X(\Delta t)$ given $X(0)$. The same holds for X_+ and X_- . Hence, we equally deal in what follows with the distribution of $X(\Delta t)$ given $X(0)$ or the one of $X(t + \Delta t)$ given $X(t)$.

Let X be the process generated by $(\mathcal{L}_x^B, \text{Dom}(\mathcal{L}_x^B))$, $\tau = \inf\{t > 0 \mid X(t) = 0\}$ and $\tau_{\pm} = \inf\{t > 0 \mid X_{\pm}(t) = 0\}$. When $X(0) = 0$,

$$X(\Delta t)\mathbb{1}_{\Delta t < \tau} \stackrel{\text{law}}{=} \begin{cases} X_+(\Delta t)\mathbb{1}_{\Delta t < \tau_+} & \text{with } X_+(0) = x \text{ if } x > 0, \\ X_-(\Delta t)\mathbb{1}_{\Delta t < \tau_-} & \text{with } X_-(0) = x \text{ if } x < 0. \end{cases}$$

The probability that X_{\pm} crosses 0 before Δt decreases at exponential as $|X_{\pm}(0)|$ increases. This event is $\{\tau < \Delta t\}$. Far from the interface, in the continuity zone, the position of X after a time step Δt is easily simulated through the Euler scheme with (6.1)-(6.2).

6.2 Algorithm in the interface layer

In the *interface layer*, even if a stochastic process X may be associated to \mathcal{L}_x^B given by (5.7), it is no longer solution to a stochastic differential equation and its short time behavior is no longer close to a Gaussian distribution. Then when $X(s)$ is in the interface layer, we use the density q of X associated to \mathcal{L}_x^B given as the Laplace inversion of the resolvent kernel of \mathcal{L}_x^B , whose expression is given in Proposition 5.3 in Section 5.

Remark 6.2. If the expression of q is cumbersome, one could also consider a scheme based on the resolvent $\mathfrak{r}(\lambda, x, y)$ as the one proposed in [41].

6.3 A general algorithm

Thanks to the Markov property of the process, which is reflected in the Chapman-Kolmogorov equation, a general algorithm for particle tracking Monte Carlo method in which we simulate the successive positions $X(k\Delta t)$ of the particles at times $k\Delta t$, $k = 0, 1, 2, \dots$ is obtained by a combination of the previous algorithms as follows:

- in the *continuity zone*, we use (6.1) or (6.2),
- in the *interface layers*, we use the expression of $q(\Delta t, x, y)$ that can be obtained as described in Subsection 6.2.

Finally, this leads to a very simple algorithm that does not require extra computation of resolvent kernels or transition density functions according to given interfaces and boundary conditions. That is why we consider in Section 5 only one interface in the free space as it is sufficient to set up a numerical algorithm to handle multiples interfaces.

Conclusion

We have shown how to compute analytic expressions of the resolvent kernel of a one-dimensional second-order differential operator with discontinuous coefficients obtained by knotting two operators with continuous coefficients. We then have shown the effectiveness of this procedure by dealing with the case of piecewise constant coefficients. This leads us to a relatively simple closed form expression for the resolvent. By inverting Laplace transforms, we then obtain some expressions for the transition density functions. We recover some formula already known that were derived by probabilistic means and derive a new one. We also show that these formula have interest in the simulation of advection-diffusion problems with discontinuous coefficients using particle tracking algorithms. Finally, we propose a general algorithm to consider the case of multiple interfaces of discontinuities. The general multidimensional case remains open.

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A Differences in interface conditions between the forward and the backward formulation.

Even though the next proposition is well known and valid for much more weaker conditions on coefficients, we give a proof in order to highlight the role of the interface conditions, and to explain why they differ between the forward and the backward formulations.

Proposition A.1. *The adjoint of $(\mathcal{L}_y^F, \text{Dom}(\mathcal{L}_y^F))$ is $(\mathcal{L}_y^B, \text{Dom}(\mathcal{L}_y^B))$ in $L^2(\mathbb{R})$.*

Proof. Let $u \in \text{Dom}(\mathcal{L}_y^F)$ (which means that we consider the version of u given by Remark 5.3). Multiplying $\mathcal{L}_y^F u$ by a test function $v \in \text{Dom}(\mathcal{L}_y^B)$ and integrating by part leads to

$$\begin{aligned} \int_{-\infty}^0 \mathcal{L}_{-,y}^F u(y) v(y) dy &= \int_{-\infty}^0 u(y) \mathcal{L}_{-,y}^B v(y) dy \\ &+ \frac{a_-(0-)}{2} u(0-) \partial_y v(0-) + \frac{a_-(0-)}{2} v(0-) \partial_y u(0-) - b_-(0-) u(0-) v(0-) \end{aligned} \quad (\text{A.1})$$

and

$$\begin{aligned} \int_0^{+\infty} \mathcal{L}_{+,y}^F u(y) v(y) dy &= \int_0^{+\infty} u(y) \mathcal{L}_{+,y}^B v(y) dy \\ &- u(0+) \frac{a_+(0+)}{2} \partial_y v(0+) - v(0+) \partial_y u(0+) + b_+(0+) u(0+) v(0+). \end{aligned} \quad (\text{A.2})$$

Then, thanks to the conditions (5.4) and (5.11) on the sum of (A.1)-(A.2),

$$\int_{-\infty}^{+\infty} \mathcal{L}_y^F u(y) v(y) dy = \int_{-\infty}^{+\infty} u(y) \mathcal{L}_y^B v(y) dy - u(0+) \left[\frac{a}{2} \partial_y v \right]_0 - \left[\frac{a}{2} \partial_y u - bu \right]_0 v(0+)$$

where $[f]_0 = f(0) + -f(0-)$ for a continuous function.

Finally, using conditions (5.10) and (5.3),

$$\int_{-\infty}^{+\infty} \mathcal{L}_y^F \mathbf{u}(y) \mathbf{v}(y) dy = \int_{-\infty}^{+\infty} \mathbf{u}(y) \mathcal{L}_y^B \mathbf{v}(y) dy, \quad \forall (\mathbf{u}, \mathbf{v}) \in \text{Dom}(\mathcal{L}_y^F) \times \text{Dom}(\mathcal{L}_y^B).$$

Such a relation holds only if $\mathcal{L}_y^B \mathbf{v} \in L^2(\mathbb{R})$ and (5.10)-(5.11) are satisfied. This is then sufficient to characterize $(\mathcal{L}_y^B, \text{Dom}(\mathcal{L}_y^B))$ as the adjoint of $(\mathcal{L}_y^F, \text{Dom}(\mathcal{L}_y^F))$ in $L^2(\mathbb{R})$. \square

B Two extra results in Laplace inversion.

To compute the transition density function in the constant Péclet case ($\mu = 0$) (See the proof of Proposition 4.4), we need the following two extra results in Laplace inversion.

Lemma B.1 ([45]). For $k, d > 0$,

$$\mathcal{L}^{-1} \left(\frac{e^{-k\sqrt{s}}}{(s-d)\sqrt{s}} \right) = \frac{e^{dt}}{2\sqrt{d}} e^{-k\sqrt{d}} \operatorname{erfc} \left(\frac{k}{2\sqrt{t}} - \sqrt{dt} \right) - \frac{e^{dt}}{2\sqrt{d}} e^{k\sqrt{d}} \operatorname{erfc} \left(\frac{k}{2\sqrt{t}} + \sqrt{dt} \right).$$

Lemma B.2. For $a \in \mathbb{R}$,

$$\begin{aligned} \mathcal{L}^{-1} \left(\sqrt{a+s} e^{-\sqrt{s}y} \right) (t, y) &= \frac{1}{\pi} \int_0^a \sin(y\sqrt{r}) \sqrt{a-r} e^{-rt} dr \\ &\quad - \frac{1}{\pi} \int_0^{+\infty} \cos(y\sqrt{r+a}) \sqrt{r} e^{-(r+a)t} dr. \end{aligned}$$

Proof. Inspired by [51], we use the Bromwich formula with the contour Γ illustrated in Figure 5.

Since the integrals on the outer and inner arcs as well as half-circles are null,

$$\begin{aligned} \mathcal{L}^{-1} \left(\sqrt{a+s} e^{-\sqrt{s}y} \right) (r, y) &= \frac{1}{2i\pi} \int_{\gamma-i\infty}^{\gamma+i\infty} \sqrt{a+s} e^{-y\sqrt{s}} e^{st} ds \\ &= \frac{1}{2i\pi} \left(\int_0^a (e^{iy\sqrt{r}} - e^{-iy\sqrt{r}}) \sqrt{a-r} e^{-rt} dr - \int_a^{+\infty} (e^{iy\sqrt{r}} + e^{-iy\sqrt{r}}) i\sqrt{r-a} e^{-rt} dr \right), \end{aligned}$$

and the result follows. \square

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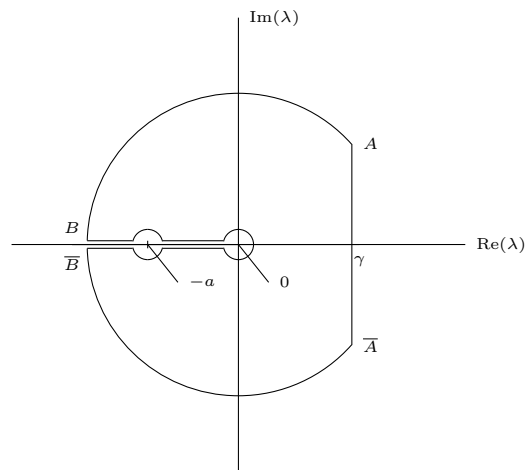


Figure 5: The contour Γ .

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