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Parametrix approximations for non constant coefficient parabolic PDEs

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1 Introduction

Closed form expressions for the fundamental solution of parabolic partial differential equations (PDE) are needed in several application domains ranging from Chemistry to Physics, from Statistics to Finance [2, 3, 5, 6]. In this paper a closed form approximation for the fundamental solution of the following parabolic PDE operator is derived

$$LU(x,t) := a(x)\partial_{xx}U(x,t) - \partial_t U(x,t) = 0,$$
(1)

on $\Omega = \mathbb{R} \times [0, t]$. The operator is uniformly parabolic and its coefficient function *a* is bounded and Hölder regular. Precisely, it is assumed that

H.1 there exists m and M such that $0 < m \le a(x) \le M < \infty, x \in \mathbb{R}$;

H.2 there exist $\alpha \in (0,1)$ and C such that $|a(x) - a(y)| \leq C|x - y|^{\alpha}, x \in \mathbb{R}$.

Under **H.1** and **H.2** the fundamental solution $\Gamma(z;\zeta) = \Gamma(x,t;\xi,\tau)$ of (1) exists and is unique [4]. When a is constant, $a(x) \equiv v$, the fundamental solution is given by $\Gamma_v(x-\xi,t-\tau)$, where

$$\Gamma_v(x,t) := \frac{1}{\sqrt{4\pi v t}} \exp\left(-\frac{x^2}{4v t}\right).$$

In general however, an explicit expression is not always available and approximations need to be computed.

A method for approximating $\Gamma(z;\zeta)$ consists on using Levi's parametrix series expansion, recently reconsidered as a computational method by Corielli and Pascucci for

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financial applications [3]. The parametrix expansion expresses $\Gamma(z;\zeta)$ in terms of the fundamental solution $Z(z;\zeta)$ of the corresponding "frozen" PDE

$$a(\xi)U_{xx}(x,t) - U_t(x,t) = 0,$$

given by $Z(x,t;\xi,\tau) = \Gamma_{a(\xi)}(x-\xi,t-\tau)$. Specifically, Γ is given by the series expansions

$$\Gamma(z;\zeta) = Z(z;\zeta) + \sum_{k=1}^{n} Z_k(z;\zeta) + E_{n+1}(z;\zeta),$$
(2)

where

$$Z_k(z;\zeta) := \int_{\tau}^t \int_{\mathbb{R}} Z(z;z_0) (LZ)_k(z_0;\zeta) dz_0, \qquad (3)$$

with $(LZ)_k$ defined by

$$(LZ)_1(z;\zeta) = LZ(z;\zeta), \qquad (LZ)_k(z;\zeta) = \int_\tau^t \int_{\mathbb{R}} LZ(z;w)(LZ)_{k-1}(w;\zeta)dw.$$

The error term E_{n+1} is of the order $O((t-\tau)^{\lfloor \frac{n+2}{2} \rfloor} \Gamma_{M+\epsilon}(z,\zeta))$, with $\epsilon > 0$.

In the following $\Gamma(z; \zeta)$ is approximated by using the first three terms of the parametrix series in (2):

$$\Gamma(z;\zeta) = Z(z;\zeta) + Z_1(z;\zeta) + Z_2(z;\zeta) + O(t^2 \Gamma_{M+\epsilon}(z;\zeta)).$$
(4)

where, for notational convenience and without loss of generality, it has been considered only the case $\zeta = (\xi, 0)$, that is $\tau = 0$.

The main practical limit of the parametric series consists in the fact that Z_k is defined in terms of a 2k dimensional integral which, in general, cannot be computed explicitly. Here a closed form approximation to Z_1 and Z_2 is derived. That approximation has errors not exceeding the remainder in (4).

With this purpose let rewrite

$$Z_1(z;\zeta) = \int_0^t I_1(t_0;z,\zeta)dt_0 \quad \text{and} \quad Z_2(z;\zeta) = \int_0^t \int_0^{t_0} I_2(t_0,t_1;z,\zeta)dt_1dt_0, \quad (5)$$

where

$$I_1(t_0; z, \zeta) = \int_{\mathbb{R}} Z(z; x_0, t_0) LZ(x_0, t_0; \zeta) dx_0,$$
(6)

$$I_2(t_0, t_1; z, \zeta) = \int_{\mathbb{R}} \int_{\mathbb{R}} Z(z; z_0) LZ(z_0; z_1) LZ(z_1; \zeta) dx_0 dx_1,$$
(7)

and $z_i = (x_i, t_i)$, i = 0, 1. Now, notice that some of the factors in the integrands in (6) and (7) tend to Dirac's deltas at the corners of the domains of the integrals in (5). Thus, at that points the computation of $I_1(t_0; z, \zeta)$ and $I_2(t_0, t_1; z, \zeta)$ reduces to simple

function evaluations. Using these values, Z_1 and Z_2 are approximated by a trapezoidal rule as follows

$$\hat{Z}_1(z;\zeta) = \frac{t}{2} \left(I_1(0^+; z, \zeta) + I_1(t^-; z, \zeta) \right)$$
(8)

and

$$\hat{Z}_2(z;\zeta) = \frac{t^2}{6} \big(I_2(0^+, 0^+; z, \zeta) + I_2(t^-, 0^+; z, \zeta) + I_2(t^-, t^-; z, \zeta) \big), \tag{9}$$

where $f(x^+)$ and $f(x^-)$ denote, respectively, the limit to x from right and left. The errors of approximations in (6) and (7) are, respectively, of order $O(t^3 ||I_1''||_{\infty,(0,t)})$ and $O(t^3 ||(\partial_{t_0t_0} + \partial_{t_0t_1} + \partial_{t_1t_1})I_2||_{\infty,D_t})$, where $D_t = \{(t_0, t_1)|0 < t_0 < t$ and $0 < t_1 < t_0\}$ is the domain of the second integral in (5)¹.

The paper is structured as follows, in next section some results concerning limits of Gaussian and parametrix functions Γ_v and Z_1 are reported. These results will be used in section 3 to derive expressions for the terms appearing in (8) and (9).

2 Preliminary results

The first lemma gives point-wise bounds on the non-constant parameter Gaussian function

$$\tilde{\Gamma}(x,t) := \Gamma_{g(x)}(x,t),$$

in terms of constant parameters Gaussians.

Lemma 1. Let g(x) bounded, that is $0 < m \le g(x) \le M < \infty$, $x \in \mathbb{R}$ then

$$\sqrt{\frac{m}{M}}\,\Gamma_m(x,t) \le \Gamma_{g(x)}(x,t) \le \sqrt{\frac{M}{m}}\,\Gamma_M(x,t), \qquad x \in \mathbb{R} \text{ and } t > 0.$$

Proof. See [3].

The following results characterize the limits of $\Gamma_v(x,t)$ and $\Gamma(x,t)$ when $t \to 0$. Lemma 2. Let f(x) have limit for $x \to 0$, v > 0 and g(x) satisfying H.1 and H.2,

$$\lim_{t \to 0} \int_{\mathbb{R}} f(x) \Gamma_{v}(x, t) dx = \lim_{t \to 0} \int_{\mathbb{R}} f(x) \tilde{\Gamma}(x, t) dx = \lim_{x \to 0} f(x)$$
(10a)

$$\lim_{t \to 0} \int_{\mathbb{R}} \frac{|x|^n}{v^{n/2} t^{n/2}} \Gamma_v(x, t) dx = \frac{2^n}{\sqrt{\pi}} \gamma((n+1)/2) = \begin{cases} (2k)!/k!, & n = 2k, \\ 2^{2k+1}k!/\sqrt{\pi}, & n = 2k+1. \end{cases}$$
(10b)

$$\lim_{t \to 0} \int_{\mathbb{R}} \frac{|x|^n}{g(x)^{k/2} t^{k/2}} \tilde{\Gamma}(x, t) dx = \begin{cases} 0, & \text{if } k < n, \\ \text{finite and positive,} & \text{if } k = n \text{ and} \\ \infty, & \text{if } k > n. \end{cases}$$
(10c)

where γ is the gamma function [1].

¹Actually, it can be proved that the errors are of order $O(t^3 ||I_1''||_{\infty} Z(z;\zeta))$ and $O(t^3 ||I_1''||_{\infty} Z(z;\zeta))$.

Proof. By Lemma 1, equation (10c) is a direct consequence of (10b) and of the boundedness of g(x).

Remark 1. Notice that (10b) is valid not only at the limit $t \to 0$ but also for any t > 0.

In the previous Lemma, (10a) characterizes the limit of $\Gamma_v(x,t)$ and $\tilde{\Gamma}(x,t)$ as a Dirac's delta. Equations (10b) and (10c) state that x^n and $t^{n/2}$ are of the same order when integrated with a Gaussian function.

The following Lemma derives a result analogous to point 3 of Lemma 2 for $\tilde{\Gamma}(x,t)$.

Lemma 3. Under the hypothesis of Lemma 2 and assuming g continuous and derivable, with bounded first derivative near 0, then

$$H_{n} = \lim_{t \to 0} \int_{\mathbb{R}} \frac{x^{n}}{g(x)^{n/2} t^{n/2}} \tilde{\Gamma}(x, t) dx = \begin{cases} \frac{n!}{(n/2)!}, & n \text{ even,} \\ 0, & n \text{ odd,} \end{cases}$$
(11)

and

$$\tilde{H}_n = \lim_{t \to 0} \int_{\mathbb{R}} \frac{1}{t^{1/2}} \frac{x^{2n+1}}{(g(x)t)^{n+1/2}} \tilde{\Gamma}(x,t) dx = \frac{(2n+1)!}{n!} \frac{g'(0)}{\sqrt{g(0)}}.$$
(12)

Proof. By (10c) in Lemma 2 the limit (11) is finite, but in a 0/0 indeterminate form. Thus, let rewrite the limit as

$$H_n = \lim_{t \to 0} \frac{\partial_t \int_{\mathbb{R}} g(x)^{-n/2} x^n \tilde{\Gamma}(x, t) dx}{(n/2) t^{n/2 - 1}}.$$

In the above limit, the derivative of $\tilde{\Gamma}(x,t)$ is given by

$$\partial_t \tilde{\Gamma}(x,t) = \left(\frac{x^2}{4g(x)t^2} - \frac{1}{2t}\right) \tilde{\Gamma}(x,t),$$

so that H_n becomes

$$H_n = \lim_{t \to 0} \int_{\mathbb{R}} \left(\frac{1}{2n} \frac{x^{n+2}}{g(x)^{n/2+1} t^{n/2+1}} - \frac{x^n}{ng(x)^{n/2} t^{n/2}} \right) \tilde{\Gamma}(x, t) dx = \frac{1}{2n} H_{n+2} - \frac{1}{n} H_n,$$

and thus $H_{n+2} = 2(n+1)H_n$. Now, since $H_0 = 1$ it follows that for n even $H_n = 2^{n/2}(n-1)!! = (n)!/(n/2)!$. For n odd, $H_n = 0$ is a direct consequence of (12).

Let thus consider (12). Proceeding as above it can be proved that $\tilde{H}_n = \frac{1}{4(n+1)}\tilde{H}_{n+1} - \frac{1}{2(n+1)}\tilde{H}_n$, so that $\tilde{H}_n = \frac{(2n+1)!}{n!}\tilde{H}_0$. It remains to show that

$$\tilde{H}_0 = \lim_{t \to 0} \int_{\mathbb{R}} \frac{x}{t\sqrt{g(x)}} \tilde{\Gamma}(x,t) dx = \frac{g'(0)}{\sqrt{g(0)}}$$

Since g is bounded, the limit can be rewritten as

$$\tilde{H}_0 = \lim_{t \to 0} \int_{-\epsilon}^{\epsilon} \frac{x}{t\sqrt{g(x)}} \tilde{\Gamma}(x, t) dx,$$

for any $\epsilon > 0$. Furthermore, again by assuming boundness and continuity of g, $\epsilon > 0$ can be choosen such that $x/\sqrt{g(x)}$ is monotone in the domain of integration.²

This allows to consider the change of variables $y = x/\sqrt{g(x)}$,

$$\frac{dy}{dx} = \frac{1}{\sqrt{g(x)}} \left(1 - x \frac{g'(x)}{2g(x)} \right)$$

and to rewrite the integral as

$$\begin{split} \int_{-\epsilon}^{\epsilon} \frac{x}{t\sqrt{g(x)}} \tilde{\Gamma}(x,t) dx &= \int_{-\epsilon}^{\epsilon} \frac{x}{t\sqrt{g(x)}} \frac{1}{\sqrt{4\pi g(x)t}} e^{-\frac{x^2}{4g(x)t}} dx \\ &= \int_{-\epsilon}^{\epsilon} \frac{y}{t} \frac{e^{-\frac{y^2}{4t}}}{\sqrt{4\pi t}} dy + \int_{-\epsilon}^{\epsilon} \frac{x}{t\sqrt{g(x)}} \left(x\frac{g'(x)}{2g(x)}\right) \frac{1}{\sqrt{4\pi g(x)t}} e^{-\frac{x^2}{4g(x)t}} dx \\ &= \int_{-\epsilon}^{\epsilon} \frac{g'(x)}{2\sqrt{g(x)}} \frac{x^2}{tg(x)} \tilde{\Gamma}(x,t) dx \end{split}$$

which, by boundedness and continuity assumptions on g, tends to $g'(0)/\sqrt{g(0)}$ for $t \to 0$.

Corollary 1. Under the same assumptions of Lemma 3, if $g \in C^2$ with g, g' and g'' bounded near the origin, then

$$\lim_{t \to 0} \int_{\mathbb{R}} \frac{x^{2n+1}}{(g(x)t)^{n+1}} \tilde{\Gamma}(x,t) dx = 0$$

Proof. By hypothesis g'' and g' are bounded in $[-\epsilon, \epsilon]$, so that, in that interval, $g^{-1/2}$ and $g^{1/2}$ can be approximated as $g(x)^{-1/2} = g(0)^{-1/2} - \frac{1}{2}g'(0)g(0)^{-3/2}x + O(x^2)$ and $g(x)^{1/2} = g(0)^{1/2} + O(x)$. Using these approximations it holds

$$\begin{aligned} \frac{x}{g(x)t} &= g(x)^{-\frac{1}{2}} \frac{x}{g(x)^{\frac{1}{2}t}} = g(0)^{-\frac{1}{2}} \frac{x}{g(x)^{\frac{1}{2}t}} - \frac{1}{2} \frac{g'(0)}{g(0)^{\frac{3}{2}}} g(x)^{\frac{1}{2}} \frac{x^2}{g(x)t} + O(x^3/t) \\ &= g(0)^{-\frac{1}{2}} \frac{x}{g(x)^{\frac{1}{2}t}} - \frac{1}{2} \frac{g'(0)}{g(0)^{\frac{3}{2}}} g(0)^{\frac{1}{2}} \frac{x^2}{g(x)t} + O(x^3/t), \end{aligned}$$

thus,

$$\lim_{t \to 0} \int_{\mathbb{R}} \frac{x}{g(x)t} \tilde{\Gamma}(x,t) dx = \lim_{t \to 0} \int_{-\epsilon}^{\epsilon} \left(g(0)^{-\frac{1}{2}} \frac{x}{g(x)^{\frac{1}{2}}t} - \frac{1}{2} \frac{g'(0)}{g(0)^{\frac{3}{2}}} g(0)^{\frac{1}{2}} \frac{x^2}{g(x)t} + O(x^3/t) \right) \tilde{\Gamma}(x,t) dx$$

² The first derivative of $x/\sqrt{g(x)}$ is null in x = 0 if and only if $\lim_{x \to 0} 2g(x) - xg'(x) = 0$, a case ruled out because, by hypothesis, g > 0 and $|g'(0)| < \infty$.

by Lemma 2 and 3

$$=\frac{1}{\sqrt{g(0)}}\frac{g'(0)}{\sqrt{g(0)}}-\frac{1}{2}\frac{g'(0)}{g(0)}\cdot 2=0$$

Finally, by proceeding in a manner analogous to the proof of Lemma 3, the thesis follows for all n.

Now, let resume rules for computing limits of integrals involving the parametrix Z. These results are used in the next section together with those provided in the corollary.

Lemma 4. If a(x) satisfy **H.1** and **H.2** then

$$\lim_{t \to \tau^+} \int_{\mathbb{R}} f(x,t) Z(x,t;\xi,\tau) dx = \lim_{\substack{t \to \tau^+ \\ x \to \xi}} f(x,t),$$
(13a)

$$\lim_{\tau \to t^-} \int_{\mathbb{R}} f(\xi, \tau) Z(x, t; \xi, \tau) d\xi = \lim_{\substack{\tau \to t^-\\\xi \to x}} f(\xi, \tau),$$
(13b)

provided that the limits in the RHSs exist and are unique. Furthermore, for n even

$$\lim_{t \to \tau^+} \int_{\mathbb{R}} \frac{(x-\xi)^n}{(a(\xi)(t-\tau))^{n/2}} Z(x,t;\xi,\tau) dx = \lim_{\tau \to t^-} \int_{\mathbb{R}} \frac{(x-\xi)^n}{(a(\xi)(t-\tau))^{n/2}} Z(x,t;\xi,\tau) d\xi = \frac{n!}{(n/2)!}$$
(14a)

and, for n odd

$$\lim_{t \to \tau^+} \int_{\mathbb{R}} \frac{(x-\xi)^n}{(a(\xi)(t-\tau))^{n/2}} Z(x,t;\xi,\tau) dx = \lim_{\tau \to t^-} \int_{\mathbb{R}} \frac{(x-\xi)^n}{(a(\xi)(t-\tau))^{n/2}} Z(x,t;\xi,\tau) d\xi = 0,$$
(14b)

$$\lim_{\tau \to t^{-}} \int_{\mathbb{R}} \frac{|x-\xi|^{n}}{(a(\xi)(t-\tau))^{n/2}} Z(x,t;\xi,\tau) dx = \frac{2^{n}}{\sqrt{\pi}} \left(\frac{n-1}{2}\right)!$$
(14c)

and

$$\lim_{\tau \to t^-} \int_{\mathbb{R}} \frac{|x-\xi|^n}{(a(\xi)(t-\tau))^{n/2}} Z(x,t;\xi,\tau) d\xi < +\infty$$
(14d)

Proof. Direct consequence of Lemma 2 and Lemma 3.

Corollary 2. With the same hypothesis of Lemma 4, if $f \in C^{2,1}$ and $\lim_{x \to \pm \infty} f(x,t)\Gamma(x,t) = 0$ and assuming a(x) twice differentiable near $x = \xi$, then

$$\lim_{t \to \tau^+} \int_{\mathbb{R}} f(x,t) LZ(x,t;\xi,\tau) dx = \lim_{\substack{t \to \tau^+ \\ x \to \xi}} \partial_{xx} \left((a(x) - a(\xi)) f(x,t) \right)$$
(15a)

$$\lim_{\tau \to t^-} \int_{\mathbb{R}} f(\xi,\tau) LZ(x,t;\xi,\tau) d\xi = -(a''(x) + 2a'(x)\partial_x)f(x,t).$$
(15b)

Proof. In order to prove (15a), let notice that $LZ = (a(x)\partial_{xx} - \partial_t)Z = a(x)\partial_{xx}Z - a(\xi)\partial_{xx}Z$ so that (15a) follows by integrating by parts:

$$\int_{\mathbb{R}} f(x,t) LZ(x,t;\xi,\tau) dx = \int_{\mathbb{R}} f(x,t) (a(x) - a(\xi)) \partial_{xx} Z(x,t;\xi,\tau) dx$$
$$= \int_{\mathbb{R}} \partial_{xx} \big((a(x) - a(\xi)) f(x,t) \big) Z(x,t;\xi,\tau) dx.$$

The last results, equation (15b), is a bit more involving. Let rewrite $LZ(z;\zeta) = A(z;\zeta)Z(z;\zeta)$, where

$$A(x,t,\xi,\tau) := \frac{a(x) - a(\xi)}{a(\xi)(t-\tau)} \left(\frac{(x-\xi)^2}{4a(\xi)(t-\tau)} - \frac{1}{2} \right)$$
(16)

By a Taylor expansion of $a(\xi)$ centered in x, A can be rewritten as

$$A(z;\zeta) = \left(a'(x)\frac{(x-\xi)}{a(\xi)(t-\tau)} - \frac{a''(x)}{2}\frac{(x-\xi)^2}{a(\xi)(t-\tau)}\right)\left(\frac{(x-\xi)^2}{4a(\xi)(t-\tau)} - \frac{1}{2}\right) + O\left(\frac{(x-\xi)^3}{t-\tau}\right),$$

so that, from the Taylor expansion $f(\xi,\tau) = f(x,\tau) - (x-\xi)f^{(1,0)}(x,\tau) + O(x-\xi)$ and defining $y = (x-\xi)/\sqrt{a(\xi)(t-\tau)}$ it gives

$$f(\zeta)A(z;\zeta) = -\frac{1}{8}a''(x)(y^4 - 2y^2)f(x,\tau) + \frac{1}{4}a'(x)\frac{(y^3 - 2y)}{\sqrt{a(\xi)(t-\tau)}}f(x,\tau) -\frac{1}{4}a'(x)(y^4 - 2y^2)f^{(1,0)}(x,\tau) + O((x-\xi)^3/(t-\tau))$$

Now, since by (14a)

$$\lim_{\tau \to t^{-}} \int_{\mathbb{R}} (y^4 - 2y^2) Z(x, t; \xi, \tau) d\xi = 8,$$

and, by Corollary 1,

$$\lim_{\tau \to t^{-}} \int_{\mathbb{R}} \frac{y^{2n+1}}{\sqrt{a(\xi)(t-\tau)}} Z(x,t;\xi,\tau) d\xi = 0, \qquad n = 0, 1,$$

it follows that

$$\lim_{\tau \to t^-} \int_{\mathbb{R}} f(\zeta) A(z;\zeta) Z(z;\zeta) d\xi = -2a'(x) \partial_x f(x,t) - a''(x) f(x,t),$$

assuming continuity of f and $f^{(1,0)}$ near (x,t). The latter requirement can be weakened by replacing f(x,t) and $f^{(1,0)}(x,t)$ with the corresponding limits and assuming existence and unicity of these.

and

3 Approximating Z_1 and Z_2

In the following it is assumed that the coefficient a(x) satisfies assumptions **H.1** and **H.2** and has enough regularity near x or ξ .

3.1 Computing $I_1(t^-)$ and $I_1(0^+)$

By rule (13b) of Lemma 4 it follows that

$$I_1(t^-; x, t; \xi, 0) = \lim_{t_0 \to t^-} \int_{\mathbb{R}} Z(x, t; x_0, t_0) LZ(x_0, t_0; \xi, 0) dx_0 = LZ(x, t; \xi, 0),$$
(17)

for t > 0. The second limit

$$I_1(0^+; x, t; \xi, 0) = \lim_{t_0 \to 0^+} \int_{\mathbb{R}} Z(x, t; x_0, t_0) LZ(x_0, t_0; \xi, 0) dx_0, \qquad t > 0,$$

is computed by using rule (15a) in Corollary 2, which gives

$$I_{1}(0^{+};x,t;\xi,0) = a''(\xi)Z(x,t;\xi,0) + 2a'(\xi)\partial_{\xi}Z(x,t;\xi,0)$$

= $\left(a''(\xi) + 2\frac{(a'(\xi))^{2}}{a(\xi)}\left(\frac{(x-\xi)^{2}}{4a(\xi)t} - \frac{1}{2}\right) + a'(\xi)\frac{x-\xi}{a(\xi)t}\right)Z(x,t;\xi,0).$ (18)

3.2 Computation of $I_2(t^-,t^-)$ and $I_2(t^-,0^+)$

Let consider the limit $\lim_{t_0 \to t^-} I_2(t_0, t_1)$, by Lemma 2 it follows that

$$I_{2}(t^{-},t_{1}) = \lim_{t_{0} \to t^{-}} \int_{\mathbb{R}} \int_{\mathbb{R}} Z(x,t;x_{0},t_{0}) LZ(z_{0};z_{1}) LZ(z_{1};\zeta) dx_{0} dx_{1}$$
$$= \int_{\mathbb{R}} LZ(z;z_{1}) LZ(z_{1};\zeta) dx_{1}.$$

Now, the limits $\lim_{t_1\to 0^+} I_2(t^-, t_1)$ and $\lim_{t_1\to t^-} I_2(t^-, t_1)$ are tackled by means of Corollary 2, equations (15a) and (15b), respectively. That is,

$$I_{2}(t^{-},0^{+}) = \lim_{t_{1}\to0^{+}} \int_{\mathbb{R}} LZ(x,t;x_{1},t_{1})LZ(x_{1},t_{1};\xi,0)dx_{1}$$

$$= (a''(\xi) + 2a'(\xi)\partial_{\xi})LZ(x,t;\xi,0)$$

$$= \left(a''(\xi) + 2\frac{(a'(\xi))^{2}}{a(\xi)}\left(\frac{(x-\xi)^{2}}{4a(\xi)t} - \frac{1}{2}\right) + a'(\xi)\frac{x-\xi}{a(\xi)t} + 2a'(\xi)\frac{\partial_{\xi}A(x,t;\xi,0)}{A(x,t,\xi,0)}\right)LZ(x,t;\xi,0)$$
(19)

and

$$I_{2}(t^{-},t^{-}) = \lim_{t_{1} \to t^{-}} \int_{\mathbb{R}} LZ(x,t;x_{1},t_{1})LZ(x_{1},t_{1};\xi,0)dx_{1}$$
$$= -(a''(x) + 2a'(x)\partial_{x})LZ(x,t;\xi,0)$$
(20)

Now, since

$$\begin{aligned} \partial_x LZ(x,t;\xi,\tau) &= L\partial_x Z(x,t;\xi,\tau) + a'(x)\partial_{xx} Z(x,t;\xi,\tau) \\ &= -L\frac{x-\xi}{2a(\xi)t} Z(x,t;\xi,\tau) + \frac{a'(x)}{a(x)-a(\xi)} LZ(x,t;\xi,\tau) \\ &= -\frac{x-\xi}{2a(\xi)t} LZ(x,t;\xi,\tau) - \frac{1}{t} \frac{x-\xi}{2a(\xi)t} Z(x,t;\xi,\tau) + \frac{a'(x)}{a(x)-a(\xi)} LZ(x,t;\xi,\tau), \end{aligned}$$

the limit in (20) can be rewritten as

$$I_{2}(t^{-},t^{-}) = -\left(a''(x) - a'(x)\frac{x-\xi}{a(\xi)t} + 2\frac{a'(x)^{2}}{a(x) - a(\xi)}\right)LZ(x,t;\xi,0) + \frac{a'(x)}{t}\frac{x-\xi}{a(\xi)t}Z(x,t;\xi,\tau),$$

3.3 Computing $I_2(0^+, 0^+)$

Before deriving an expression for $I_2(0^+, 0^+)$ it is convenient to prove the following Lemma.

Lemma 5. Let assume $f(x) \in C^2$ on $B = [\xi - \epsilon, \xi + \epsilon]$, then

$$\lim_{t \to \tau} \int_{\mathbb{R}} f(x) \partial_{\xi} Z(x, t; \xi, \tau) dx = f'(\xi).$$
(21)

Proof. Firstly,

$$\partial_{\xi} Z(x,t;\xi,\tau) = \left(\frac{a'(\xi)}{a(\xi)} \left(\frac{(x-\xi)^2}{4a(\xi)(t-\tau)} - \frac{1}{2}\right) + \frac{x-\xi}{2a(\xi)(t-\tau)}\right) Z(x,t;\xi,\tau).$$

Then, from $f(x) = f(\xi) + (x - \xi)f'(\xi) + O((x - \xi)^2 ||f''||_{\infty,B})$ it follows that (21) can be rewritten as

$$\begin{split} \lim_{t \to \tau} \int_B f(x) \partial_{\xi} Z(x,t;\xi,\tau) dx &= \lim_{t \to \tau} \int_B \frac{a'(\xi)}{a(\xi)} \left(\frac{(x-\xi)^2}{4a(\xi)(t-\tau)} - \frac{1}{2} \right) f(\xi) Z(x,t;\xi,\tau) dx \\ &+ \lim_{t \to \tau} \int_B \frac{(x-\xi)^2}{2a(\xi)(t-\tau)} f'(\xi) Z(x,t;\xi,\tau) dx. \end{split}$$

where it has been used the fact that integral of odd terms is null and that the remaining omitted terms vanish for $t \to \tau$ by virtue of Lemma 4, equation (14a). The result in (21) follows by noting that by (14a) the first limit converges to 0 and the second one to $f'(\xi)$.

Let consider now the computation of $I_2(0^+, 0^+)$. From (15a) it follows that

$$I_{2}(t_{0}, 0^{+}) = \lim_{t_{1} \to 0} \int_{\mathbb{R}} \int_{\mathbb{R}} Z(x, t; x_{0}, t_{0}) LZ(z_{0}; z_{1}) LZ(z_{1}; \zeta) dx_{0} dx_{1}$$
$$= \int_{\mathbb{R}} Z(z; z_{0}) (a''(\xi) + 2a'(\xi)\partial_{\xi}) LZ(z_{0}; \zeta) dx_{0}.$$

so that,

$$I_{2}(0^{+},0^{+}) = \lim_{t_{0}\to0} \int_{\mathbb{R}} a''(\xi)Z(z;z_{0})LZ(z_{0};\zeta)dx_{0} + \lim_{t_{0}\to0} \int_{\mathbb{R}} 2a'(\xi)Z(z;z_{0})\partial_{\xi}LZ(z_{0};\zeta)dx_{0}$$
$$= a''(\xi) \left[\partial_{x_{0}x_{0}}(a(x_{0}) - a(\xi))Z(z;x_{0},0)\right]_{x_{0}=\xi} + 2a'(\xi)C$$

where

$$C = \lim_{t_0 \to 0} \int_{\mathbb{R}} Z(z; z_0) \partial_{\xi} LZ(z_0; \zeta) dx_0.$$

Now, since $LZ(z_0;\zeta) = (a(x_0) - a(\xi))\partial_{x_0x_0}Z(z_0,\zeta)$, C can be rewritten as

$$C = -\lim_{t_0 \to 0} \int_{\mathbb{R}} a'(\xi) Z(z; z_0) \partial_{x_0 x_0} Z(z_0; \zeta) dx_0 + \lim_{t_0 \to 0} \int_{\mathbb{R}} Z(z; z_0) (a(x_0) - a(\xi)) \partial_{x_0 x_0} \partial_{\xi} Z(z_0; \zeta) dx_0 = -a'(\xi) \partial_{\xi\xi} Z(z; \zeta) + \lim_{t_0 \to 0} \int_{\mathbb{R}} \left(\partial_{x_0 x_0} (a(x_0) - a(\xi)) Z(z; z_0) \right) \partial_{\xi} Z(z_0; \zeta) dx_0 = -a'(\xi) \partial_{\xi\xi} Z(z; \zeta) + \left[\partial_{x_0 x_0 x_0} (a(x_0) - a(\xi)) Z(z; x_0, 0) \right]_{x_0 = \xi}.$$

Thus,

$$I_2(0^+, 0^+) = \left[(a''(\xi) + 2a'(\xi)\partial_{x_0})\partial_{x_0x_0}(a(x_0) - a(\xi))Z(z; x_0, 0) \right]_{x_0 = \xi} - 2a'(\xi)^2 \partial_{\xi\xi} Z(z; \zeta).$$
(22)

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