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Abstract

In this article, we provide a general methodology to compute the resolvent kernel as well as the density when available for a one-dimensional second-order differential operators with discontinuous coefficients. In a sequel, the computed resolvent kernel will be used to set-up an efficient and accurate simulation scheme.

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

1 Introduction

Diffusive phenomena in media with permeable or semi-permeable barriers, often called *skew diffusions*, are ubiquitous. Precisely, they can be encountered in (with only a few references) geophysics for soil [10, 24, 26, 43, 48], air [47] and ocean [45]; astrophysics [53]; molecular dynamics [7]; population ecology [8, 30]; finance [9, 21, 51], ... Examples of such media with permeable or semi-permeable barrier in thermodynamics or electronics are the materials built with layers of 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.

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In this article, our motivation is to simulate the diffusive phenomena in heterogeneous media which is modeled by an advection-diffusion equation with discontinuous coefficients. To illustrate the interest of this particular phenomena, we consider the propagation of a solute in the underground [54]. In this case, due to the high heterogeneity of the media (inclusions of rocks of different natures, fissures, ...), there is absolutely no reason for the diffusivity and the advective term in the advection-diffusion equation which govern the transport of this solute to be continuous. As it will be discussed, discontinuities are seen as permeable barriers which impose some conditions on the mass of a solute as well as on its flow.

The main contribution of this paper is to address the problem of obtaining explicit, closed form formula for the resolvent (or Green) kernel and the density for a one-dimensional medium with a diffusivivity a and an advective (drift) term b that may be discontinuous at the same place. To do so, we consider the advection-diffusion in free space with only a single barrier. Not only our method is easily generalized to deal with multiple interfaces and boundary conditions, but also the formula we provide here may be sufficient for numerical purposes. The formula we propose generalize the one obtained by the *method of images* when the symmetries in the coefficients allow it [52]. It also allows to derive density transition functions, traditionally computed through probabilistic arguments [2, 6, 14, 20, 50].

In addition, our contribution could also be applied to multidimensional media with a structure close to one dimensional media (graphs, orthotropic diffusivity with plane discontinuities, ...) or to coefficients that are discontinuous at different positions. Hence, the results here extend the ones of [23] in which no advection term was treated.

Moreover, such closed form formula open the door to numerical simulation using a class of Monte Carlo methods called *particles tracking techniques* [44, 54]. In a sequel [34], we use the expressions of the resolvent kernel obtained in this article in a new and efficient numerical scheme which allows to simulate the case where both the diffusivity and the drift term may be discontinuous. Compared to other schemes in the literature, this is a novelty: in [13, 14, 33, 36, 39, 5, 24, 44, 48], the proposed scheme do not take an advective term $b \neq 0$ into account. In [12, 35] (random walk based methods) — which are not sensitive with regard to the values of the drifts — as well as in [11, 14] (*exact simulation techniques*), either a or b is discontinuous but not both. In [34], we show in particular that the resolvent kernel is a useful tool to deal with the transient regime as well while relying on much more simpler expressions than the density transition function. The general multidimensional case remains open.

Outline. The present article is divided in two sections which can be read almost independently. The second section contained explicit formula for the case of piecewise constant coefficients and one can go directly to it without difficulties.

In Section 2, we explain the relationship between the forward (Fokker-Planck) and the backward equations. Then we provide a general methodology to derive analytic closed form expression for the density transition function and resolvent kernel associated to the Fokker-Planck equation in presence of discontinuities. In particular, we compute the resolvent kernel from particular, analytic functions obtained from simpler problems without discontinuity.

In Section 3, 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. With inverse Laplace transforms, we derive some explicit expressions for the density transition function (or the fundamental solution) for some particular situations, from which we recover some known results by a simple way and provide a new one.

2 Problem settings: coefficients with a discontinuity at 0.

Let $\mathcal{C}(I, J)$ be the class of continuous functions from I to J. For ξ_+ and ξ_- in $\mathcal{C}(\mathbb{R}, \mathbb{R}^d)$ where $d \geq 1$, we define their *knotting* as

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

and associate the sets $\mathfrak{C}^{\bowtie}(\mathbb{R}^d)$ and $\mathfrak{B}^{\bowtie}(\mathbb{R}^d)$, containing every *knotting* of two functions which respectively belong to the sets

$$\mathfrak{C} := \big\{ a \in \mathcal{C}(\mathbb{R}, \mathbb{R}^d) \,\big|\, 0 < c \leq a(x) \leq C, \forall x \in \mathbb{R} \text{ for } c, C > 0 \big\},$$

and

$$\mathfrak{B} := \big\{ b \in \mathcal{C}(\mathbb{R}, \mathbb{R}^d) \,\big|\, \|b\|_\infty \leq C \big\},$$

where $\|\cdot\|_\infty$ is the uniform norm.

Remark 2.1. The elements of $\mathfrak{C}^{\bowtie}$ and $\mathfrak{B}^{\bowtie}$ might be continuous or discontinuous at 0. Here we are naturally interested by discontinuous functions.

Remark 2.2. We choose to *knot* functions at 0 for convenience of the presentation. Actually, everything we are going to 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 *knotting*.

2.1 The advection-diffusion problem with discontinuous coefficients

Let us consider a solute evolving in an infinite one dimensional porous medium described by a diffusivity $a = a_- \bowtie a_+ \in \mathfrak{C}^{\bowtie}$ and an advective force $b = b_- \bowtie b_+ \in \mathfrak{B}^{\bowtie}$. The point $y = 0$ is then an interface between two layers possessing different diffusion/advective coefficients.

According to the Lagrangian point of view, 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 and whose concentration $\mathfrak{u}(t, \cdot)$ at time t is given by the solution of the advection-diffusion equation:

$$\partial_t \mathfrak{u}(t, y) - \mathcal{L}_y^F \mathfrak{u}(t, y) = 0, \ t > 0, \ y \neq 0, \tag{2.1}$$

$$\mathfrak{u}(t, \cdot) \xrightarrow[t\to 0]{\text{weakly}} \nu, \tag{2.2}$$

$$a_-(0-)\partial_y \mathfrak{u}(t, 0-) - b_-(0-)\mathfrak{u}(t, 0-) = a_+(0+)\partial_y \mathfrak{u}(t, 0+) - b_+(0+)\mathfrak{u}(t, 0+), \tag{2.3}$$

$$\mathfrak{u}(t, 0-) = \mathfrak{u}(t, 0+), \tag{2.4}$$

where

$$\mathcal{L}_y^F \mathfrak{u}(t, y) = \begin{cases} \mathcal{L}_{-,y}^F \mathfrak{u}(t, y) = \dfrac{1}{2}\partial_y(a_-(y)\partial_y \mathfrak{u}(t, y)) - \partial_y(b_-(y)\mathfrak{u}(t, y)) & \text{if } y < 0, \\ \mathcal{L}_{+,y}^F \mathfrak{u}(t, y) = \dfrac{1}{2}\partial_y(a_+(y)\partial_y \mathfrak{u}(t, y)) - \partial_y(b_+(y)\mathfrak{u}(t, y)) & \text{if } y > 0. \end{cases} \tag{2.5}$$

Remark 2.3. When $\operatorname{div}(b_\pm(y)) = 0$ at a point $y \neq 0$ (the fluid is incompressible around y), then $\partial_y(b_\pm(y)\mathfrak{u}(t, y)) = b_\pm(y)\partial_y \mathfrak{u}(t, y)$.

Remark 2.4. The conditions (2.3)-(2.4) ensure the mass conservation and the continuity of the density $\mathfrak{u}(t,y)$ at the interface. They have a completely natural interpretation in term of modeling.

The differential operator $\mathcal{L}_y^F$ appears as the *knotting* of $\mathcal{L}_{-,y}^F$ and $\mathcal{L}_{+,y}^F$. Yet (2.5) 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 [31].

Let $\mathrm{L}^2(\mathbb{R})$ be the space of square summable functions equipped with the usual norm $\|\cdot\|_2$ and $\mathrm{H}^1(\mathbb{R})$ be the Sobolev space of functions in $\mathrm{L}^2(\mathbb{R})$ admitting a weak derivative in $\mathrm{L}^2(\mathbb{R})$. When the initial mass repartition ν has a density n with respect to the Lebesgue measure which belongs to $\mathrm{L}^2(\mathbb{R})$, then the advection-diffusion equation (2.1)-(2.4) has to be understood in its variational form. Therefore, its solution $\mathfrak{u}(t,x)$ is sought in the intersection of $\mathrm{L}^2([0,T];\mathrm{H}^1(\mathbb{R}))$ and $\mathcal{C}([0,T];\mathrm{L}^2(\mathbb{R}))$ and we are naturally lead to let $\mathcal{L}_y^F$ act on $\mathrm{L}^2(\mathbb{R})$. Its domain $\mathrm{Dom}(\mathcal{L}_y^F)$ is thus defined as

$$\mathrm{Dom}(\mathcal{L}_y^F) := \big\{\mathfrak{u} \in \mathrm{H}^1(\mathbb{R}) \;\big|\; \mathcal{L}_y^F\mathfrak{u} \in \mathrm{L}^2(\mathbb{R})\big\}.$$

Remark 2.5. If $\mathfrak{u} \in \mathrm{H}^1(\mathbb{R})$ and $\mathcal{L}_y^F\mathfrak{u} \in \mathrm{L}^2(\mathbb{R})$, then it is easily seen that $y \mapsto a(y)\partial_y\mathfrak{u}(y) + b(y)\mathfrak{u}(y)$ belongs to $\mathrm{H}^1(\mathbb{R})$. As there exists a continuous version (the one we implicitly use) of a function in $\mathrm{H}^1(\mathbb{R})$, $\mathfrak{u}(y)$ and $a(y)\partial_y\mathfrak{u}(y)$ are really defined for $y = 0-$ (resp. $y = 0+$) by continuity. Hence, the definition of $\mathrm{Dom}(\mathcal{L}_y^F)$ directly implies the transmission conditions $[\mathfrak{u}]_0 = 0$ and $[a\partial_y\mathfrak{u} + b\mathfrak{u}]_0 = 0$, where $[f]_0 = f(0+) - f(0-)$ for a function f. Meanwhile, for a solution $\mathfrak{u}$ to (2.1)-(2.2) with $\mathfrak{u}(t,\cdot) \in \mathrm{Dom}(\mathcal{L}_x^F)$, for any $t > 0$, this naturally leads to the conditions (2.3)-(2.4).

Remark 2.6. The problem (2.1)-(2.4) 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 [27, 28, 29].

The formulation (2.1)-(2.4) 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. We refer it as the *forward formulation*. On the other hand, the *backward formulation* presented below is the classical one used for defining and studying stochastic processes [22, 49].

2.2 The backward formulation

For suitable functions $\mathfrak{v} : \mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}$, we introduce similarly to (2.5) the operator

$$\mathcal{L}_y^B\mathfrak{v}(t,y) := \begin{cases} \mathcal{L}_{-,y}^B\mathfrak{v}(t,y) = \dfrac{1}{2}\partial_y(a_-(y)\partial_y\mathfrak{v}(t,y)) + b_-(y)\partial_y\mathfrak{v}(t,y) & \text{if } y < 0, \\ \mathcal{L}_{+,y}^B\mathfrak{v}(y) = \dfrac{1}{2}\partial_y(a_+(y)\partial_y\mathfrak{v}(t,y)) + b_+(y)\partial_y\mathfrak{v}(t,y) & \text{if } y > 0. \end{cases} \tag{2.6}$$

Hence we could deal with the equation

$$\partial_t\mathfrak{v}(t,y) - \mathcal{L}_y^B\mathfrak{v}(t,y) = 0,\ t > 0,\ y \neq 0, \tag{2.7}$$

$$\mathfrak{v}(t,y) \xrightarrow[t\to 0]{} f(y) \in \mathrm{L}^2(\mathbb{R}), \tag{2.8}$$

$$a_-(t,0-)\partial_y\mathfrak{v}(t,0-) = a_+(t,0+)\partial_y\mathfrak{v}(t,0+), \tag{2.9}$$

$$\mathfrak{v}(t,0-) = \mathfrak{v}(t,0+). \tag{2.10}$$

As above, we define

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

Since $\mathcal{L}_y^B \mathfrak{v} \in \mathrm{L}^2(\mathbb{R})$ for $\mathfrak{v} \in \mathrm{Dom}(\mathcal{L}_y^B)$, $a(y)\partial_y \mathfrak{v}(y) \in \mathrm{H}^1(\mathbb{R})$. Using the same argument as in Remark 2.5, $\mathrm{Dom}(\mathcal{L}_y^B)$ is well defined. Besides, for a variational solution $\mathfrak{v}$ to (2.7)-(2.8) with $\mathfrak{v}(t,\cdot) \in \mathrm{Dom}(\mathcal{L}_y^B)$, the condition (2.9)-(2.10) are implicitly satisfied for the proper choice of the version of $a\nabla \mathfrak{v}(t,\cdot)$ which is continuous over $\mathbb{R}$ (and so is $\mathfrak{v}(t,\cdot)$). 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 both formulations. In fact, no advective term is involved in the interface conditions for 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 2.1. *The adjoint of* $(\mathcal{L}_y^F, \mathrm{Dom}(\mathcal{L}_y^F))$ *is* $(\mathcal{L}_y^B, \mathrm{Dom}(\mathcal{L}_y^B))$ *in* $\mathrm{L}^2(\mathbb{R})$.

Proof. Let $\mathfrak{u} \in \mathrm{Dom}(\mathcal{L}_y^F)$ (which means that we consider the version of $\mathfrak{u}$ given by Remark 2.5). Multiplying $\mathcal{L}_y^F \mathfrak{u}$ by a test function $\mathfrak{v} \in \mathrm{Dom}(\mathcal{L}_y^B)$ and integrating by part leads to

$$\begin{aligned}\int_{-\infty}^{0} \mathcal{L}_{-,y}^F \mathfrak{u}(y)\mathfrak{v}(y)\,\mathrm{d}y = \int_{-\infty}^{0} \mathfrak{u}(y)\mathcal{L}_{-,y}^B \mathfrak{v}(y)\,\mathrm{d}y \\ + \frac{a_-(0-)}{2}\mathfrak{u}(0-)\partial_y \mathfrak{v}(0-) + \frac{a_-(0-)}{2}\mathfrak{v}(0-)\partial_y \mathfrak{u}(0-) - b_-(0-)\mathfrak{u}(0-)\mathfrak{v}(0-) \quad (2.11)\end{aligned}$$

and

$$\begin{aligned}\int_{0}^{+\infty} \mathcal{L}_{+,y}^F \mathfrak{u}(y)\mathfrak{v}(y)\,\mathrm{d}y = \int_{0}^{+\infty} \mathfrak{u}(y)\mathcal{L}_{+,y}^B \mathfrak{v}(y)\,\mathrm{d}y \\ - \mathfrak{u}(0+)\frac{a_+(0+)}{2}\partial_y \mathfrak{v}(0+) - \mathfrak{v}(0+)\partial_y \mathfrak{u}(0+) + b_+(0+)\mathfrak{u}(0+)\mathfrak{v}(0+). \quad (2.12)\end{aligned}$$

Then, thanks to the conditions (2.4) and (2.10) on the sum of (2.11)-(2.12),

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

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

Finally, using conditions (2.9) and (2.3),

$$\int_{-\infty}^{+\infty} \mathcal{L}_y^F \mathfrak{u}(y)\mathfrak{v}(y)\,\mathrm{d}y = \int_{-\infty}^{+\infty} \mathfrak{u}(y)\mathcal{L}_y^B \mathfrak{v}(y)\,\mathrm{d}y,\ \forall (\mathfrak{u},\mathfrak{v}) \in \mathrm{Dom}(\mathcal{L}_y^F) \times \mathrm{Dom}(\mathcal{L}_y^B).$$

Such a relation holds only if $\mathcal{L}_y^B \mathfrak{v} \in \mathrm{L}^2(\mathbb{R})$ and (2.9)-(2.10) are satisfied. This is then sufficient to characterize $(\mathcal{L}_y^B, \mathrm{Dom}(\mathcal{L}_y^B))$ as the adjoint of $(\mathcal{L}_y^F, \mathrm{Dom}(\mathcal{L}_y^F))$ in $\mathrm{L}^2(\mathbb{R})$. □

2.3 Characterization of the probability transition function

One of the motivations of this paper is the design of particle tracking techniques to solve (2.1)-(2.4). For that purpose, we display a stochastic process X such that $\mathfrak{u}(t,\cdot)$ is the density of $X(t)$ when the particles are initially distributed according to the measure ν.

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

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

where $\mathbf{E}_x$ is the expectation of X given $X(0)=x$. The backward operator $\mathcal{L}_x^B$ is called the *infinitesimal generator* of X. This is one of the reasons why we decide to deal with the backward formulation.

Let us consider the family indiced by x of solutions to (2.1)-(2.4) where the initial condition $\nu=\delta_x$, the Dirac mass at x. We denotes by $\mathfrak{q}(t,x,y)=\mathfrak{u}(t,y)$ the elements of this family.

This function $\mathfrak{q}(t,x,y)$, called a *probability transition function*, has a lot of important properties. In particular, $y\mapsto\mathfrak{q}(t,x,y)$ is the density of $X(s+t)$ given $X(s)=x$, for any $s,t\geq 0$, since the problem is time-homogeneous. Hence, knowing $\mathfrak{q}(t,x,y)$ allows one to set-up a numerical scheme or to study the properties of the process (see Section 2.4).

Proposition 2.2 ([4] or [46, Theorem II.3.8])**.** *There exists a kernel $\mathfrak{q}(t,x,y)$, $t>0$, $x,y\in\mathbb{R}$ such that ($\mathcal{L}_x^B$ applies on the x-variable, while $\mathcal{L}_y^F$ applies on the y-variable):*

$$\begin{gathered}
\partial_t\mathfrak{q}(t,x,y)=\mathcal{L}_x^B\mathfrak{q}(t,x,y),\ \forall t>0,\ x,y\neq 0,\\
\partial_t\mathfrak{q}(t,x,y)=\mathcal{L}_y^F\mathfrak{q}(t,x,y),\ \forall t>0,\ x,y\neq 0,\\
\mathfrak{q}(t,x,y)\xrightarrow[t\to 0]{\text{weakly}}\delta_y(x)\ \textit{and}\ \mathfrak{q}(t,x,y)\xrightarrow[t\to 0]{\text{weakly}}\delta_x(y),\\
\forall t>0,\ y\neq 0,\ x\mapsto\mathfrak{q}(t,x,y)\ \textit{satisfies}\ (2.9)\text{-}(2.10),\\
\forall t>0,\ x\neq 0,\ y\mapsto\mathfrak{q}(t,x,y)\ \textit{satisfies}\ (2.3)\text{-}(2.4).
\end{gathered}$$

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

This kernel $\mathfrak{q}$ is also called the *fundamental solution*. The solution $\mathfrak{u}(t,y)$ to (2.1)-(2.4) as well as the solution $\mathfrak{v}(t,y)$ to (2.7)-(2.10) are then given by

$$\mathfrak{u}(t,y)=\int_{\mathbb{R}}\nu(\,\mathrm{d}x)\mathfrak{q}(t,x,y)\ \text{and}\ \mathfrak{v}(t,x)=\int_{\mathbb{R}}\mathfrak{q}(t,x,y)f(y)\,\mathrm{d}y. \tag{2.13}$$

Hence, the same kernel $\mathfrak{q}$ allows to consider both the forward and the backward equations. With suitable bounds on $\mathfrak{q}$, it may be proved that a stochastic process X whose infinitesimal generator is $\mathcal{L}_x^B$ exists.

Corollary 2.1 ([46, Theorem II.3.8])**.** *The operator $(\mathcal{L}_x^B,\mathrm{Dom}(\mathcal{L}_x^B))$ is the infinitesimal generator of a Feller (hence strong Markov) process X with continuous paths.*

2.4 Application to a particle tracking technique

When a and b are not discontinuous but constant on the entire domain, a stochastic process X may be associated to the forward operator $\frac{1}{2}a\partial_y^2 \cdot - \partial_y(b\cdot) = \frac{1}{2}a\partial_y^2 \cdot - b \cdot \partial_y \cdot$. For each $t \geq 0$, the dynamic of this X is simply $X(t) = x + \sqrt{2a}W_t + bt$ where W is a Brownian motion. This dynamic is read from the backward operator $\frac{1}{2}\partial_y^2 \cdot + b \cdot \partial_y$ which explains why the sign in front of the drift changes.

In this paper, both a and b may be discontinuous. In this case, two possible methodologies can be derived to simulate such a process. The first one consists in using explicit expressions for the density transition function $\mathfrak{q}$ according to the interfaces and the boundary conditions. The expressions therefore changed if the boundary conditions are changed. The other approach, chosen here and *e.g.* in [37], 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). That is why we consider only one interface in the free space as it may be sufficient to set up numerical algorithms up to neglecting errors due to event with a very low probability of appearance.

A possible choice is to combine algorithms in different zones as proposed in [37]:

- a *continuity zone* far enough from the discontinuity to guarantee with a high level of confidence no crossing of the interface,
- an *interface layer*, around the discontinuity.

Remark 2.7. In bounded domains with prescribed boundary conditions, boundary layers could be considered as well (see for example in [37]).

In the *continuity zone*, one can respectively associate to $\mathcal{L}^B_{-,y}$ and $\mathcal{L}^B_{+,y}$ (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

$$X_-(t + \Delta t) = x_- + \sqrt{2\, a_-(x_-)}(W_{t+\Delta t} - W_t) + b_-(x_-)\, \Delta t, \tag{2.14}$$

$$X_+(t + \Delta t) = x_+ + \sqrt{2\, a_+(x_+)}(W_{t+\Delta t} - W_t) + b_+(x_+)\, \Delta t. \tag{2.15}$$

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 $(\mathcal{L}^B_x, \mathrm{Dom}(\mathcal{L}^B_x))$, $\tau = \inf\{t > 0 \mid X(t) = 0\}$ and $\tau_\pm = \inf\{t > 0 \mid X_\pm(t) = 0\}$. When $X(0) = 0$,

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

Therefore, far from the discontinuity and up to neglecting the event $\{\tau < \Delta t\}$, that the particle crosses 0 before Δt, the distribution of $X_\pm(\Delta t)$ approximates the one of $X(\Delta t)$ with $X_\pm(0) = x$. Thanks to the exponential decay of the probability of $\{\tau < \Delta t\}$ regarding the distance between the interface and the starting point. Hence, the successive positions of X at times $\Delta t, 2\Delta t, \ldots$ can easily be simulated through the Euler scheme. Indeed, from (2.14), the distribution of $X(t + \Delta t)$ given $X(t) = x$ is close to the one of a Gaussian distribution with mean $b_\pm(x)\Delta t$

and variance $2a_{\pm}(x)\Delta t$ where the choice of $+$ or $-$ depends on the sign of x. Yet such an approximation is only valid far from the interface.

In the *interface layer*, when $X(s)$ is close to the discontinuity, we have to design a specific way of simulating $X(s+\Delta t)$ when $X(s)$ is known. The reason is the following. Even if a stochastic process X may be associated to $\mathcal{L}_x^B$ given by (2.6), it is no longer solution to a stochastic differential equation and its short time behavior is no longer close to a Gaussian distribution. One main goal is thus to derive the density $\mathfrak{q}$ of X associated to $\mathcal{L}_x^B$ in the interface layer.

Thanks to the Markov property of the process, which is reflected in the Chapman-Kolmogorov equation, knowing how to approximate $\mathfrak{q}(\Delta t, x, y)$ in the interface layer (for x close to 0) as well as using (2.14) or (2.15) in the zone of constant diffusivity (or any other suitable scheme) is sufficient to set up a particle tracking Monte Carlo method in which we simulate the successive positions $X(k\Delta t)$ of the particles at times $k\Delta t$, $k = 0, 1, 2, \ldots$.

Finally, not only this leads to usually very simple algorithms, but also it has a natural interpretation: each particle carries some part of the mass of the solute.

2.5 Computation of resolvent kernels

We have motivated our interest for the density as a way to construct particle tracking schemes. As we will see later on, even if the coefficients are simply piecewise constant in free space with only one discontinuity, the expression of $\mathfrak{q}$ may be cumbersome. Yet we will derive in a subsequent paper a scheme which use the resolvent kernel [34] in spite of $\mathfrak{q}$ as it is simpler to compute. Moreover $\mathfrak{q}$ may be recovered from the resolvent kernel [40] through the inversion of the Laplace's transform. Consequently, we are only going to focus in this paper on the resolvent kernel.

2.5.1 The resolvent kernel

We recall here two classical definitions and a property.

The *resolvent kernel* is the Laplace transform of the density kernel $\mathfrak{q}$, that is

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

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

$$R_\lambda f(x) := \int_{\mathbb{R}} \mathfrak{r}(\lambda; x, y) f(y)\,\mathrm{d}y,\ f \in \mathrm{L}^2(\mathbb{R}). \tag{2.16}$$

Following formal application of the Laplace transform to (2.7)-(2.10), $x \mapsto \mathfrak{r}(\lambda; x, y)$ solves for any $y \in \mathbb{R}$,

$$(\lambda - \mathcal{L}_x^B)\mathfrak{r}(\lambda; x, y) = \delta_y(x). \tag{2.17}$$

2.5.2 Differential operators and their factorized forms

We now consider a different class of operators whose properties will be used to obtain an explicit expression of the resolvent kernel. In Section 2.6 below, we will link this new class of operators with the ones which we consider in Section 2.2.

The sets of coefficients we consider is, for some constants $0 < c \leq C$,

$$\begin{aligned}\mathfrak{M} &= \big\{(a,\rho,b) : \mathbb{R} \to \mathbb{R}^3 \text{ measurable } \big|\, 0 < c \leq a(x), \rho(x) \leq C,\ |b(x)| \leq C\big\},\\ \mathfrak{H} &= \big\{(a,\rho,b) : \mathbb{R} \to \mathbb{R}^3 \,\big|\, a,\rho \in \mathfrak{C},\ b \in \mathfrak{B}\big\} \subset \mathfrak{M},\\ \text{and } \mathfrak{H}^{\bowtie} &= \big\{(a,\rho,b) : \mathbb{R} \to \mathbb{R}^3 \,\big|\, a,\rho \in \mathfrak{C}^{\bowtie}, b \in \mathfrak{B}^{\bowtie}\big\} \subset \mathfrak{M}.\end{aligned}$$

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 $(a,\rho,b) \in \mathfrak{H}$, we associate the differential (backward) operator

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

Following the approach of W. Feller, we look at a *factorized form* of $\mathcal{A}^B_{x,(a,\rho,b)}$ [19]. There are several reasons to use it. It is particularly suitable for a proper definition of the interface conditions as well as 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 $G : \mathbb{R} \to \mathbb{R}$ is defined as*

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

when the limit exists.

Remark 2.8. When $G(x) = x$, the differentiability is just the classical differentiability. Hence, we write ∂_x in spite of $\mathrm{D}^{G:x\mapsto x}_x$.

Proposition 2.3. *Let $(a,\rho,b) \in \mathfrak{M}$. The differential operator $\mathcal{A}^B_{x,(a,\rho,b)}$ is well defined and can be factorized as:*

$$\mathcal{A}^B_{x,(a,\rho,b)} = \frac{1}{2}\mathrm{D}^M_x \mathrm{D}^S_x,$$

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

$$S(x) = \int_0^x \frac{\kappa(y)}{a(y)}\,\mathrm{d}y \text{ and } M(x) = \int_0^x \frac{1}{\rho(y)\kappa(y)}\,\mathrm{d}y, \tag{2.18}$$

$$s(x) = \frac{\kappa(x)}{a(x)},\ m(x) = \frac{1}{\kappa(x)\rho(x)},\ h(x) = \int_0^x \frac{2b(y)}{a(y)\rho(y)}\,\mathrm{d}y \text{ and } \kappa(x) = e^{-h(x)}. \tag{2.19}$$

Remark 2.9. Using Definition 2.1,

$$\mathrm{D}^S_x f(x) = s(x)^{-1}\partial_x f(x) \text{ and } \mathrm{D}^M_x f(x) = m(x)^{-1}\partial_x f(x).$$

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

$$\mathrm{Dom}(\Omega) = \{f \in \mathcal{C}_0 \mid \Omega f \in \mathcal{C}_0\}, \tag{2.20}$$
$$= \{f \in \mathcal{C}_0 \mid \forall \lambda > 0,\ \exists w \in \mathcal{C}_0 \text{ s.t. } (\lambda - \Omega)f = w\}. \tag{2.21}$$

The existence of $(\Omega, \mathrm{Dom}(\Omega))$ as well as the equivalence between (2.20) and (2.21) follows from classical results of W. Feller [15, 18, 16, 17].

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

$$\mathcal{A}^B_{x,(a,\rho,b)}(f\circ\Phi)(x) = \left(\frac{\rho(x)}{2}a(x)\Phi^{''}(x) + b(x)\Phi^{'}(x)\right)\partial_z f(\Phi(x)) + \frac{\rho(x)}{2}\Phi^{'}(x)\partial_x(a(x)(\Phi^{'})^{-1}(x)\partial_x f(\Phi(x))).$$

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 (2.19) ensures that

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

and

$$\mathcal{A}^B_{x,(a,\rho,b)}(f\circ\Phi)(x) = \frac{\rho(x)}{2}\Phi^{'}(x)\partial_x\left(a(x)\left(\frac{1}{\Phi'(x)}\partial_x(f\circ\Phi)(x)\right)\right)$$
$$= \frac{1}{2}m(x)^{-1}\partial_x(s(x)^{-1}\partial_x(f\circ\Phi)(x)) = \frac{1}{2}\mathrm{D}_x^M\mathrm{D}_x^S(f\circ\Phi)(x) = \Omega(f\circ\Phi)(x).$$

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

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

Using this representation, we characterize the functions in the domain $\mathrm{Dom}(\mathcal{A}^B_{x,(a,\rho,b)})$. We will use it later in Proposition 2.8.

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

Proof. From the definition of the domain of $\mathcal{A}^B_{x,(a,\rho,b)}$ (see (2.20)), the problem $(\lambda - \mathcal{A}^B_{x,(a,\rho,b)})f(x) = w(x)$ 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. □

The following synthesized one of the purpose of this section.

Proposition 2.4 ([16, 25, 40])**.** *When $(a,\rho,b) \in \mathfrak{M}$, the operator $(\mathcal{A}^B_{x,(a,\rho,b)}, \mathrm{Dom}(\mathcal{A}^B_{x,(a,\rho,b)}))$ is the infinitesimal generator of a Feller process X.*

We finish this parts by recalling a convenient property of stability of the coefficients (a, ρ, b) under a change of variable. This is one of our justification to introduce the parameter ρ in addition to a and b. We will use it later in Section 3.1 to reduce the number of parameters.

Proposition 2.5. *Let us consider piecewise $\mathcal{C}^1$ change of variable G from $\mathbb{R}$ to an interval $I \subset \mathbb{R}$. Let $(a, \rho, b) \in \mathfrak{M}$ and let X be the corresponding process. Then $Y = G(X)$ is the process living in I which is associated to a family $(a \cdot G', \rho \cdot G', b \cdot G')$ in the system of coordinates defined by $y = G(x)$.*

2.5.3 The resolvent kernel for knitted operators under their factorized form

With the factorized form of the operator comes two particular families of functions from which the resolvent kernel can be computed.

Proposition 2.6 ([18, 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*

$$(\lambda - \mathcal{A}^B_{x,(a,\rho,b)})u(\lambda;x) = 0,\ \forall x \in \mathbb{R},\ \lambda > 0, \textit{ for } u = \phi \textit{ or } \psi,$$
$$\phi(\lambda;0) = \psi(\lambda;0) = 1,\ \phi \textit{ is decreasing from } +\infty \textit{ to } 0,$$
$$\psi \textit{ is valued increasing from } 0 \textit{ to } +\infty.$$

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

Remark 2.10. As in the proof of Lemma 2.1, $\mathrm{D}^S_x\phi(\lambda;\cdot)$ and $\mathrm{D}^S_x\psi(\lambda;\cdot)$ are themselves continuous on $\mathbb{R}$.

We define the *Wronskian* of two suitable functions f and g as $\mathrm{Wr}[f,g](x) := f(x)\mathrm{D}^S_x g(x) - g(x)\mathrm{D}^S_x f(x)$.

Proposition 2.7 ([18, page 475, §7], [25])**.** *For the functions ψ and ϕ of Proposition 2.6, let us define*

$$g(\lambda;x,y) := \frac{2}{W}\begin{cases}\psi(\lambda;x)\phi(\lambda;y) & \textit{if } x < y,\\ \phi(\lambda;x)\psi(\lambda;y) & \textit{if } x \geq y\end{cases} \tag{2.22}$$

with $W = \mathrm{Wr}[\phi(\lambda;\cdot),\psi(\lambda;\cdot)](x)$ (this function is constant in x). With

$$\mathfrak{r}_{\mathcal{A}^B_{x,(a,\rho,b)}}(\lambda;x,y) := g(\lambda;x,y)m(y),$$

the family $(G_\lambda)_{\lambda>0}$ of linear operators defined by

$$G_\lambda f(x) := \int_{\mathbb{R}} \mathfrak{r}_{\mathcal{A}^B_{x,(a,\rho,b)}}(\lambda;x,y)f(y)\,\mathrm{d}y\ \forall f \in \mathcal{C}_0 \tag{2.23}$$

is the resolvent of $(\mathcal{A}^B_{x,(a,\rho,b)}, \mathrm{Dom}(\mathcal{A}^B_{x,(a,\rho,b)}))$, meaning that $G_\lambda = (\lambda - \mathcal{A}^B_{x,(a,\rho,b)})^{-1}$ in $\mathcal{C}_0$ and that $\mathfrak{r}_{\mathcal{A}^B_{x,(a,\rho,b)}}(\lambda;x,y)$ is the resolvent kernel of $\mathcal{A}^B_{x,(a,\rho,b)}$.

Remark 2.11. It is immediate from (2.22) that $g(\lambda;x,y)$ is continuous and symmetric in (x,y).

We use this construction to characterize the resolvent kernel of the operators $\mathcal{A}^B_{x,(a,\rho,b)}$ for knitted coefficients. For that purpose, we first set a few hypothesis, notations and similar stuff.

Hypothesis 2.1. 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 2.1. To $(a_\pm, \rho_\pm, b_\pm) \in \mathfrak{H}$ we associate the corresponding operators $\mathcal{A}^B_{x,(a_\pm,\rho_\pm,b_\pm)}$, scales functions $S_\pm$, speed measures $M_\pm$ with density $m_\pm$, the minimal functions $(\phi_\pm, \psi_\pm)$, ...

Remark 2.12. With (2.19) and (2.18), the scale measure S and the density m of speed measure M of $\mathcal{A}^B_{x,(a,\rho,b)}$ satisfies $S = S_- \bowtie S_+$ and $m = m_- \bowtie m_+$.

Proposition 2.8. *Let $(a, \rho, b) \in \mathfrak{H}^{\bowtie}$ as in Hypothesis 2.1. The kernel $g(\lambda; x, y)$ given by* (2.22) *associated to $(\mathcal{A}^B_{x,(a,\rho,b)}, \mathrm{Dom}(\mathcal{A}^B_{x,(a,\rho,b)}))$ solves:*

$$(\lambda - \mathcal{A}^B_{x,(a,\rho,b)})g(\lambda; x, y) = 0,\ x, y \in \mathbb{R}, \tag{2.24}$$

$$g(\lambda; 0-, y) = g(\lambda; 0+, y),\ y \neq 0, \tag{2.25}$$

$$g(\lambda; y-, y) = g(\lambda; y+, y),\ y \neq 0, \tag{2.26}$$

$$\mathrm{D}^{S_-}_x g(\lambda; 0-, y) = \mathrm{D}^{S_+}_x g(\lambda; 0+, y),\ y \neq 0, \tag{2.27}$$

$$\begin{cases} \mathrm{D}^{S_-}_x g(\lambda; y-, y) - \mathrm{D}^{S_-}_x g(\lambda; y+, y) = 2, \text{ if } y < 0, \\ \mathrm{D}^{S_+}_x g(\lambda; y-, y) - \mathrm{D}^{S_+}_x g(\lambda; y+, y) = 2, \text{ if } y > 0. \end{cases} \tag{2.28}$$

Proof. Eq. (2.24) follows from (2.22). From Remark 2.10, $u(\lambda; \cdot)$ and $\mathrm{D}^S u(\lambda; \cdot)$ are continuous for $u = \phi, \psi$. Thus $x \mapsto g(\lambda; x, y)$ is continuous, which leads to (2.25). In addition, $x \mapsto \mathrm{D}^S_x g(\lambda; x, y)$ is continuous when $x \neq 0$. As $S = S_- \bowtie S_+$, this leads to (2.27).

Let us assume that $y > 0$. When $x \geq y$, $\mathrm{D}^{S_+}_x g(\lambda; y + h, y) = \dfrac{2}{W} \mathrm{D}^{S_+}_x \phi(\lambda; y + h)\psi(\lambda; y)$. Using the expression of W, for a small $h > 0$,

$$\psi(\lambda; y + h)\mathrm{D}^{S_+}_x \phi(\lambda; y + h) = -W + \phi(\lambda; y + h)\mathrm{D}^{S_+}_x \psi(\lambda; y + h).$$

Thus,

$$\mathrm{D}^{S_+}_x g(\lambda; y + h, y) = \frac{2}{W} \left(-W + \phi(\lambda; y + h)\mathrm{D}^{S_+}_x \psi(\lambda; y + h)\right) \frac{\psi(\lambda; y)}{\psi(\lambda; y + h)}. \tag{2.29}$$

Similarly, when $x < y$, $\mathrm{D}^{S_+}_x g(\lambda; y - h, y) = \dfrac{2}{W} \mathrm{D}^{S_+}_x \psi(\lambda; y - h)\phi(\lambda; y)$. Using the expression of W, for a small $h > 0$ yields

$$\mathrm{D}^{S_+}_x g(\lambda; y - h, y) = \frac{2}{W} \left(W + \psi(\lambda; y - h)\mathrm{D}^{S_+}_x \phi(\lambda; y - h)\right) \frac{\phi(\lambda; y)}{\phi(\lambda; y - h)}. \tag{2.30}$$

Summing the two expressions (2.29) and (2.30) and using the continuity of ϕ, ψ, $\mathrm{D}^{S_+}_x \psi$ and $\mathrm{D}^{S_+}_x \phi$ at y yields (2.28) for the case $y > 0$ as $h \to 0$.

For the case $y < 0$, use the same arguments with the operator $\mathrm{D}^{S_-}_x$. □

We are now in position by using (2.24)-(2.28) to provide an explicit expression of g when $(\phi_\pm, \psi_\pm)$ are known. This is basically the case when the coefficients $(a_\pm, \rho_\pm, b_\pm)$ are constant. It will be treated in full details later in Section 3.

Notation 2.2. We consider two suitable continuous functions u and v The *Wronskian* (negative side) of u and v is defined by

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

Theorem 2.1. *Let $(a,\rho,b)\in\mathfrak{H}^{\bowtie}$ be as in Hypothesis 2.1.*

Let $g(\lambda;x,y)$ be the kernel associated to $(\mathcal{A}^B_{x,(a,\rho,b)},\mathrm{Dom}(\mathcal{A}^B_{x,(a,\rho,b)}))$ through (2.22)*. Then*

$$g(\lambda;x,y) := \begin{cases} g_{y\geq 0}(\lambda;x,y) & \text{if } y\geq 0,\\ g_{y<0}(\lambda;x,y) & \text{if } y<0, \end{cases} \tag{2.31}$$

where for $y\geq 0$

$$\begin{aligned}
g_{y\geq 0}(\lambda;x,y) = {}& c_1^+\phi_+(\lambda;y)\psi_-(\lambda;x)\mathbb{1}_{x\leq 0}\\
&+ \big(c_2^+\phi_+(\lambda;y)\phi_+(\lambda;x) + c_3^+\phi_+(\lambda;y)\psi_+(\lambda;x)\big)\mathbb{1}_{x\in]0,y[}\\
&+ (c_2^+\phi_+(\lambda;y)\phi_+(\lambda;x) + c_3^+\psi_+(\lambda;y)\phi_+(\lambda;x))\mathbb{1}_{x\geq y}
\end{aligned} \tag{2.32}$$

with

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

while for $y<0$,

$$\begin{aligned}
g_{y<0}(\lambda;x,y) := {}& c_1^-\psi_-(\lambda;y)\phi_+(\lambda;x)\mathbb{1}_{x\geq 0}\\
&+ \big(c_2^-\psi_-(\lambda;y)\psi_-(\lambda;x) + c_3^-\psi_-(\lambda;y)\phi_-(\lambda;x)\big)\mathbb{1}_{x\in]y,0[}\\
&+ (c_2^-\psi_-(\lambda;y)\psi_-(\lambda;x) + c_3^-\phi_-(\lambda;y)\psi_-(\lambda;x))\mathbb{1}_{x\leq y}
\end{aligned} \tag{2.33}$$

with

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

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

Remark 2.13. 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 $\psi_+(\lambda;\cdot)$.

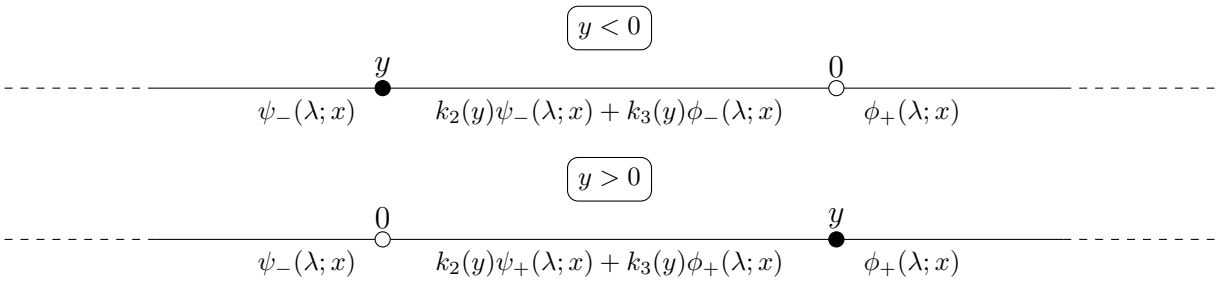

Figure 1: Splitting the state space to define superpositions.

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

We have the following picture: To take (2.24)-(2.25) 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 (2.32). Our choice ensures from that as $x \to \infty$, $g(\lambda;x,y)$ 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 (2.27), (2.25) and (2.28), leads 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

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

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 (2.33). Conditions (2.27), (2.25) and (2.28), leads 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

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

The general formula follows from algebraic manipulations. □

Remark 2.14. The distribution of some random variables (hitting time, occupation time, ...) related to a diffusion may be recovered from the minimal solutions $\phi(\lambda;\cdot)$ and $\psi(\lambda;\cdot)$ (see *e.g.* [41]). From the expression of g, one finds also the minimal solutions ϕ and ψ of $\mathcal{A}^B_{x,(a,\rho,b)}$ through (2.22). Since $\phi(\lambda;0)=\psi(\lambda;0)=\phi_\pm(0)=\psi_\pm(0)=1$, the Wronskian W between ϕ and ψ is given by

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

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 (2.32) 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 $c_3^\pm+c_2^\pm=c_1^\pm$.

2.6 Relationship between the resolvent kernels

Let us consider $(a,b)\in\mathfrak{C}^\bowtie\times\mathfrak{B}^\bowtie$, so that $(a,1,b)\in\mathfrak{H}^\bowtie$ satisfies Hypothesis 2.1.

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

Lemma 2.2. *Let $(a,1,b)\in\mathfrak{H}^\bowtie$. There exists a set D which is dense in both $\mathrm{Dom}(\mathcal{L}^B_x)$ equipped with graph norm $f\mapsto\|f\|_{\mathrm{L}^2(\mathbb{R})}+\|\mathcal{L}^B_x f\|_{\mathrm{L}^2(\mathbb{R})}$ and $\mathrm{Dom}(\mathcal{A}^B_{x,(a,1,b)})$ also equipped with the graph norm $f\mapsto\|f\|_\infty+\|\mathcal{A}^B_{x,(a,1,b)}f\|_\infty$ such that $\mathcal{L}^B_x f=\mathcal{A}^B_{x,(a,1,b)}f$ for any $f\in D$.*

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

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

so that $D\subset\mathrm{Dom}(\mathcal{A}^B_{x,(a,1,b)})$ by Proposition 2.3. The subset D does not depend on λ. Since $\mathcal{C}_0\cap\mathrm{L}^2(\mathbb{R})$ is dense in $\mathcal{C}_0$, D is dense for the graph norm in $\mathrm{Dom}(\mathcal{A}^B_{x,(a,1,b)})$.

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

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

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

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

We deduce immediately the following result on the associated processes.

Corollary 2.2. *When $(a, 1, b) \in \mathfrak{H}^{\bowtie}$, the processes constructed by Corollary 2.1 with $\rho = 1$ and Proposition 2.4 are the same.*

Again with Lemma 2.2, comparing (2.16) with (2.23) links the resolvent kernel $\mathfrak{r}(\lambda; x, y)$ of $\mathcal{L}^B_x$ with ones of $\mathcal{A}^B_{x,(a,1,b)}$. Combining Proposition 2.7 with Lemma 2.2 leads to the following result.

Proposition 2.9. *Let $(a, 1, b) \in \mathfrak{H}^{\bowtie}$. The resolvent kernel $\mathfrak{r}(\lambda; x, y)$ of $\mathcal{L}^B_{x,(a,b)}$ solution to the problem* (2.17) *is*

$$\mathfrak{r}(\lambda, x, y) = \mathfrak{r}_{\mathcal{A}^B_{x,(a,1,b)}}(\lambda; x, y) := g(\lambda; x, y)m(y)$$

where g is given by Theorem 2.1.

The next proposition shows that $\mathfrak{r}(\lambda; x, y)$ and consequently $\mathfrak{q}(t, x, y)$ satisfy (2.3)-(2.4) with respect to the variable y (forward equation) as well as (2.9)-(2.10) with respect to the variable x (backward equation).

Proposition 2.10. *Let $(a, 1, b) \in \mathfrak{H}^{\bowtie}$. Let f be continuous and differentiable so that $\mathrm{D}^S_x f$ is also continuous (such as $x \mapsto g(\lambda; x, y)$). Then $[a\partial_x f]_0 = 0$ and $[a\partial_x(fm) - bfm]_0 = 0$.*

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

$$\mathrm{D}^S_x f(\pm\epsilon) = \frac{a(\pm\epsilon)}{\kappa(\pm\epsilon)}\partial_x f(\epsilon) \xrightarrow[\epsilon\to 0]{} a(0\pm)\partial_x f(0\pm).$$

Hence, $[D^S_x f]_0 = [a\partial_x f]_0$.

For m given in Proposition 2.3, $D^S_x m(x) = -b(x)/\kappa(x)^2$. Let f is such that $[f]_0 = [D^S_x f]_0 = 0$. Hence for $x \neq 0$,

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

This proves the result. □

3 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. Precisely, we consider $(a, \rho, b) = (a_-, \rho_-, b_-) \bowtie (a_+, \rho_+, b_+) \in \mathfrak{H}^{\bowtie}$ obtained by knitting two families of constant coefficients $(a_\pm, \rho_\pm, b_\pm)$.

3.1 Expression of the resolvent kernel

We introduce a convenient change of variable which allows to express the resolvent kernel of $\mathcal{A}^B_{x,(a,\rho,b)}$ in terms of the one of a process called the drifted Skew Brownian motion.

Definition 3.1 (Drifted Skew Brownian motion)**.** *A process Y associated to a coefficient of the form*

$$\mathrm{DSBM}(\beta, \gamma_+, \gamma_-) := \begin{cases} (\beta, \beta^{-1}, \gamma_+) & \text{if } x \geq 0, \\ (1-\beta, (1-\beta)^{-1}, \gamma_-) & \text{if } x < 0 \end{cases}$$

with $\beta \in (0, 1)$, $\gamma_-, \gamma_+ \in \mathbb{R}$ is called a drifted Skew Brownian motion *(DSBM). It is a* Skew Brownian motion *if $\gamma_- = \gamma_+ = 0$ [32]. 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 is immediate from Proposition 2.5.

Lemma 3.1. *Let X be associated to the piecewise constant coefficients $(a, \rho, b) \in \mathfrak{H}^{\bowtie}$ as above. For $\kappa_-, \kappa_+ > 0$ we set $G(x) := \kappa(x) \cdot x$ be a piecewise linear change of variable with $\kappa(x) := (\kappa_- \bowtie \kappa_+)(x)$. Then $Y = G(X)$ is associated to the piecewise constant coefficients $(a\kappa, \rho\kappa, b\kappa) \in \mathfrak{H}^{\bowtie}$.*

Proposition 3.1 (Reduction to a drifted Skew Brownian motion)**.** *Let X be associated to the piecewise constant coefficients $(a, \rho, b) \in \mathfrak{H}^{\bowtie}$ as above.*

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

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

with

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

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

$$\mathfrak{r}_{\mathcal{A}^B_{x,(a,\rho,b)}}(\lambda; x, y) = \frac{\mathfrak{r}_{\mathrm{DSBM}(\beta,\gamma_+,\gamma_-)}(\lambda; \phi(x), \phi(y))}{\sqrt{a(y)\rho(y)}}$$

where $\mathfrak{r}_{\mathrm{DSBM}(\beta,\gamma_+,\gamma_-)}$ 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 3.1. 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 $\mathrm{DSBM}\,(\beta, \gamma_+, \gamma_-)$. □

The advantage of using G is that the number of parameters defining $(a, \rho, b) \in \mathfrak{H}^{\bowtie}$, 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 [32, 35]. Hence, we could 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 $Y = G(X)$.

3.2 Explicit computations of the resolvent kernel of the DSBM

The coefficients of the DSBM are piecewise constant ones. The results of Section 2 can therefore be used. According to Proposition 3.1, it is enough to compute $\mathfrak{r}_{\mathrm{DSBM}(\beta,\gamma_+,\gamma_-)}$ to get an expression for the resolvent kernel $\mathfrak{r}_{\mathcal{A}^B_{x,(a,\rho,b)}}$ with $(a, \rho, b) = (a_-, \rho_-, b_-) \bowtie (a_+, \rho_+, b_+)$ for any $(a_\pm, \rho_\pm, b_\pm)$.

The speed measure m of the process Y associated to a $\mathrm{DSBM}(\beta, \gamma_+, \gamma_-)$ is

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

and its scale function S is $S(x) = \int_0^x s(y)\,\mathrm{d}y$ with $s(x) = 1/m(x)$. According to Proposition 2.9,

$$\mathfrak{r}_{\mathrm{DSBM}(\beta,\gamma_+,\gamma_-)}(\lambda, x, y) = g(\lambda, x, y)m(y), \tag{3.1}$$

where $g(\lambda, x, y)$ is given by Theorem 2.1 in which the following minimal functions $\phi_\pm(\lambda; \cdot)$ and $\psi_\pm(\lambda; \cdot)$ are

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

It is here noteworthy to remark that these minimal functions do not depend on β.

The next proposition is an application of Theorem 2.1 and (3.1) after some algebraic manipulation. Its formulation requires the following bunch of notations

Notation 3.1. We set

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

and define the constants

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

Proposition 3.2. *With the above notations on* Θ, Θ_+, Θ_-, λ_+ *and* λ_-, *for any* $\lambda > 0$, $x, y \in \mathbb{R}$,

$$\mathfrak{r}_{\mathrm{DSBM}(\beta,\gamma_+,\gamma_-)}(\lambda; x, y) = \frac{1}{\Theta} \times \begin{cases} 2\beta \exp(\gamma_+ y - \sqrt{\lambda_+} y - \gamma_- x + \sqrt{\lambda_-} x) \\ \qquad \textit{if } x \le 0 \le y, \\ \lambda_+^{-1/2} \exp(\gamma_+(y-x)) \times \left[\Theta \exp(-\sqrt{\lambda_+}(y-x)) + \Theta_+ \exp(-\sqrt{\lambda_+}(x+y))\right] \\ \qquad \textit{if } 0 < x \le y, \\ \lambda_+^{-1/2} \exp(-\gamma_+(x-y)) \times \left[\Theta \exp(-\sqrt{\lambda_+}(x-y)) + \Theta_+ \exp(-\sqrt{\lambda_+}(x+y))\right] \\ \qquad \textit{if } 0 < y \le x, \\ 2(1-\beta) \exp(\gamma_- y - \gamma_+ x + \sqrt{\lambda_-} y - \sqrt{\lambda_+} x) \\ \qquad \textit{if } y < 0 \le x, \\ \lambda_-^{-1/2} \exp(-\gamma_-(x-y)) \times \left[\Theta \exp(-\sqrt{\lambda_-}(x-y)) + \Theta_- \exp(\sqrt{\lambda_-}(y+x))\right] \\ \qquad \textit{if } y \le x < 0, \\ \lambda_-^{-1/2} \exp(\gamma_-(y-x)) \times \left[\Theta \exp(-\sqrt{\lambda_-}(y-x)) + \Theta_- \exp(\sqrt{\lambda_-}(y+x))\right] \\ \qquad \textit{if } x \le y < 0. \end{cases} \tag{3.2}$$

3.3 Some explicit expressions for the density transition function

Here we propose various explicit expressions of the density transition function $\mathfrak{q}_{\mathrm{DSBM}(\beta,\gamma_+,\gamma_-)}$ whenever we manage to derive the Laplace inversions of $\mathfrak{r}_{\mathrm{DSBM}(\beta,\gamma_+,\gamma_-)}$.

Notation 3.2.

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

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

3.3.1 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 found 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.

3.3.2 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,

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

Let us recall some classical formula on inverse Laplace.

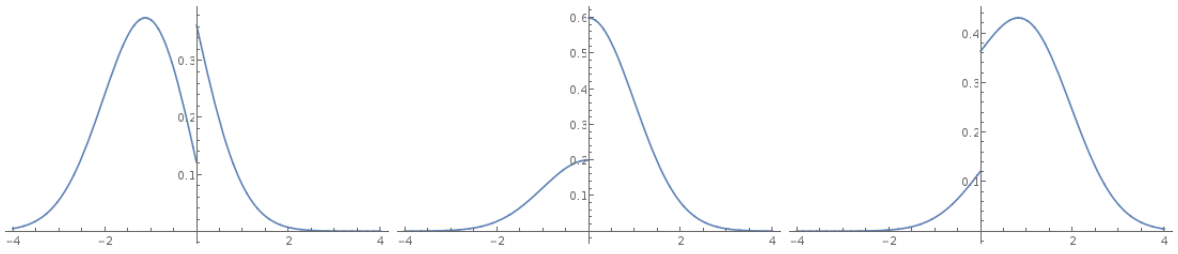

Figure 2: The density $\mathfrak{q}_{\mathrm{DSBM}(\beta,0,0)}(t,x,y)$ of the SBM for $\beta = \frac{3}{4}$ at time $t = 1$ for the initial positions: $x = -1$, $x = 0$ and $x = 1$ (from left to right).

Lemma 3.2 (See [1]). *For $k \geq 0$, $c > 0$, $\mu \in \mathbb{R}$,*

$$\mathcal{L}^{-1}\left(\frac{1}{\sqrt{\lambda}}\, e^{-k\sqrt{\lambda}}\right) = \frac{1}{\sqrt{\pi t}}\, e^{-\frac{k^2}{4t}}, \tag{3.3}$$

$$\mathcal{L}^{-1}(f(c\lambda + d)) = \frac{1}{c}\, e^{-\frac{d}{c}t}\, \mathcal{L}^{-1}(f)\left(\frac{t}{c}\right), \tag{3.4}$$

$$\mathcal{L}^{-1}\left(\frac{e^{-k\sqrt{\lambda}}}{\mu + \sqrt{\lambda}}\right) = \frac{1}{\sqrt{\pi t}}\, e^{-\frac{k^2}{4t}} - \mu e^{\mu k}\, e^{\mu^2 t}\, \operatorname{erfc}\left(\mu\sqrt{t} + \frac{k}{2\sqrt{t}}\right). \tag{3.5}$$

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

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

so that

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

The formula of Lemma 3.2 are sufficient to compute termwise the inverse Laplace transforms of the resolvent kernel when $\lambda_+ = \lambda_-$.

3.3.3 The Skew Brownian Motion

The SBM of parameter $\beta \in (0,1)$ is given by the choice of the coefficients $\mathrm{DSBM}(\beta,0,0)$. Hence, $\lambda_+ = \lambda_-$ and $\mu = 0$. Thus, after an application of (3.3)-(3.4) to (2.16) as well as some rewriting,

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

This density was obtained in [50] through a probabilistic argument. Some plots are given in Figure 2.

3.3.4 The Skew Brownian Motion with a constant drift

The density of the SBM with a constant drift, which corresponds to the coefficient $\mathrm{DSBM}(\beta,\gamma,\gamma)$ for some $\gamma \neq 0$ was computed in [2, 3, 14, 21] with different probabilistic arguments.

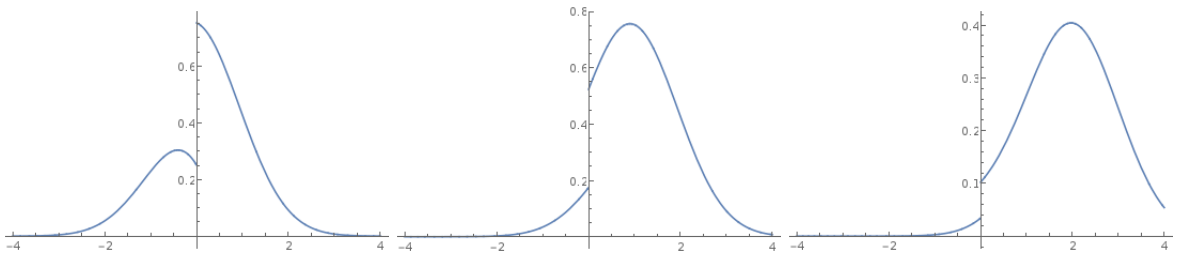

Figure 3: The density $p(t,x,y)$ of the SBM for $\beta = \frac{3}{4}$ with a constant drift $\gamma = 2$ at time $t = 1$ for the initial positions: $x = -1$, $x = 0$ and $x = 1$ (from left to right).

In this case, $\lambda_+ = \lambda_- = \sqrt{\gamma^2 + 2\lambda}$ and $\mu = (2\beta - 1)\gamma$. With the formula of Lemma 3.2 (see Figure 3),

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

We recover the density obtained in [2, 14] up to a conversion of erfc to its probabilistic counterpart.

3.3.5 The Bang-Bang Skew Brownian Motion

The Bang-Bang SBM is the diffusion corresponding to the choice of the coefficients $\mathrm{DSBM}(\beta, \gamma, -\gamma)$ for some $\gamma \neq 0$. This process was introduced in [20]. 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 3.2 (see Figure 4)

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

This is the expression given in [20] up to a conversion of erfc into its probabilistic counterpart. It is also the one given in [6].

3.3.6 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

$$\gamma_- = \kappa\gamma_+ \text{ with } \kappa = \frac{\beta}{1-\beta} \text{ or equivalently } \mu = 0 \text{ when } \beta \neq \frac{1}{2}. \tag{3.6}$$

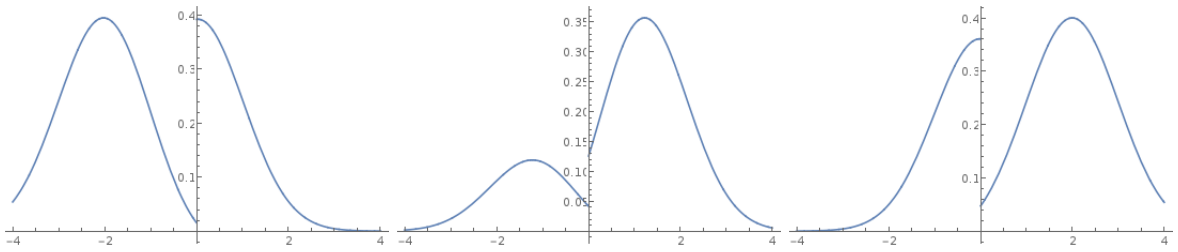

Figure 4: The density $\mathfrak{q}_{\mathrm{DSBM}(\beta,\gamma,\gamma)}(t,x,y)$ of the SBM for $\beta=\frac{3}{4}$ with a Bang bang drift $\gamma=2$ at time $t=1$ for the initial positions $x=-1$, $x=0$ and $x=1$ (from left to right).

Remark 3.1. This assumption on γ_+ and γ_- is natural. Then Y is obtained through the transformation of Proposition 3.1 from a process X with piecewise constant coefficients (a,ρ,b), then (3.6) 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.

To deal with this case, we need two extra results in Laplace inversion.

Lemma 3.3 ([38])**.** *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 3.4. *For $a\in\mathbb{R}$,*

$$\mathcal{L}^{-1}\left(\sqrt{a+s}e^{-\sqrt{s}\,y}\right)(t,y)=\frac{1}{\pi}\int_0^a\sin(y\sqrt{r})\sqrt{a-r}\,e^{-rt}\,\mathrm{d}r \\ -\frac{1}{\pi}\int_0^{+\infty}\cos(y\sqrt{r+a})\,\sqrt{r}\,e^{-(r+a)t}\,\mathrm{d}r.$$

Proof. Inspired by [42], 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,

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

hence the result. □

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

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

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 $y<0<x$.

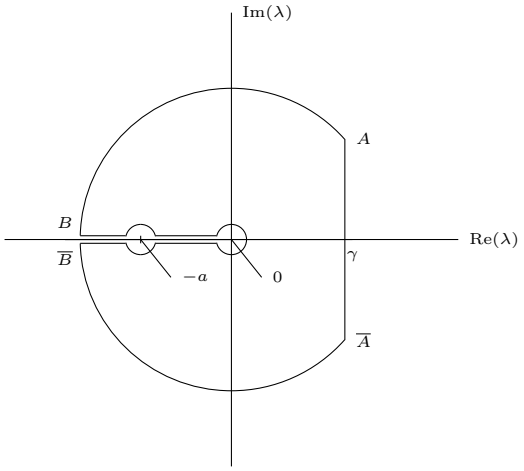

Figure 5: The contour Γ.

Proposition 3.3. *For any $t \geq 0$ and* $\mathrm{DSBM}(\beta, \gamma, \kappa\gamma)$*, with $\gamma(y) = ((\kappa\gamma) \bowtie \gamma)(y)$,*

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

Proof. When (3.6) holds,

$$\frac{1}{\Theta} = \frac{\beta\sqrt{\lambda_+}-(1-\beta)\sqrt{\lambda_-}}{\beta^2\lambda_+-(1-\beta)^2\lambda_-} = \frac{\beta\sqrt{\lambda_+}-(1-\beta)\sqrt{\lambda_-}}{2\lambda(2\beta-1)}. \tag{3.7}$$

In addition,

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

Each line in the right-hand side of (3.2) is easily inverted using (3.3) excepted when $y < 0 \leq x$ and $x \leq 0 < y$.

To simplify the formula, we consider starting at $x = 0$. With (3.7),

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

We focus on the term for $y > 0$, the other term being treated by symmetry. With (3.4), 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 3.3 while the second term is inverted using (3.3).

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

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

We conclude using Lemma 3.4.

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

Conclusion

We have shown how to compute analytic expressions of the resolvent kernel of a 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 density transition functions. We recover some formula already known that were derived by probabilistic means and derive a new one.

In the sequel [34], we show how these formula for the resolvent kernels allow one to set up a simple numerical scheme in presence of discontinuities both for the diffusivity and the advective terms.

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