APPROXIMATE SOLUTIONS TO SECOND ORDER PARABOLIC EQUATIONS I: ANALYTIC ESTIMATES

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Abstract. We establish a new type of local asymptotic formula for the Green's function of a parabolic linear operator with non-constant coefficients. Our procedure leads to an elementary, algorithmic construction of approximate solutions to parabolic equations which are accurate to arbitrary prescribed order in the short-time limit.

Contents

1. Introduction

We establish a new type of local estimate for the Green's function of a parabolic linear operator with non-constant coefficients that *do not depend on time.* More precisely, we consider second-order differential

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operators L of the form

$$Lu(x) := \sum_{i,j=1}^{N} a_{ij}(x)\partial_i\partial_j u(x) + \sum_{k=1}^{N} b_k(x)\partial_k u(x) + c(x)u(x), \tag{1.1}$$

where $x = (x_1, ..., x_N) \in \mathbb{R}^N$, $\partial_k := \frac{\partial}{\partial x_k}$, and the coefficients a_{ij}, b_i, and c and all their derivatives are assumed to be smooth and uniformly bounded. (We then write $a_{ij}, b_j, c \in \mathcal{C}_b^\infty\left(\mathbb{R}^N\right)$ and we denote the class of these operators by $\mathbb{L}$.)

We further assume that L is *uniformly strongly elliptic*, namely that there exists a constant $\gamma > 0$ such that

$$\sum_{ij} a_{ij}(x)\xi_i\xi_j \geq \gamma\|\xi\|^2, \quad \|\xi\|^2 := \sum_{i=1}^{N} \xi_i^2, \tag{1.2}$$

for all $(\xi, x) \in \mathbb{R}^N \times \mathbb{R}^N$. We define the matrix $A(x) := [a_{ij}(x)]$, which, without loss of generality, we can assume to be symmetric. In view of the applications we are interested in, we take the coefficients of L to be real-valued. (The set of operators $L \in \mathbb{L}$ satisfying (1.2) will be denoted by $\mathbb{L}_\gamma$.)

We study the initial value problem (IVP) for the parabolic operator $\partial_t - L$, namely we want

$$\begin{cases} \partial_t u(t,x) - Lu(t,x) = g(t,x) & \text{in } (0,\infty) \times \mathbb{R}^N \\ u(0,x) = f(x), & \text{on } \{0\} \times \mathbb{R}^N, \end{cases} \tag{1.3}$$

for u, f, and g in suitable function spaces. We can also replace $\mathbb{R}^N$ with a manifold of bounded geometry [13, 35]. In view of Duhamel's principle, we may assume $g = 0$.

Then it is known that there exists $\mathcal{G}^L \in \mathcal{C}^\infty((0,\infty) \times \mathbb{R}^N \times \mathbb{R}^N)$ such that

$$u(t,x) = \int_{\mathbb{R}^N} \mathcal{G}^L(t,x,y)f(y)dy, \quad t > 0, \tag{1.4}$$

is a solution of the above equation, and it is unique if f and hence u satisfy certain growth conditions, specified later (see for instance [18], page 237). We will often write $\mathcal{G}^L(t,x,y) = \mathcal{G}_t^L(x,y)$. In case we have uniqueness, we shall also use the notation $u(t) = e^{tL}f$. The operator e^{tL} is then called the *solution operator* of the problem (1.3), and its kernel $\mathcal{G}_t^L$ the *Green's function*, or *fundamental solution* of L, or *conditional probability density* in applications to probability.

When $b(x), c(x) \neq 0$ in (1.1), the corresponding parabolic equation $\partial_t u - Lu = 0$ is collectively referred to as a Fokker-Planck equation.

Fokker-Planck equations arise in many applications, for example in statistical mechanics [16, 21], and more generally in probability.

For L with constant coefficients and for a few other cases, one can explicitly compute the kernel $\mathcal{G}^L$. In general however, it is not known how to provide explicit formulas for $\mathcal{G}^L$, though there is a large literature on developing methods to obtaining good asymptotic formulas for the Green's function for t small and x close to y. For example, interpreting the operator L as a Laplace-Beltrami operator on a manifold plus lower order terms, lead to formal asymptotic expansions of the form

(1.5)
$$\mathcal{G}_t(x,y) = \frac{e^{-\frac{d(x,y)^2}{4t}}}{(4\pi t)^{N/2}} \left(\mathcal{G}^{(0)}(x,y) + \mathcal{G}^{(1)}(x,y)t + \mathcal{G}^{(2)}(x,y)t^n + \dots\right),$$

as $t \to 0_+$, where $d(x,y)$ is the geodesic distance between x and y and $\mathcal{G}^{(j)}(x,y)$ are smooth functions in x and y. Among the vast literature we refer to [3, 26, 29, 38, 40, 48, 48, 50], (see also [23] for a pseudo-differential perspective). However, one difficulty in the practical implementation of this geometric approach is that, except again in special cases, there is no closed form solution to the geodesic equations used in defining $d(x,y)$, which thus needs to be accurately approximated or computed numerically.

A related short-time asymptotic approach uses oscillatory type integrals, which gives:

(1.6)
$$\mathcal{G}^L(t,x,y) \sim \sum_{j\geq 0} t^{(j-n)/2} p_j\left(x, t^{-1/2}(x-y)\right) e^{-(x-y)^T A(x)^{-1}\cdot(x-y)/4t},$$

as $t \to 0_+$, where $p_j(x,w)$ is a polynomial of degree j in w, and $A(x) := [a_{ij}(x)]$. (We follow here Taylor [43, Chapter 7, Section 13], where an asymptotic parametrix for the heat equation on compact manifolds was constructed.) Finally, we mention the recent approach in [2] using multivariate Hermite expansions.

The point of departure of this paper is an expansion of the form (1.6) above. We generalize such asymptotic expansion to obtain a *new* type of approximation of the fundamental solution for the operator L, which may prove more accurate and more stable in practical implementations [14, 13]. The main goal is to provide an *algorithmic, explicit* method to compute each term in the expansion, while at the same time obtain sharp error bounds in both weighted and unweighted Sobolev spaces. We do not work on compact manifolds, rather in $\mathbb{R}^N$, so that the error needs to be globally controlled (see below for a connection with operators on non-compact manifolds of bounded geometry). In particular, our approximation is valid uniformly in x and y, provided t is small enough.

Our approach is more elementary than the ones found in the literature and rely on an iterative time-ordered perturbative formula for the solution operator e^{tL}, Equation (2.15), a parabolic rescaling argument, and a suitable Taylor's expansion of the coefficients of L (equation 3.8). Since the iterative formula is obtained via repeated applications of Duhamel's principle, we could also treat certain classes of semilinear equations following Kato's method, which allows to take rougher data as well (see [33] in the context of the Navier-Stokes equations). We remark here that a similar parabolic scaling combined with Taylor expansions has been used in obtaining a short-time expansion for stochastic flows (see [7, 17]).

The approach in this paper can be extended to the case of certain operators with unbounded coefficients that appear in applications, such as $\partial_t - (ax^2\partial_x^2 + bx\partial_x + c)$ acting on $\mathbb{R}_t \times \mathbb{R}_{x+}$. This extension is work in progress [13]. See also below for a more detailed discussion of this point.

Our main result is the following theorem. We introduce the weight $\langle x\rangle = (1 + |x|^2)^{1/2}$. Below, $W_a^{m,p} := W_a^{m,p}(\mathbb{R}^N)$ is the exponentially weighted Sobolev space defined by

$$W_a^{m,p}(\mathbb{R}^N) := \{u : \mathbb{R}^N \to \mathbb{C},\ \partial_x^\alpha\big(e^{a\langle x\rangle}u(\cdot)\big) \in L^p(\mathbb{R}^N),\ |\alpha| \le m\},$$

for $1 < p < \infty$, $m \in \mathbb{Z}_+$, and $a \in \mathbb{R}$. (See also Equation (2.4)). When $a = 0$, we recover the usual Sobolev spaces. The need to consider exponentially weighted spaces arises in applications to probability, in particular in stochastic volatility models. For instance, after making the substitution $x = e^y$, the payoff usually associated with the Black-Scholes equation (equation (1.9) below) belongs to $W_a^{m,p}$ with $m = 1$, $a < -1$, and p large. We also denote

$$G(z; x) = (4\pi)^{-N/2} \det(A(z))^{-1/2} e^{-x^T A(z)^{-1} x/4}, \tag{1.7}$$

where z is a given point in $\mathbb{R}^N$. It is interesting to mention that the Black-Scholes equation fits into the framework of manifolds with cylindrical ends, to which the results of Krainer [31] apply. Manifolds with cylindrical ends are the simplest examples of manifolds with bounded geometry.

To approximate the value of the Green function $\mathcal{G}_t(x, y)$ at some point (x, y), we will use a Taylor-type expansion at the point z of a suitable parabolic rescaling of the coefficients of L, which, however will be chosen depending of x and y, $z = z(x,y)$. Typically $z(x,y) = \lambda x + (1-\lambda)y$, for some fixed λ, but we can allow more general choices. Namely, we shall say that $z(x,y)$ is *admissible* if $z(x,x) = x$ and all derivatives $\partial^\alpha z$ are bounded for $\alpha \neq 0$.

Theorem 1.1. *Let $\mu \in \mathbb{Z}_+$, $L \in \mathbb{L}_\gamma$, $z = z(x,y)$ be an admissible function. Then for each integer $0 \leq \ell \leq \mu$, there exist* explicitly computable *functions* $\mathfrak{P}^\ell(z,x,y) = \sum a_{\alpha,\beta}(z)(x-z)^\alpha(x-y)^\beta$, $|\alpha| \leq \ell$, $\beta \leq 3\ell$, $a_{\alpha,\beta} \in \mathcal{C}_b^\infty(\mathbb{R}^N)$*, with the following property. Let*

$$\mathcal{G}_t^{[\mu,z]}(x,y) := t^{-N/2} \sum_{\ell=0}^{\mu} t^{\ell/2}\, \mathfrak{P}^\ell(\,z,\, z + \frac{x-z}{t^{1/2}}\,,\, z + \frac{y-z}{t^{1/2}}\,) G(z;\, \frac{x-y}{t^{1/2}}\,),$$

where $z = z(x,y)$. Define the error term $\mathcal{E}_t^{[\mu,z]}$ in the approximation of the Green's function by:

$$e^{tL} f(x) = \int_{\mathbb{R}^N} \mathcal{G}_t^{[\mu,z]}(x,y) f(y) dy + t^{(\mu+1)/2} \mathcal{E}_t^{[\mu,z]} f(x).$$

Then, for any $f \in W_a^{m,p}(\mathbb{R}^N)$, $a, m \in \mathbb{R}$, $1 < p < \infty$, we have

$$\|\mathcal{E}_t^{[\mu,z]} f\|_{W_a^{m+k,p}} \leq C t^{-k/2} \|f\|_{W_a^{m,p}}, \tag{1.8}$$

for any $t \in [0,T]$, $0 < T < \infty$, $k \in Z\!\!Z_+$, with C independent of $t \in [0,T]$.

The function $\mathcal{G}_t^{[\mu,z]}(x,y)$ will be called the *μth-order approximation kernel* for the solution operator e^{tL}.

See Subsection 1.1 at the end of this introduction for a more detailed description of how the approximation kernel $\mathcal{G}_t^{[\mu,z]}(x,y)$ is obtained. In Section 4 we give an explicit iterative construction of the functions $\mathfrak{P}^\ell$. The main interest is, of course, in the derivation of the approximation kernel. However, without good error estimates, this kernel will not be of great use in practice.

For $z = x$ we have checked that the first few polynomials $p_j(x, x - y) := \mathfrak{P}^j(x,x,y)$ coincide with the ones in the expansion (1.6) above (see [43, Chapter 7, Section 13]). Our result is more general, however. We discuss in [13] different choices of the additional function $z = z(x,y)$ in the framework of the usual Black-Scholes equation. It turns out that the choice $z = x$ is not always the most appropriate. In fact, for the Black-Scholes equation, the choice $z = \sqrt{xy}$ can lead to a better approximation, whereas, surprisingly, the choice $z = (x+y)/2$ yields worse numerical results than simply choosing $z = x$.

A localization procedure as in [35] will allow us to pass from operators on $\mathbb{R}^N$ to operators on manifolds M of bounded geometry (again following [11] and [35]). More precisely, our results will extend to operators of the form $L = \sum_{ij}^N a_{ij}\partial_i\partial_j + \sum_{ij}^N b_i\partial_i + c$, defined on a subset Ω of $\mathbb{R}^N$ such that the coefficients are bounded in *normal coordinates* with respect to the metric $g = \sum_{ij}^N a^{ij} dx_i dx_j$, assumed to be complete of bounded geometry on Ω. Here the matrix $[a^{ij}]$ is the inverse of the matrix A, following the usual convention. Such metrics arise naturally when resolving boundary singularities. We refer to [1, 11, 32, 46] for recent papers dealing with partial differential equations on manifolds with metrics of this form. In particular, we can deal with certain operators having polynomial coefficients such as those arising in probability and its applications, for example in the Black-Scholes option pricing equation [6]

$$Lu(x) = \sigma x^2 \partial_x^2 u(x)/2 + r(x\partial_x u(x) - u(x)), \tag{1.9}$$

where in this context t is the time to option expiry. Our results also apply to differential operators arising in stochastic volatility models (c.f. [4, 20, 22, 25, 36, 37]). On the other hand, our results apply to operators of the form $x^{2\beta}\partial_x^2$, $0 < \beta < 1$ *only locally.* A good framework for obtaining differential operators with unbounded coefficients that satisfy our assumptions is that of Lie manifolds [1]. This point will be discussed in detail in [13]. Explicit calculations and concrete, practical applications of our method will be given in [14, 15].

In addition, our methods generalize to operators with *time-depdendent* coefficients, satisfying certain conditions. This extension is addressed in a forthcoming paper [12].

We conclude this first part of the introduction with an outline of the paper. In Section 2, we define the weighted and regular Sobolev spaces of initial data for the parabolic equation and introduce the class of operators L under study. We also briefly discuss mapping properties of the semigroup generated by L and use them to justify the time-ordered perturbation expansion of e^{tL}. In Section 3, we exploit local in space and time dilations of the Green's function together with a certain Taylor expansion of the operator L to rewrite the perturbation expansion as a formal power series in $s = \sqrt{t}$. In Section 4, we employ commutator estimates to derive computable formulas for each term in the expansion. Finally, in Section 5, we rigorously justify our expansion and derive error bounds in time by means of pseudodifferential calculus.

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1.1. **The approximate Green function.** We close this Introduction by describing in more details how the approximation kernel $\mathcal{G}_t^{[n,z]}$ is defined. Given an operator T with smooth kernel, we denote its kernel by $T(x,y)$ as customary.

We consider a *uniformly strongly elliptic* differential operator L of the form $L := \sum_{i,j=1}^N a_{ij}\partial_i\partial_j + \sum_{k=1}^N b_k\partial_k + c$, where $a_{ij}, b_k, c \in C_b^\infty(\mathbb{R}^N)$ are *real valued*. Given a fixed point $z \in \mathbb{R}^N$ and $s > 0$, we define $L^{s,z} := \sum_{i,j=1}^N a_{ij}^{s,z}(x)\partial_i\partial_j + s\sum_{i=1}^N b_i^{s,z}(x)\partial_i + s^2 c^{s,z}(x)$, where for a generic function f we set $f^{s,z}(x) = f(z + s(x - z))$. Hence, z acts as a fixed dilation center. We then Taylor expand this operator in s around 0 to order n:

$$L^{s,z} = \sum_{m=0}^{n} s^m L_m^z + V_{n+1}^{s,z} = \sum_{m=0}^{n+1} s^m L_m^z, \tag{1.10}$$

where L_j^z, $0 \le j \le n$, are differential operators with *polynomial coefficients* that do not depend on s, whereas L_{n+1}^z has smooth coefficients that, however, do depend on s (although this dependence is not shown in the notation). Hence, $V_{n+1}^{s,z} = s^{n+1}L_{n+1}^z$ is the remainder of the Taylor expansion. The order n will be chosen later. In particular, we observe that

$$L_0^z = \sum_{i,j} a_{ij}(z)\partial_i\partial_j. \tag{1.11}$$

For any fixed, positive integers $k \le n+1$ and ℓ, we shall denote by $\mathfrak{A}_{k,\ell}$ the set of multi-indexes $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_k) \in \mathbb{N}^k$, such that $|\alpha| := \sum \alpha_j = \ell$. (Hence, $k \le \ell$.) Then, for each multi-index $\alpha = (\alpha_1, \ldots, \alpha_k) \in \mathfrak{A}_{k,\ell}$, $k \le n$, we introduce

$$\Lambda_{\alpha,z} := \int_{\Sigma_k} e^{\tau_0 L_0^z} L_{\alpha_1}^z e^{\tau_1 L_0^z} L_{\alpha_2}^z \cdots L_{\alpha_k}^z e^{\tau_k L_0^z} d\tau. \tag{1.12}$$

Observe that k, ℓ are unique given α.

The main point is that the operators Λ_α can be computed explicitly as follows. Let us denote by $\mathcal{D}(a,b)$ the vector space of all differentiations of polynomial degree at most a and order at most b. (By *polynomial degree* of a differentiation we mean the highest power of the polynomials appearing as coefficients.) Then, for any $L_0 \in \mathcal{D}(0,2)$ that is uniformly strongly elliptic and for any $L_m \in \mathcal{D}(m,2)$, we have a differential operator $P_m(L_0, L_m; \theta, x, \partial)$ given by the formula $e^{\theta L_0} L_m = P_m(L_0, L_m; \theta, x, \partial)e^{\theta L_0}$, where $\theta > 0$ (see Lemma 4.5). Let Σ_k be the unit k-dimensional simplex. Next, for any given multi-index $\alpha \in \mathfrak{A}_{k,\ell}$ with $k \le n$, we define $\mathcal{P}_\alpha(x,z,\partial) := \int_{\Sigma_k} \prod_{i=1}^k P_{\alpha_i}(L_0^z, L_{\alpha_i}^z; 1 -$

$\sigma_i, x, \partial)d\sigma$. Then

$$\Lambda_{\alpha,z} = \mathcal{P}_\alpha(x, z, \partial_x)e^{L_0^z}, \tag{1.13}$$

where the product is the composition of operators and $\mathcal{P}_\alpha$ is a differential operator of order $2k + \ell$ in x and polynomial degree $\leq \ell$ in $(x - z)$ (see Lemma 4.6).

Since z is arbitrary, but fixed at this stage, if L_0^z is the operator in (1.11) then $e^{L_0^z}(x, y)$ can be explicitly calculated and it agrees with the function $G(z, x - y)$ introduced in equation (1.7). Therefore, it can be easily seen from (1.13), that

$$\Lambda_{\alpha,z}(x, y) = \mathfrak{P}^\ell(z, x, y)G(z; x - y),$$

for some $\mathfrak{P}^\ell(z, x, y) = \sum a_{\alpha,\beta}(z)(x - z)^\alpha(x - y)^\beta$, $|\alpha| \leq \ell$, $\beta \leq 3\ell$, $a_{\alpha,\beta} \in \mathcal{C}_b^\infty(\mathbb{R}^N)$. In particular, all $\Lambda_{\alpha,z}$ are operators with smooth kernels, thus denoted $\Lambda_{\alpha,z}(x, y)$.

We will show that e^{tL} as well is an operator with smooth kernels, henceforth denoted $\mathcal{G}_t^L(x, y)$.

Let us fix for the time being a smooth function $z : \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}^N$ whose properties will be made precise below. (Two typical examples are $z(x, y) = (x+y)/2$ and $z(x, y) = x$, which suffice in many applications.)

Our approximation will be obtained by combining Lemma 3.2 with the perturbative estimate of Equation (3.18) at some point $z = z(x, y)$ using the dilation with center $z(x, y)$ and denoting $s^2 = t$. Then, for any $\mu \geq n$, we define

$$\begin{aligned}\mathcal{G}_t^{[\mu,z]}(x, y) &:= s^{-N}e^{L_0^z}(z + s^{-1}(x - z), z + s^{-1}(y - z)) \\ &+ \sum_{\ell=1}^{\mu}\sum_{k=1}^{\ell}\sum_{\alpha\in\mathfrak{A}_{k,\ell}} s^\ell\Lambda_{\alpha,z}(z + s^{-1}(x - z), z + s^{-1}(y - z)).\end{aligned} \tag{1.14}$$

The operator L is not shown explicitly in the notation $\mathcal{G}_t^{[\mu,z]}(x, y)$, although $\mathcal{G}_t^{[\mu,z]}(x, y)$ does depend on L. This is not likely to cause any confusion, since L is usually fixed in our discussions.

The justification of the above definition for the approximation is that a Dyson series expansion of order $n + 1$ gives us

$$\begin{aligned}\mathcal{G}_t(x, y) &:= s^{-N}e^{L_0^z}(z + s^{-1}(x - z), z + s^{-1}(y - z)) \\ &+ \sum_{\ell=1}^{(n+1)^2}\sum_{k=1}^{\max\{\ell,n+1\}}\sum_{\alpha\in\mathfrak{A}_{k,\ell}} s^\ell\Lambda_{\alpha,z}(z + s^{-1}(x - z), z + s^{-1}(y - z)),\end{aligned} \tag{1.15}$$

where for $k = n + 1$ and $\alpha = (\alpha_1, \ldots, \alpha_k) \in \mathfrak{A}_{k,\ell}$, we introduce

$$\Lambda_{\alpha,z} := \int_{\Sigma_k} e^{\tau_0 L_0^z} L_{\alpha_1}^z e^{\tau_1 L_0^z} L_{\alpha_2}^z \cdots L_{\alpha_k}^z e^{\tau_k L^{s,z}} d\tau. \tag{1.16}$$

The difference between equations (1.14) and (1.15) is that the sum in the first equation contains exactly the terms with s^ℓ, $\ell \leq n$, from the second equation. The difference between equations (1.12) and (1.16) is in the last exponential. Note that $\Lambda_{\alpha,z}$ does not depend on s if $\ell = |\alpha| \leq n$, but it may depend on s otherwise. In any case, all the terms $\Lambda_{\alpha,z}$ that depend on s will be included in the error term. All terms $\Lambda_{\alpha,z}$ with $\mu < |\alpha| \leq n$, which do not depend on s, will also be included in the error. We remark that the error term is never computed explicitly, as only the μth order approximation kernel is needed. Therefore, while μ will usually be small in applications, we can take n as large as needed to justify the error bounds of Theorem 1.1. In Section 5, we will show that $n > \mu + N - 1$ suffices.

2. Preliminaries

We begin by discussing in more details the class of second-order operators L of the form (1.1) that are the focus of our work. Below we set

$$C_b^\infty(\mathbb{R}^N) := \{f : \mathbb{R}^N \to \mathbb{C}, \partial^\alpha f \text{ bounded for all } \alpha\}. \tag{2.1}$$

Definition 2.1. *We shall denote by $\mathbb{L}$ the set of differential operators L of the form*

$$L := \sum_{i,j=1}^N a_{ij}\partial_i\partial_j + \sum_{k=1}^N b_k\partial_k + c, \tag{2.2}$$

where $a_{ij}, b_k, c \in C_b^\infty(\mathbb{R}^N)$ are real valued. *We shall denote by $\mathbb{L}_\gamma$ the subset of operators $L \in \mathbb{L}$ satisfying the uniform strong ellipticity estimate* (1.2) *with the ellipticity constant γ. We let $A = [a_{ij}]$ and assume additionally that A is symmetric, which can be achieved simply by replacing A with its symmetric part, since this does not change our differential operator.*

The above definition can be extended to operators on manifolds of bounded geometry M (see [11, 35, 42]). For example, when $M = \mathbb{R}^N$ with the Euclidean metric, the class $\mathbb{L}$ considered in [35] coincides with the class $\mathbb{L}$ considered in this paper.

In what follows, we denote the inner product on $L^2(\mathbb{R}^N)$ by $(u, v) = \int_{\mathbb{R}^N} u(x)\overline{v(x)}dx$. Let us denote $\langle\xi\rangle := (1 + |\xi|^2)^{1/2}$ and let $\hat{u}$ be the

Fourier Transform of u. We also recall the definition of and some basic facts about L^p-based Sobolev spaces $W^{r,p}(\mathbb{R}^N)$. For $1 < p < \infty$, $r \in \mathbb{R}$:

$$(2.3) \quad W^{r,p}(\mathbb{R}^N) := \{u : \mathbb{R}^N \to \mathbb{C}\,,\ \langle \xi \rangle^r \hat{u} \in L^p(\mathbb{R}^N)\}$$
$$= W^{r,p}(\mathbb{R}^N) := \{u : \mathbb{R}^N \to \mathbb{C}\,,\ (1-\Delta)^{r/2} u \in L^p(\mathbb{R}^N)\},$$

If $r \in \mathbb{Z}_+$,

$$W^{r,p}(\mathbb{R}^N) = \{u : \mathbb{R}^N \to \mathbb{C},\ \partial^\alpha u \in L^p(\mathbb{R}^N),\ |\alpha| \leq r\}.$$

Since the dimension N is fixed throughout the paper, we will usually write $W^{r,p}$ for $W^{r,p}(\mathbb{R}^N)$. When $1 < p < \infty$, the dual of $W^{r,p}$ is the Sobolev space $W^{-r,p'}$ with $1/p + 1/p' = 1$.

We are interested in considering the initial value problem (1.3) in the largest-possible space of initial data f that includes the typical initial conditions that arise in applications and where uniqueness holds. We therefore introduce exponentially weighted Sobolev spaces. Given a fixed point $y \in \mathbb{R}^N$, we set $\langle x \rangle_w := \langle x - w \rangle = (1 + |x-w|^2)^{1/2}$ and define $W^{m,p}_{a,w}(\mathbb{R}^N)$ for $m \in \mathbb{Z}_+$, $a \in \mathbb{R}$, $1 < p < \infty$, by

$$(2.4) \quad W^{r,p}_{a,w}(\mathbb{R}^N) := e^{-a\langle x \rangle_w} W^{r,p}(\mathbb{R}^N)$$
$$= \{u : \mathbb{R}^N \to \mathbb{C},\ \partial^\alpha_x\big(e^{a\langle x \rangle_w} u(\cdot)\big), \in L^p(\mathbb{R}^N),\ |\alpha| \leq r\}, \quad \text{if } r \in \mathbb{Z}_+,$$

with norm

$$\|u\|^p_{W^{m,p}_{a,w}} := \|e^{a\langle x \rangle_w} u\|^p_{W^{m,p}} = \sum_{|\alpha| \leq m} \|\partial^\alpha_\xi\big(e^{a\langle x \rangle_w} u(x)\big)\|^p_{L^p}.$$

When it is clear from the context, we may drop the subscript w from the above notation. We observe that $W^{m,p}_0 = W^{m,p}_{0,w} = W^{m,p}$. The spaces $W^{r,p}_{a,w}$ and $W^{-r,p'}_{-a,w}$ are naturally duals to each other if $1/p + 1/p' = 1$.

A crucial observation is that, for any $L \in \mathbb{L}_\gamma$ and any $a \in \mathbb{R}$, the operators $L_a := e^{a\langle x \rangle_w} L e^{-a\langle x \rangle_w}$ are also in $\mathbb{L}_\gamma$. They moreover define a bounded family in $\mathbb{L}_\gamma$ if a is in a bounded set, while w is *arbitrary*. Since proving a result for L acting between weighted Sobolev spaces $W^{s,p}_{a,w}$ is the same as proving the corresponding result for L_1 acting between the Sobolev spaces $W^{s,p} = W^{s,p}_{0,w}$, we may assume that $a = 0$ and w is arbitrary. In particular, $L : W^{s+2,p}_{a,y} \to W^{s,p}_{a,w}$ is well defined and continuous for any a and w, since this is true for $a = 0$.

In fact, it will be crucial for us to establish mapping properties that are *independent* of w. This will be the case in all estimates below, unless stated otherwise. One of the most important example is provided by Corollary 3.9. Moreover, the spaces $W^{m,p}_{a,w}$ do not depend on the choice of the point y (although their norm obviously does). Because of this observation, we shall often omit the point w from the notation, when this does not affect the clarity of the presentation.

We begin by recalling some properties of L and the associated solution operator e^{tL} to the initial value problem (1.3).

2.1. **Mapping properties.** Given a Banach X and an interval I of the real line, we shall denote by $\mathcal{C}(I, X)$ the space of continuous functions $u : I \to X$. By $\mathcal{C}^k(I, X)$ we shall denote the space of functions $u \in \mathcal{C}(I, X)$ such that $u^{(j)} \in \mathcal{C}(I, X)$ for all $0 \le j \le k$. We assume that $X \subset L^1_{\text{loc}}(\mathbb{R}^N)$, and that L is a closed unbounded operator on X with domain $\mathcal{D}(L) \subset X$.

Let $g \in \mathcal{C}([0, \infty), X)$. By a *classical solution in* X of (1.3) we mean a function

$$u \in \mathcal{C}([0, \infty), X) \cap \mathcal{C}^1((0, \infty), X) \cap \mathcal{C}((0, \infty), \mathcal{D}(L)), \tag{2.5}$$

such that $\partial_t u(t) = Lu(t) + g(t)$ in X for all $t > 0$ and $u(0) = f$ in X. (The domain of L is given the graph norm $|||u||| := \|u\| + \|Lu\|$, which makes $\mathcal{D}(L)$ a complete normed space, since we have assumed that L is closed and X is complete.) In particular, $u(0) = f$ must belong to the closure of $\mathcal{D}(L)$ in X. In the case of interest here, if $X = W^{s,p}_a$, then $\mathcal{D}(L) = W^{s+2,p}_a$, which is dense in X.

In view of Duhamel's formula (which will be justified below), we can assume $g = 0$ in Equation (1.3). We shall take our Banach space where the solution is defined to be $X = L^p_a$ for some arbitrary, but fixed, $p \in (1, \infty)$ and $a \ge 0$. Then Equation (1.3) becomes

$$\begin{cases} \partial_t u(t) - Lu(t) = 0 & \text{in } L^p_a(\mathbb{R}^N), \\ u(0) = f & f \in L^p_a(\mathbb{R}^N). \end{cases} \tag{2.6}$$

Let us notice that if $f \in \mathcal{C}^\infty(\mathbb{R}^N)$ also, then we recover Equation (1.3). The growth condition $u(t) \in L^p_a$ is needed, however, in order to insure uniqueness.

A family of (bounded) linear operators $U(t)$ on X, $t \ge 0$, will be called a $\mathcal{C}^0$ or *strongly continuous* semigroups of operators if $U(t)$ forms a semigroup in t and $U(t)u \to u$ in X as $t \to 0+$. This last property shows that the function $[0, \infty) \ni t \to U(t)f \in X$ is continuous for any $f \in X$.

We shall need the following standard result. Recall the subset $\mathbb{L}_\gamma \subset \mathbb{L}$ introduced in Definition 2.1.

Lemma 2.2. *(i) Let $L \in \mathbb{L}_\gamma$, then there exists a constant $C > 0$ such that*

$$\gamma(\nabla u, \nabla u) - C(u, u) \le -(Lu, u) \le C(\nabla u, \nabla u) + C(u, u).$$

(ii) The norm $|||v|||_{2m} := \|u\|_{L^p} + \|L^m u\|_{L^p}$ *is equivalent to the norm* $\|\cdot\|_{W^{2m,p}}$ *on* $W^{2m,p}(\mathbb{R}^N)$*, for any* $m \in \mathbb{Z}_+$ *and* $1 < p < \infty$.

Proof. (Sketch.) (i) follows from a direct calculation. See [42] or [35] for (ii). □

It follows from this lemma that $L : W^{2,p} \to L^p$ is a closed, densely defined unbounded operator on L^p. This technical fact is important because it is often needed for the general results that we will use below.

For the sake of clarity and completeness, we include here a quick review and some proofs of the main properties of the semigroup generated by L. Our proofs also serve the purpose of justifying the perturbative expansion described in Section 2.2, which is discussed extensively in the literature, but usually not in the setting that we need. Further details can be found in [34, 30, 41]. Below $p \in (1, \infty)$ and $\gamma > 0$ will be arbitrary but fixed, and the constants appearing in the estimates depend on p and γ, but not on $L \in \mathbb{L}_\gamma$.

Proposition 2.3. *Let* $a \in \mathbb{R}$, $1 < p < \infty$, *and* $L \in \mathbb{L}_\gamma$.

(i) For each $f \in W^{2,p}_a$*, the problem* (1.3) *has a unique classical solution*

$$u \in \mathcal{C}([0,\infty), L^p_a) \cap \mathcal{C}^1((0,\infty), L^p_a) \cap \mathcal{C}((0,\infty), W^{2,p}_a).$$

(ii) Let $e^{tL} f := u(t)$*, then we have* $e^{tL} W^{r,p}_a \subset W^{r,p}_a$ *and, moreover,* $\|e^{tL} f\|_{W^{r,p}_a} \le C e^{\omega t} \|f\|_{W^{r,p}_a}$*, for a constant* C *independent of* r, a*, and* $L \in \mathbb{L}_\gamma$ *in* bounded *sets..*

Proof. We can assume $a = 0$, as explained above. Lemma 2.2 (i) gives that L satisfies the assumptions of the Hille-Yosida theorem [19, 34, 41], and hence e^{tL} is defined, is a C^0 semigroup, and $u(t) := e^{tL} f$ is indeed a classical solution. This proves (i).

It also follows from standard properties of C^0-semigroups in Banach spaces that $\|e^{tL} f\|_{L^p} \le C e^{\omega t} \|f\|_{L^p}$ for some constants $C > 0$ and $\omega \in \mathbb{R}$ independent of $L \in \mathbb{L}_\gamma$. To prove (ii), we then notice that

$$\begin{aligned}
(2.7)\quad \|e^{tL} f\|_{W^{2m,p}} &\le C|||e^{tL} f|||_{2m,p} = C\big(\|e^{tL} f\|_{L^p} + \|L^m e^{tL} f\|_{L^p}\big) \\
&= C\big(\|e^{tL} f\|_{L^p} + \|e^{tL} L^m f\|_{L^p}\big) \le C e^{\omega t}\big(\|f\|_{L^p} + \|L^m f\|_{L^p}\big) \\
&= C e^{\omega t} |||f|||_{2m} \le C e^{\omega t} \|f\|_{W^{2m,p}},
\end{aligned}$$

with constants depending on m, p, and L, but not on t. Though L may not be self-adjoint, the adjoint L^* is an operator of the same type, in the sense that $L^* \in \mathbb{L}_\gamma$. Hence the estimate above holds for L^*, with possibly different constants. We can then extend Equation (2.7) to $W^{-2m,p'}$, $m \in \mathbb{Z}_+$, by duality and to any $W^{r,p}$ by interpolation (see for example [8, 45] for results on interpolation). This completes the proof. □

From now on we shall denote by e^{tL} the $\mathcal{C}^0$-semigroup generated by L on $L^p_a = e^{a\langle x\rangle_z} L^p(\mathbb{R}^N)$, with p and a determined by the context (usually arbitrary, but fixed).

We recall that for $f \in \mathcal{D}(L)$, the map $t \to e^{tL}f$ is in $\mathcal{C}^1([0,\infty), X)$ and $\partial_t e^{tL} f = e^{tL} L f = L e^{tL} f$. For any two normed spaces X and Y, we denote by $\mathcal{B}(X,Y)$ the normed space of continuous, linear operators $T : X \to Y$ with norm $\|T\|_{X\to Y}$. When $X = Y$, we shall also write $\|T\|_X := \|T\|_{X\to X}$ and $\mathcal{B}(X) := \mathcal{B}(X,X)$. The identity operator of any space will be denoted by 1.

Lemma 2.4. *Let $L \in \mathbb{L}_\gamma$. We have $\|e^{tL} - 1\|_{W^{s+2,p}_a \to W^{s,p}_a} \le Ct$, for any $t \in (0,1]$. In particular, $[0,\infty) \ni t \to e^{tL} \in \mathcal{B}(W^{s+2,p}_a, W^{s,p}_a)$ is continuous.*

Proof. We have $e^{tL}f - f = \int_0^t e^{sL} L f ds$ for any $f \in W^{2,p}_a$, by standard properties of $\mathcal{C}^0$-semigroups. Lemma 2.3 (ii) then gives

$$\|e^{tL}f - f\|_{W^{s,p}_a} \le \int_0^t \|e^{sL}\|_{W^{s,p}_a} \|Lf\|_{W^{s,p}_a} ds \le C t e^{\omega t} \|f\|_{W^{s+2,p}_a},$$

which proves the first part of the result.

Let now $t_1 \ge t_2$. Then

$$\|e^{t_1 L} - e^{t_2 L}\|_{W^{s+2,p}_a \to W^{s,p}_a} \le \|e^{(t_1 - t_2)L} - 1\|_{W^{s+2,p}_a \to W^{s,p}_a} \|e^{t_2 L}\|_{W^{s,p}_a}.$$

This completes the second part of the proof. □

Remark 2.5. Let $\delta \in (0,2]$. Then an interpolation argument gives $\|e^{tL} - 1\|_{W^{s+\delta,p}_a \to W^{s,p}_a} \le C t^{\delta/2}$, for any $t \in (0,1]$. Hence the function $[0,\infty) \ni t \to e^{tL} \in \mathcal{B}(W^{s+\delta,p}_a, W^{s,p}_a)$ is also continuous.

We discuss smoothing properties of e^{tL}, it is convenient to first assume $L^* = L$, that is that L is self-adjoint. This will require us to set $a = 0$ in our weighted Sobolev spaces $W^{s,p}_a = W^{s,p}_a(\mathbb{R}^N)$. This assumption will be removed later on. The following result is known, we sketch a proof for completeness. (See for example [41] and [35] in the more general case of manifolds with bounded geometry.)

Corollary 2.6. *Let $t > 0$. There exist constants $C_{r,s} > 0$ such that, for any $L \in \mathbb{L}_\gamma$ with $L = L^*$:*

(i) $\|e^{tL}f\|_{W^{r,p}(\mathbb{R}^N)} \le C_{r,s} t^{(s-r)/2} \|f\|_{W^{s,p}(\mathbb{R}^N)}$, $r \ge s$ real.

(ii) There exists $\mathcal{G}^L_t(x,y) \in \mathcal{C}^\infty((0,\infty) \times \mathbb{R}^N \times \mathbb{R}^N)$ such that

$$e^{tL} f(x) = \int_{\mathbb{R}^N} \mathcal{G}^L_t(x,y) f(y) dy. \tag{2.8}$$

Proof. The part (i) can be proved using resolvent estimates and a scaling-in-time argument. Part (ii) folllows from the Schwartz kernel theorem (see for example [43, Chapter 7]), since from (i) e^{tL} maps compactly supported distributions in $\mathcal{E}'(\mathbb{R}^N)$ to smooth functions in $C^\infty(\mathbb{R}^N)$. In fact, if we denote by $<,>$ the duality pairing between C^∞ and $\mathcal{E}'$, we explicitly have:

$$\mathcal{G}_t^L(x,y) =< \delta_x, e^{tL}\delta_y >, \tag{2.9}$$

where δ_z, $z \in \mathbb{R}^N$, represents the Dirac delta distributions supported at z (*i.e.*, $\delta_z(f) = f(z)$). □

We now proceed to eliminate the assumption that $L^* = L$ in the above result. First, let us notice that if $L, L_0 \in \mathbb{L}_\gamma$, and if we denote $V = L - L_0$ and $g(t,x) = Vu(x,t)$, then (1.3) becomes

$$\begin{cases} \partial_t u - L_0 u = g & \text{in } (0,\infty) \times \mathbb{R}^N, \\ u(0,x) = f(x) & \text{on } \{0\} \times \mathbb{R}^N. \end{cases} \tag{2.10}$$

It is well-know that applying Duhamel's formula, gives a Volterra integral equation of the first kind for u. If $L = L_0^*$, the solution of the integral equation is a classical solution of (2.10). in fact, it is enough that e^{tL_0} generates an analytic semigroup (see [41, Theorem 2.4, page 107]). For simplicity, we want to avoid using the theory of analytic semigroups, and rather use instead Corrolary 2.6.

Lemma 2.7. *Let us assume that $g \in \mathcal{C}([0,\infty), L^p)$. Then the classical L^p-solution of the problem* (2.10) *is given by*

$$u(t) = e^{tL_0} f + \int_0^t e^{(t-\tau)L_0} g(\tau) d\tau. \tag{2.11}$$

Assume that $L \in \mathbb{L}_\gamma$, and let $L_0 = (L^* + L)/2$. Then, the classical L^p-solution $u(t) =: e^{tL} f$ to the problem (2.6) *is given by:*

$$e^{tL} f = e^{tL_0} f + \int_0^t e^{(t-\tau)L_0} (L - L_0) e^{\tau L} f d\tau, \tag{2.12}$$

for any initial data $f \in L^p$, $1 < p < \infty$.

Proof. Let us notice that u is defined since $e^{(t-\tau)L_0} g(\tau)$ is continuous in τ. For $f \in W^{2,p}$ and $g \in \mathcal{C}([0,\infty), W^{2,p})$, the function u is also differentiable and

$$u'(t) = L_0 e^{tL_0} f + \int_0^t L_0 e^{(t-\tau)L_0} g(\tau) d\tau + g(t) = L_0 u(t) + g(t).$$

Since $\mathcal{C}([0,\infty), W^{2,p})$ is dense in $\mathcal{C}([0,\infty), L^p)$ (for the topology of uniform convergence on compacta), this proves the first part.

To prove the second part, let us chose $f \in W^{1,p}$, then the function $[0,\infty) \ni \tau \to (L - L_0)e^{\tau L} f = g(\tau) \in L^p$ is continuous (since $L - L_0$ is in $\mathbb{L}$ and has order at most one), and hence we can apply the first part to obtain the formula (2.12).

In general, using Proposition 2.3, part (ii), and the fact that $V \in \mathbb{L}$ and has order at most one, we obtain by Corollary 2.6, part (i) that $\|e^{(t-\tau)L_0}(L - L_0)e^{\tau L} f\|_{L^p} \leq C t^{-1/2} \|f\|_{L^p}$, so that the integral on the right hand side of (2.12) is defined and continuous in $f \in L^p$. Since the left hand side of (2.12) is also continuous in $f \in L^p$, the result then follows by continuity and by density of $W^{1,p}$ in L^p. □

Remark 2.8. The integral $\int_0^t e^{(t-\tau)L_0}(L - L_0)e^{\tau L} f d\tau$ is defined either as a Bochner integral (for the definition of the Bochner integral see e.g. [39]) or as the limit $\lim_{\epsilon \searrow 0} \int_\epsilon^{t-\epsilon} e^{(t-\tau)L_0}(L - L_0)e^{\tau L} f d\tau$ of Riemann integral for continuous functions.

We now extend Corollary 2.6 to non self-adjoint operators L and to the exponentially weighted spaces $W_a^{s,p}$.

Proposition 2.9. *Let $L \in \mathbb{L}_\gamma$ arbitrary. We have $e^{tL} W_a^{s,p} \subset W_a^{r,p}$ for all $r, s, a \in \mathbb{R}$, $1 < p < \infty$, and $t > 0$. Let $r \geq s$, then*

$$\|u(t)\|_{W_a^{r,p}} \leq C t^{(s-r)/2} \|f\|_{W_a^{s,p}}, \quad t \in (0,1].$$

The constant C above is independent r, s, a, p, and L, as long as they belong to bounded sets.

We recall that $W_a^{s,p}$ is independent of the choice of the point z (see Equation (2.4)). The constant C in the above proposition is also independent of $z \in \mathbb{R}^N$ since the family $e^{a\langle x\rangle_z} L e^{-a\langle x\rangle_z}$ is uniformly bounded in $\mathbb{L}_\gamma$ for $z \in \mathbb{R}^N$ and a in a bounded set. For this reason, we shall sometimes drop the index z from the notation $\langle x\rangle_z$.

Proof. As discussed above, we may assume that $a = 0$. Also, note that we already know that $e^{tL} W_a^{s,p} \subset W_a^{r,p}$ for all $r \leq s$, so let us concentrate on the non-trivial case $r \geq s$. Let $L_0 := (L + L^*)/2$ and $V = L - L_0$. Then $V \in \mathbb{L}$ is a differential operator of order at most one. By Lemma 2.7,

$$e^{tL} = e^{tL_0} + \int_0^t e^{(t-\tau)L_0} V e^{\tau L} d\tau.$$

Let us assume also that $s \leq r < s + 1$. Using also Proposition 2.3, part ii, we obtain that the norm $\|e^{tL}\|_{W^{s,p} \to W^{r,p}}$ of e^{tL} as linear map

$W^{s,p} \to W^{r,p}$ can be bounded as

$$\|e^{tL}\|_{W^{s,p}\to W^{r,p}} \leq \|e^{tL_0}\|_{W^{s,p}\to W^{r,p}} + \int_0^t \|e^{(t-\tau)L_0}\|_{W^{s-1,p}\to W^{r,p}} \|V\|_{W^{s,p}\to W^{s-1,p}} \|e^{\tau L_1}\|_{W^{s,p}} d\tau$$
$$\leq C\Big(t^{(s-r)/2} + \int_0^t (t-\tau)^{(s-1-r)/2} d\tau\Big) = Ct^{(s-r)/2}(1+t^{1/2}) \leq Ct^{(r-s)/2},$$

where in the last inequality we have used that $0 < t \leq 1$, and where $C > 0$ is a generic constant, different at each appearance. The general case follows from this one as follows. Let $\delta = (r-s)/m$, for $m > r-s$. We first notice that $\|e^{tL/m}\|_{W^{s+(j-1)\delta,p}\to W^{s+j\delta,p}} \leq C(t/m)^{(s-r)/(2m)}$ by the result that we have just proved, since $\delta < 1$. We then write $e^{tL} = \big(e^{tL/m}\big)^m$ and we use the submultiplicative property of the norm to obtain $\|e^{tL}\|_{W^{s,p}\to W^{r,p}} \leq C(t/m)^{m(s-r)/(2m)} = C' t^{(s-r)/2}$. □

In particular, Proposition 2.9 gives the existence of the Green's function $\mathcal{G}_t^L(x,y)$ for any $L \in \mathbb{L}_\gamma$, defined again via formula (2.9). In particular for $t > 0$, this kernel is a smooth function of x and y. We will also use the notation $\mathcal{G}_t^L(x,y) = e^{tL}(x,y)$. The following corollary is a consequence of Proposition 2.9.

Corollary 2.10. *Let $L \in \mathbb{L}_\gamma$ and $s, r \in \mathbb{R}$ be arbitrary. We then have that the map*

$$(0,\infty) \ni t \to e^{tL} \in \mathcal{B}(W_a^{s,p}, W_a^{r,p})$$

is infinitely many times differentiable.

Proof. We have $\partial_t^k e^{tL} = e^{tL} L^k$, so it is enough to show that the map $(0,\infty) \ni t \to e^{tL} \in \mathcal{B}(W_a^{s-k,p}, W_a^{r,p})$ is continuous. Now, for each $\delta > 0$, let $t \geq \delta > 0$. Then $e^{\delta L}$ maps $W_a^{s-k,p}$ to $W_a^{r+2,p}$ continuously, by Proposition 2.9. Writing $e^{tL} = e^{(t-\delta)L} e^{\delta L}$ and using the continuity of $[\delta,\infty) \ni t \to e^{(t-\delta)L} \in \mathcal{B}(W_a^{r+2,p}, W_a^{r,p})$, by Lemma 2.4, we obtain the result. □

Let us notice for further reference that for constant coefficient operators, the Green's function can be determined explicitly.

Remark 2.11. If L (1.1) is a constant coefficient operator

$$L^0 = \sum_{i,j=1}^n a_{ij}^0 \partial_i \partial_j + \sum_{k=1}^n b_k^0 \partial_k + c^0 \tag{2.13}$$

and $A^0 := (a^0_{ij})$ is the matrix of highest order coefficients, assumed to satisfy $a^0_{ij} = a^0_{ji}$, we have the explicit formula
(2.14)
$$\mathcal{G}_t^{L^0}(x,y) = e^{tL^0}(x,y) = \frac{e^{c^0 t}}{\sqrt{(4\pi t)^n \det(A^0)}} e^{\frac{(x+b^0t-y)^t(A^0)^{-1}(x+b^0t-y)}{4t}}.$$

2.2. **Perturbative expansion.** The purpose of this section is to obtain a time-ordered perturbative expansion of e^{tL}, $L \in \mathbb{L}_\gamma$, in terms of e^{tL_0} for a fixed element $L_0 \in \mathbb{L}_\gamma$. Later, L_0 will be obtained by freezing the highest-order coefficients of L at a given point z and dropping the lower-order terms. This expansion is the well-known Dyson series [27, 28, 30]. Here, we concentrate on justifying this expansion in our setting and in obtaining global error estimates in weighted Sobolev spaces.

For each $k \in \mathbb{Z}_+$, we denote by

$$\begin{aligned}\Sigma_k &:= \{\tau = (\tau_0, \tau_1, \dots, \tau_k) \in \mathbb{R}^{k+1},\ \tau_j \geq 0, \sum \tau_j = 1\} \\ &\simeq \{\sigma = (\sigma_1, \dots, \sigma_k) \in \mathbb{R}^k,\ 1 \geq \sigma_1 \geq \sigma_2 \geq \dots \sigma_{k-1} \geq \sigma_k \geq 0\}\end{aligned}$$

the *standard unit simplex* of dimension k. The identification above is given by $\sigma_j = \tau_j + \tau_{j+1} + \dots + \tau_k$. Using this bijection, for any operator-valued function f of $\mathbb{R}^N$ we can write

$$\begin{aligned}\int_{\Sigma_k} f(\tau)d\tau &= \int_0^1\int_0^{\sigma_1}\dots\int_0^{\sigma_{k-1}} f(1-\sigma_1, \sigma_1-\sigma_2, \dots, \sigma_{k-1}-\sigma_k, \sigma_k)d\sigma_k \dots d\sigma_1 \\ &= \int_{\Sigma_k} f(1-\sigma_1, \sigma_1-\sigma_2, \dots, \sigma_{k-1}-\sigma_k, \sigma_k)d\sigma\end{aligned}$$

We recall that, if $g : [a,b] \to X$ is a *continuous* function to a Banach space X, $\int_a^b g(t)dt$ is defined as a Riemann integral. We begin with a preliminary lemma. We further recall that $\mathcal{B}(X,Y)$ the Banach space of continuous, linear maps between two Banach spaces X and Y.

Lemma 2.12. *Let $L_j \in \mathbb{L}_\gamma$ and let V_j be such that $e^{-b_j\langle x\rangle}V_j \in \mathbb{L}$, $j = 1, \dots, k$, for some $b = (b_1, \dots, b_k) \in \mathbb{R}^k_+$, $k \in \mathbb{Z}_+$. Then*

$$\Phi(\tau) = e^{\tau_0 L_0} V_1 e^{\tau_1 L_1} \dots e^{\tau_{k-1}L_{k-1}} V_k e^{\tau_k L_k}, \qquad \tau \in \Sigma_k$$

defines a continuous function $\Phi : \Sigma_k \to \mathcal{B}(W^{s,p}_a(\mathbb{R}^N), W^{r,p}_{a-|b|}(\mathbb{R}^N))$ for any $a \in \mathbb{R}$ and $1 < p < \infty$.

Above we use the standard multi index notation $|b| = \sum_{j=1}^k b_j$.

Proof. It is enough to prove that Φ is continuous on each of the sets $\mathcal{V}_j := \{\tau_j > 1/(k+2)\}$, $j = 0, \ldots, k$, since they cover Σ_k. Let us assume that $j = 0$, for the simplicity of notation.

By assumption and by Lemma 2.4, each of the functions

$$[0, \infty) \ni \tau_j \to V_j e^{\tau_j L_j} \in \mathcal{B}(W^{r_j+4,p}_{c_j}, W^{r_j,p}_{c_j - b_j}), \quad 1 \le j \le k,$$

is continuous. For a suitable choice of c_j and r_j (more precisely, $c_j = c_{j+1} - b_{j+1}$, $c_k = a$, $r_j = r_{j+1} - 4$, $r_k = s$), we obtain that the map

$$[0, \infty)^k \ni (\tau_j) =: \tau' \to \Psi(\tau') := V_1 e^{\tau_1 L_1} ... V_k e^{\tau_k L_k} \in \mathcal{B}(W^{s,p}_a, W^{s-4k,p}_{a-|b|})$$

is continuous.

Corollary 2.10 gives that the map $\tau_0 \to e^{\tau_0 L_0} \in \mathcal{B}(W^{s-4k,p}_{a-|b|}, W^{r,p}_{a-|b|})$ is continuous for $\tau_0 \ge 1/(k+2)$. This proves the continuity of Φ on $\mathcal{V}_0$ and completes the proof of the lemma. □

By iterating Duhamel's formula in Lemma 2.7, we obtain a time-ordered expansion of e^{tL}.

Proposition 2.13. *Let $d \in \mathbb{Z}_+$. Then, for each $L, L_0 \in \mathbb{L}_\gamma$,*

$$\begin{aligned} e^{tL} = {} & e^{tL_0} + t \int_{\Sigma_1} e^{t\tau_0 L_0} V e^{t\tau_1 L_0} d\tau \\ & + t^2 \int_{\Sigma_2} e^{t\tau_0 L_0} V e^{t\tau_1 L_0} V e^{t\tau_2 L_0} d\tau + \cdots + \\ & + t^d \int_{\Sigma_p} e^{t\tau_0 L_0} V e^{t\tau_1 L_0} \ldots e^{t\tau_{d-1} L_0} V e^{t\tau_d L_0} d\tau \\ & + t^{d+1} \int_{\Sigma_{d+1}} e^{t\tau_0 L_0} V e^{t\tau_1 L_0} \ldots e^{t\tau_d L_0} V e^{\tau_{d+1} L} d\tau, \end{aligned} \tag{2.15}$$

where $V = L - L_0$, and each integral is a well-defined Riemann integral of a Banach valued function.

The positive integer d will be called the *iteration level* of the approximation. As $d \to \infty$, formula (2.15) above gives rise to an asymptotic series (*Dyson series*, see [27, 28, 30] and the references therein).

Later in the paper, V will be replaced by a Taylor approximation of L, so that V will have polynomial coefficients in x, so we have included this case in the lemma above.

Proof. Recall that Lemma 2.7 gives

$$e^{tL} - e^{tL_0} = \int_0^t e^{(1-\zeta)L_0} V e^{\zeta L} d\zeta = \int_0^1 e^{t(1-\tau)L_0} V e^{t\tau L} t d\tau.$$

with the substitution $\zeta = t\tau$. This is in fact our result for $k = 1$.

The result for any p then follows by induction using the above formula.

Recall that on each simplex Σ_p, we denoted $\sigma_k = \tau_k + \tau_{k+1} + \ldots + \tau_p$. Explicitly, for $t = 1$ we have

$$
\begin{aligned}
e^L = e^{L_0} &+ \int_{\Sigma_1} e^{(1-\sigma_1)L_0} V e^{\sigma_1 L_0} d\sigma + \int_{\Sigma_2} e^{(1-\sigma_1)L_0} V e^{(\sigma_1-\sigma_2)L_0} V e^{\sigma_2 L_0} d\sigma \\
&+ \cdots + \int_{\Sigma_{d-1}} e^{(1-\sigma_1)L_0} V \ldots V e^{(\sigma_{d-2}-\sigma_{d-1})L_0} V e^{\sigma_{d-1} L} d\sigma \\
= e^{L_0} &+ \int_{\Sigma_1} e^{(1-\sigma_1)L_0} V e^{\sigma_1 L_0} d\sigma + \int_{\Sigma_2} e^{(1-\sigma_1)L_0} V e^{(\sigma_1-\sigma_2)L_0} V e^{\sigma_2 L_0} d\sigma \\
&+ \cdots + \int_{\Sigma_{d-1}} e^{(1-\sigma_1)L_0} V \ldots V e^{(\sigma_{d-2}-\sigma_{d-1})L_0} V e^{\sigma_{d-1} L_0} d\sigma + \ldots \\
&+ \int_{\Sigma_{d-1}} \int_0^{\sigma_{d-1}} e^{(1-\sigma_1)L_0} V \ldots e^{(\sigma_{d-2}-\sigma_{d-1})L_0} V e^{(\sigma_{d-1}-\sigma_d)L_0} V e^{\sigma_d L} d\sigma d\sigma_n \\
= e^{L_0} &+ \int_{\Sigma_1} e^{(1-\sigma_1)L_0} V e^{\sigma_1 L_0} d\sigma + \int_{\Sigma_2} e^{(1-\sigma_1)L_0} V e^{(\sigma_1-\sigma_2)L_0} V e^{\sigma_2 L_0} d\sigma \\
&+ \cdots + \int_{\Sigma_d} e^{(1-\sigma_1)L_0} V e^{(\sigma_1-\sigma_2)L_0} \ldots e^{(\sigma_{d-1}-\sigma_d)L_0} V e^{\sigma_d L} d\sigma,
\end{aligned}
$$

where each integral is well defined as a Riemann integral by the Lemma 2.12. □

3. Local dilations and perturbative expansions

In this section, we tackle the task of deriving an algorithmically computable approximation to e^{tL}. We exploit the perturbative expansion (2.15) with L_0 the operator obtained by freezing the highest-order coefficents of L at a given, but arbitrary, point $z \in \mathbb{R}^N$, and dropping the lower-order terms (see (3.11a) below). Then, we approximate $L - L_0$ by an appropriate Taylor expansion, so that each of the terms in (2.15) except the last one can be explicitly computed using commutator formulas, as discussed in Section 4. Recall that the sets of second order differential operators $\mathbb{L}_\gamma \subset \mathbb{L}$ were introduced in Definition 2.1.

First, using a suitable rescaling in space and time, we replace the problem of determining an asymptotic expansion of the kernel

$$\mathcal{G}_t^L(x, y) := e^{tL}(x, y)$$

of e^{tL} by the problem of determining an asymptotic expansion of the kernel $\mathcal{G}_1^{L^{s,z}}(x, y) = e^{L^{s,z}}(x, y)$ of $e^{L^{s,z}}$ for a suitable family of operators $L^{s,z}$ parameterized by $s = \sqrt{t}$, and by the point $z \in \mathbb{R}^N$. The point

z is fixed throughout this section, but it will be allowed to vary later on as a function of x and y satisfying some conditions, for example $z = (x+y)/2$. For some results, we will set $z = x$. The family $L^{s,z}$ has limit precisely L_0 as $s \to 0$. Since we will let z vary later, we shall sometimes write $L_0 = L_0^z$.

For any $s > 0$, we consider the action on functions of dilating x by s about z and t by s^2 about 0. If $f : \mathbb{R}^N \to \mathbb{R}$, $u : [0,\infty) \times \mathbb{R}^N \to \mathbb{R}$, we then set

$$f^{s,z}(x) := f(z + s(x - z)), \tag{3.1}$$

$$u^{s,z}(t,x) := u(s^2 t, z + s(x - z)), \tag{3.2}$$

and,

$$L^{s,z} := \sum_{i,j=1}^{N} a_{ij}^{s,z}(x)\partial_i\partial_j + s\sum_{i=1}^{N} b_i^{s,z}(x)\partial_i + s^2 c^{s,z}(x). \tag{3.3}$$

We immediately see that

$$L^{s,z}u^{s,z} = s^2(Lu)^{s,z}, \quad (\partial_t - L^{s,z})u^{s,z} = s^2[(\partial_t - L)u]^{s,z} \tag{3.4}$$

In particular, we have the following simple lemma, which we record for further reference.

Lemma 3.1. *If u solves* (2.10)*, then $u^{s,z}$ solves*

$$\begin{cases} \partial_t u^{s,z} - L^{s,z}u^{s,z} = 0 & \text{in } (0,\infty) \times \mathbb{R}^N \\ u^{s,z} = f^{s,z} \in \mathcal{C}_c^\infty(\mathbb{R}^N) & \text{on } \{0\} \times \mathbb{R}^N. \end{cases} \tag{3.5}$$

3.1. **Dilations and Green's functions.** We want to study the Initial Value Problem (3.5) and the Green's function of its associated solution operator $e^{tL^{s,z}}$. We can reduce to study the special case $z = 0$.

The definition of the Green's function and Lemma 3.1 then gives

$$\begin{aligned} u^{s,0}(t,x) &= \int_{\mathbb{R}^N} \mathcal{G}_t^{L^{s,0}}(x,y) f^{s,z}(y)dy = \int_{\mathbb{R}^N} \mathcal{G}_t^{L^{s,0}}(x,y) f(sy)dy \\ &= s^{-N}\int_{\mathbb{R}^N} \mathcal{G}_t^{L^{s,0}}(x,\frac{y}{s}) f(y)dy. \end{aligned} \tag{3.6}$$

On the other hand,

$$u^{s,0}(t,x) = u(s^2t, sx) = \int_{\mathbb{R}^N} \mathcal{G}_{s^2t}^{L}(sx,y) f(y)dy,$$

which implies

$$\mathcal{G}_t^{L^{s,0}}(x,\frac{y}{s}) = s^N \mathcal{G}_{s^2t}^{L}(sx,y) \;\Leftrightarrow\; \mathcal{G}_t^{L^{s,0}}(x,y) = s^N \mathcal{G}_{s^2t}^{L}(sx,sy).$$

In other words

$$\mathcal{G}_t^L(x,y) = s^{-N}\mathcal{G}_{s^{-2}t}^{L^{s,0}}(s^{-1}x, s^{-1}y)$$

If we now translate to $z \neq 0$ and choose $s = \sqrt{t}$, we obtain the desired correspondence between $\mathcal{G}_t^L$ and $\mathcal{G}_1^{L^{s,z}}$, which we also record for further reference.

Lemma 3.2. *Assume $L \in \mathbb{L}$ and let z be a fixed, but arbitrary, point in $\mathbb{R}^N$. Then, for any $s > 0$,*

$$\begin{aligned}\mathcal{G}_t^L(x,y) &= s^{-N}\mathcal{G}_1^{L^{s,z}}(z + s^{-1}(x-z), z + s^{-1}(y-z)) \\ &= t^{-\frac{N}{2}}\mathcal{G}_1^{L^{\sqrt{t},z}}(z + t^{-\frac{1}{2}}(x-z), z + t^{-\frac{1}{2}}(y-z)), \text{ if } s = t^{-\frac{1}{2}}.\end{aligned}$$

3.2. **Perturbative expansion of $e^{L^{s,z}}$.** Since Lemma 3.2 gives us an immediate procedure for obtaining the Green function $\mathcal{G}_t^L(x,y)$ of $\partial_t - L$ from the Green's function $\mathcal{G}_t^{L^{s,z}}(x,y)$ of $\partial_t - L^{s,z}$, we now concentrate on obtaining a perturbative expansion for the latter.

Recall that $L_0^z = L^{0,z} = \lim_{s\searrow 0} L^{s,z}$. Let us write $V_1^{s,z} := L^{s,z} - L_0^z$. Then, $V_1^{s,z}$ takes the role of V in the perturbative expansion (2.15) for the operator $e^{L^{s,z}}$, that is:

$$\begin{aligned}e^{L^{s,z}} = \; & e^{L_0^z} + \int_{\Sigma_1} e^{\tau_0 L_0^z} V_1^{s,z} e^{\tau_1 L_0^z} d\tau \\ & + \int_{\Sigma_2} e^{\tau_0 L_0^z} V_1^{s,z} e^{\tau_1 L_0^z} V_1^{s,z} e^{\tau_2 L_0^z} d\tau + \dots \\ & \quad + \int_{\Sigma_d} e^{\tau_0 L_0^z} V_1^{s,z} e^{\tau_1 L_0^z} \dots e^{\tau_{d-1} L_0^z} V_1^{s,z} e^{\tau_d L_0^z} d\tau \\ & \qquad + \int_{\Sigma_{d+1}} e^{\tau_0 L_0^z} V_1^{s,z} e^{\tau_1 L_0^z} \dots e^{\tau_d L_0^z} V_1^{s,z} e^{\tau_{d+1} L^{s,z}} d\tau.\end{aligned} \tag{3.7}$$

In a sense to be made precise below, we have $V_1^s = \mathcal{O}(s)$. Consequently, if we let the iteration level $d \to \infty$ in (2.15), we obtain a formal power series in s. We will rigorously show in Section 5 using the exponentially weighted Sobolev spaces $W_a^{s,p}$ that (2.15) indeed gives rises to an asymptotically convergent series in s as $s \to 0$ and will derive global error bounds in $W^{s,p}$ and $W_a^{s,p}$ for the partial sums.

Let $n \in \mathbb{Z}_+$ be a fixed integer and consider the Taylor expansion of the operator $L^{s,z}$ up to order n in s around $s = 0$,

$$L^{s,z} = \sum_{m=0}^{n} s^m L_m^z + V_{n+1}^{s,z} \tag{3.8}$$

were $V_{n+1}^{s,z}$ is the remainder term in the expansion. Let

$$V_{n+1}^{s,z} = s^{n+1} L_{n+1}^{s,z}.$$

The operators L_m^z, $1 \le m \le n$, are given by

$$L_m^z := \frac{1}{m!}\left(\frac{d^m}{ds^m}L^{s,z}\right)\bigg|_{s=0}, \tag{3.9}$$

and are independent of s, while

$$L_{n+1}^{s,z} := \frac{1}{(n+1)!}\left(\frac{d^{n+1}}{d\theta^{n+1}}L^{\theta,z}\right)\bigg|_{\theta=\alpha s}, \tag{3.10}$$

for some $0 < \alpha < 1$, and hence it still depends on s.

Remark 3.3. From the form of $L^{s,z}$ in equation (3.3) it follows that the operator L_m^z, $m \le n$, (respectively $L_{n+1}^{s,z}$) has coefficients that are *polynomials in $x - z$ of degree at most m* (respectively of degree $n+1$). The coefficients of the polynomials themselves are bounded functions of z. More precisely, the coefficients of the second order derivative terms are of degree at most m in $x - z$, while the coefficients of the first order derivatives term are of degree at most $m-1$ in $x-z$, and the coefficients of the zero order derivative term is of degree at most $m-2$ in $x - z$. The coefficients of these polynomials in $x - z$ are *bounded* functions of z, together will all their derivatives, a fact that will be exploited later.

The first few terms of the Taylor expansions are explicitly:

$$L_0^z = \sum_{i,j=1}^N a_{ij}(z)\partial_i\partial_j, \tag{3.11a}$$

$$L_1^z = \sum_{i,j=1}^N \left((x-z)\cdot\nabla a_{ij}(z)\right)\partial_i\partial_j + \sum_{i=1}^N b_i(z)\partial_i, \tag{3.11b}$$

$$\begin{aligned} L_2^z = \sum_{i,j=1}^N \frac{1}{2}\big((x-z)^T\ \nabla^2 a_{ij}(z)\ (x-z)\big)\partial_i\partial_j + \\ + \sum_{i=1}^N ((x-z)\cdot\nabla b_i(z))\partial_i + c(z). \end{aligned} \tag{3.11c}$$

Since L_0^z has coefficients that are constant in x, from formula (2.14) we obtain

$$e^{tL_0^z} = \frac{1}{\sqrt{(4\pi t)^N \det A^0}} e^{\frac{(x-y)^t (A^0)^{-1}(x-y)}{4t}}, \tag{3.12}$$

where $A^0 := A(z)$.

Furthermore $V_1^s := L^{s,z} - L_0^z$ can be written as

$$V_1^s := \sum_{m=0}^{n} s^m L_m^z + s^{n+1} L_{n+1}^{s,z}. \tag{3.13}$$

This Taylor polynomial expansion can then be substituted into (3.7), yielding another polynomial in s. To describe each term of this polynomial and to formulate the main results in this section, we need to introduce some notation. Let $\mathbb{N} := \{1, 2, 3, \dots\}$ denote the set of natural numbers (always assumed to be > 0).

Definition 3.4. *For any integers $1 \leq k \leq d+1$ and ℓ, we shall denote by $\mathfrak{A}_{k,\ell}$ the set of multi-indexes $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_k) \in \mathbb{N}^k$, such that $|\alpha| := \sum \alpha_j = \ell$. Furthermore, we denote $\mathfrak{A}_\ell := \bigcup_{k=1}^{\ell} \mathfrak{A}_{k,\ell}$. For symmetry, it will be convenient to set $\mathfrak{A}_{\ell,k} = \{\emptyset\}$ if $\ell < k$, including when $\ell \leq 0$.*

We note that, since $\alpha_i \geq 1$, the set $\mathfrak{A}_{k,\ell}$ is empty if $\ell < k$. The meaning of ℓ is that of the corresponding power of s and the meaning of k is that of the iteration level in the Dyson series (3.7).

Proposition 3.5. *The set $\mathfrak{A}_\ell$ contains $2^{\ell-1}$ elements.*

Proof. For any given, $1 \leq k \leq \ell$, the number of elements in the set $\mathfrak{A}_{k,\ell}$ is the number of sequences $\{\alpha_1, \alpha_2, ...\alpha_k\}$ of size k which add up to ℓ and is, therefore, given by $\binom{\ell-1}{k-1}$. Consequently, the number of elements in $\mathfrak{A}_\ell$ is given by $\sum_{k=1}^{\ell} \binom{\ell-1}{k-1} = \sum_{k=0}^{\ell-1} \binom{\ell-1}{k} = 2^{\ell-1}$. □

We are now in the position to describe the expansion 3.7 more explicitly. We recall that d is the iteration level of the approximation and n is the order of the Taylor expansion. In the following definition, by abuse of notation, it will be convenient to write L_{n+1}^z instead of $L_{n+1}^{s,z}$, that is, we shall omit s from the notation. We also recall that $\mathfrak{A}_{k,\ell} \equiv \emptyset$, if $\ell < k$. This condition will be understood.

Definition 3.6. *For each multi-index $\alpha = (\alpha_1, \dots, \alpha_k) \in \mathfrak{A}_{k,\ell}$, we let*

$$\Lambda_{\alpha,z} := \int_{\Sigma_k} e^{\tau_0 L_0^z} L_{\alpha_1}^z e^{\tau_1 L_0^z} L_{\alpha_2}^z \cdots L_{\alpha_k}^z e^{\tau_k L_0^z} d\tau, \tag{3.14}$$

if $1 \leq k \leq d$, and

$$\Lambda_{\alpha,z} := \int_{\Sigma_{d+1}} e^{\tau_0 L_0^z} L_{\alpha_1}^z e^{\tau_1 L_0^z} L_{\alpha_2}^z \cdots L_{\alpha_{d+1}}^z e^{\tau_{d+1} L^{s,z}} d\tau. \tag{3.15}$$

if $k = d+1$. Then, we set

$$\Lambda_z^\ell := \sum_{\alpha \in \mathfrak{A}_\ell} \Lambda_{\alpha,z}, \tag{3.16}$$

with the convention that $\Lambda_z^0 = e^{L_0^z}$.

We observe that α uniquely determines k and ℓ, so that our notation is justified. Let $\alpha = (\alpha_j) \in \mathfrak{A}_{k,\ell}$. We remark that if $k = n+1$ or some $\alpha_j = n+1$ (in which case $L_{\alpha_j}^z$ stands in fact for $L_{n+1}^{s,z}$), then $\Lambda_{\alpha,z}$ and Λ_z^ℓ depend on s, so we shall sometimes denote these terms by $\Lambda_{\alpha,s,z}$ and $\Lambda_{s,z}^\ell$.

Also, in what follows, when no confusion can arise, we will drop the explicit dependence on z. However, in Section 5, z will be allowed to vary and we will reinstate the full notation. We also observe that each Λ_z^ℓ or $\Lambda_{s,z}^\ell$ is well defined as a Riemann integral by Lemma 2.12 and by the following lemmas. Let us recall that $\langle x\rangle_w = (1+|x-w|^2)^{1/2}$.

Lemma 3.7. *The family*

$$\{\langle x\rangle_z^{-j} L_j^z;\ s \in (0,1],\ z \in \mathbb{R}^N,\ j = 0,\dots,n+1\}$$

defines a bounded subset of $\mathbb{L}$.

Proof. This is an immediate consequence of Remark 3.3 if $j \le n$ and of directly estimating the remainder in the Taylor series for $j = n+1$. $\square$

In the following Lemma, we shall use an *arbitrary* center for our weight.

Lemma 3.8. *For each given* $\epsilon > 0$*, the family*

$$\{e^{-\epsilon\langle z-w\rangle} e^{-\epsilon\langle x\rangle_w} L_j^z;\ s \in (0,1],\ z \in \mathbb{R}^N,\ j = 0,\dots,n+1\}$$

is a bounded subset of $\mathbb{L}$.

Proof. Let us assume first that $w = z$. We need to prove that the family

$$\{e^{-\epsilon\langle x\rangle_z} L_j^z;\ s \in (0,1],\ z \in \mathbb{R}^N,\ j = 0,\dots,n+1\}$$

is bounded in $\mathbb{L}$. Indeed, this follows from Lemma 3.7 and the simple observation that $\langle x\rangle_z^j e^{-\epsilon\langle x\rangle_z} \le C$, with C independent of z and j.

To obtain the statement of the theorem, we then apply the triangle inequality to the vectors $(0,x), (1,z), (1,w) \in \mathbb{R}^{1+N}$ to conclude that $\langle x-z\rangle - \langle x-w\rangle \le |z-w| \le \langle z-w\rangle$. This shows that $e^{\epsilon(\langle x-z\rangle - \langle x-w\rangle - \langle z-w\rangle)} \le 1$. Hence the family

$$\{e^{\epsilon(\langle x-z\rangle - \langle x-w\rangle - \langle z-w\rangle)} e^{-\epsilon\langle x\rangle_z} L_j^z = e^{-\epsilon\langle z-w\rangle} e^{-\epsilon\langle x\rangle_w} L_j^z\},$$

$s \in (0,1],\ z \in \mathbb{R}^N,\ j = 0,\dots,n+1$, is bounded in $\mathbb{L}$, as claimed. $\square$

Lemma 2.12 together with Lemma 3.8 then give the following result.

Corollary 3.9. *We have* $\Lambda_{\alpha,z} \in \mathcal{B}(W^{s,p}_a, W^{r,p}_{a-\epsilon})$*, for any* $\alpha \in \mathfrak{A}_{k,\ell}$*,* $z \in \mathbb{R}^N$*,* $r, s \in \mathbb{R}$*,* $1 < p < \infty$*, and* $\epsilon > 0$*. Moreover, we have that*

$$\|\Lambda_{\alpha,z}\|_{W^{q,p}_{a,z} \to W^{r,p}_{a-\epsilon,z}} \le C_{q,r,p,a,\epsilon} e^{k\epsilon\langle z-w\rangle},$$

for a constant $C_{q,r,p,a,\epsilon}$ *that does not depend on* z*. In particular, each* $\Lambda_{\alpha,z}$ *is an operator with smooth kernel* $\Lambda_{\alpha,z}(x,y)$*.*

Therefore, we can write

$$\Lambda_{\alpha,z} f(x) = \int_{\mathbb{R}^N} \Lambda_{\alpha,z}(x,y) f(y) dy. \tag{3.17}$$

The point of the above definition and results is to rewrite the perturbative expansion (partial Dyson series) in the form

Lemma 3.10. *Denote* $M = (d+1)(n+1)$*. We have*

$$e^{L^{s,z}} = e^{L^z_0} + \sum_{\ell=1}^{M} \sum_{k=1}^{\min\{\ell,d+1\}} \sum_{\alpha \in \mathfrak{A}_{k,\ell}} s^\ell \Lambda_{\alpha,z} = \sum_{\ell=0}^{M} s^\ell \Lambda^\ell_z.$$

We now assume that $n \le d$ and write the perturbative expansion of the above Lemma as follows:

$$\begin{aligned} e^{L^{s,z}} &= e^{L^z_0} + \sum_{\ell=1}^{n} s^\ell \Lambda^\ell_z + \sum_{\ell=n+1}^{M} s^\ell \Lambda^\ell_z \\ &= e^{L^z_0} + \sum_{\ell=1}^{n} s^\ell \Lambda^\ell_z + s^{n+1}\mathbb{E}^{s,z}_{d,n} = \sum_{\ell=0}^{n} s^\ell \Lambda^\ell_z + s^{n+1}\mathbb{E}^{s,z}_{d,n}, \end{aligned} \tag{3.18}$$

where $\mathbb{E}^{s,z}_{d,n}$ represents the error in the approximation and depends on s, whereas the terms Λ^ℓ_z, $1 \le \ell \le n$ *do not depend* on s or d, since we have assumed that $n \le d$. Since $\mathbb{E}^{s,z}_{d,n}$ is independent of d for $d \ge n$, we shall eventually restrict to $d = n$.

4. Commutator calculations

The purpose of this section is to give an explicitly computable representation of the perturbative expansion (3.18) as

$$e^{L^{s,z}} \sim e^{L^z_0} + \sum_{\ell=1}^{n} s^\ell \mathcal{P}^\ell(x,z,\partial) e^{L^z_0}$$

where $\mathcal{P}^j(x,z,\partial)$ is a differential operator with smooth coefficients that depend polynomialy on $x - z$ and s, and are bounded with all derivatives in z. Both the order of the operator as well as the degree of the polynomial coefficients depend on the order of the Taylor expansion n, which also equals the iteration level d. We give an explicit characterization of $\mathbb{P}_n$ and an iterative procedure to calculate it in Theorem 4.7. The main idea is to show that each $\Lambda_{\alpha,z}$ in (3.14) can be written as an explicitly computable differential operator $\mathcal{P}_\alpha$ acting on the distribution kernel of $e^{L_0^{\tilde{z}}}$, and thus using (3.16) show that the perturbative expansion (3.18) can be rewritten in this form as well. Throughout this section, z is kept *fixed*, though arbitrary, and ∂ will always mean differentiation with respect to x.

Definition 4.1 (Spaces of Differentiatial Operators)**.** *For any nonnegative integers a, b we denote by $\mathcal{D}(a,b)$ the vector space of all differentiations of polynomial degree at most a and order at most b. We extend this definition to negative indices by defining $\mathcal{D}(a,b) = \{0\}$ if either a or b is negative. By polynomial degree of A we mean the highest power of the polynomials appearing as coefficients in A.*

We remark that $\mathcal{D}(0,b)$ consists of differential operators with *constant coefficients*.

Definition 4.2 (Adjoint Representation)**.** *For any two differentiations $A_1 \in \mathcal{D}(a_1,b_1)$ and $A_2 \in \mathcal{D}(a_2,b_2)$ we define $\mathrm{ad}_{A_1}(A_2)$ by*

$$\mathrm{ad}_{A_1}(A_2) := [A_1, A_2] = A_1A_2 - A_2A_1, \tag{4.1}$$

as usual, and for any integer $j \geq 1$ we define $\mathrm{ad}^j_{A_1}(A_2)$ recursively by

$$\mathrm{ad}^j_{A_1}(A_2) := \mathrm{ad}_{A_1}(\mathrm{ad}^{j-1}_{A_1}(A_2)) \tag{4.2}$$

Proposition 4.3. *Suppose $A_1 \in \mathcal{D}(a_1,b_1)$ and $A_2 \in \mathcal{D}(a_2,b_2)$. Then for any integer $k \geq 1$, $\mathrm{ad}^k_{A_1}(A_2) \in \mathcal{D}(k(a_1-1)+a_2, k(b_1-1)+b_2)$.*

Proof. We first notice that

$$\mathrm{ad}_{A_1}(A_2) \in \mathcal{D}(a_1 - 1 + a_2, b_1 - 1 + b_2). \tag{4.3}$$

Next, from (4.2) we have

$$\mathrm{ad}^k_{A_1}(A_2) = \mathrm{ad}_{A_1}(\mathrm{ad}_{A_1}(\mathrm{ad}_{A_1}(\mathrm{ad}_{A_1}(\dots)))), \quad k - \text{times}, \tag{4.4}$$

so that an application of (4.3) k times yields the result. ☐

Lemma 4.4. *Let m, k be fixed integers ≥ 1. Let $L_0 \in \mathcal{D}(0,2)$ and $L_m \in \mathcal{D}(m,2)$. Then, $\mathrm{ad}^k_{L_0}(L_m) \in \mathcal{D}(m-k, k+2)$. In particular,*

$$\mathrm{ad}^k_{L_0}(L_m) = 0, \qquad \textit{if } k > m. \tag{4.5}$$

Proof. Applying Lemma 4.4 we see that $\mathrm{ad}^k_{L_0^z}(L_m^z) \in \mathcal{D}(m-k, k+2)$. If $k > m$, then by definition $\mathcal{D}(m-k, k+2) = \{0\}$ and we obtain (4.5). ☐

Lemma 4.5. *Let $L_0 \in \mathcal{D}(0,2) \cap \mathbb{L}_\gamma$, and let $L_m \in \mathcal{D}(m,2)$. Then for any $\theta > 0$,*

$$e^{\theta L_0} L_m = P_m(L_0, L_m; \theta, x, \partial) e^{\theta L_0},$$

where $P_m(\theta) = P_m(L_0, L_m; \theta, x, \partial) \in \mathcal{D}(m, m+2)$ is given by

$$P_m(\theta) := \sum_{k=0}^{m} \frac{\theta^k}{k!} \operatorname{ad}_{L_0}^k (L_m) = L_m + \theta [L_0, L_m] + \frac{\theta^2}{2} [L_0, [L_0, L_m]] + \cdots .$$

Proof. Recall the Baker-Campbell-Hausdorff formula (see for instance [5, 9, 24])

$$\Phi(t) := e^{tA} B - \left(\sum_{k=0}^{\infty} t^k \operatorname{ad}_A^k (B)/k! \right) e^{tA} = 0. \tag{4.6}$$

In general, this formula is a formal infinite series, and the equality $\Phi(t) = 0$ must be justified.

Setting $A = L_0$, $B = L_m$, we have that $\operatorname{ad}_A^{m+1}(B) = 0$, by Lemma 4.4, so the sum becomes finite, and the function $\Phi(t)$ is well defined as a bounded operator $W_1^{m,p} \to L^p$. Since $\Phi(0) = 0$, to prove that $\Phi(t) = 0$ for all t, it is enough to show that $\partial_t \Phi(t) f = 0$ for all $f \in W_1^{m,p}$. Indeed, we have

$$\begin{aligned}
\partial_t \Phi(t) f &= e^{tA} A B f \\
&\quad - \left(\sum_{k=0}^{\infty} k t^{k-1} \operatorname{ad}_A^k (B)/k! \right) e^{tA} f - \left(\sum_{k=0}^{\infty} t^k \operatorname{ad}_A^k (B)/k! \right) A e^{tA} f \\
&= e^{tA} A B f - \left(\sum_{k=0}^{\infty} t^k \operatorname{ad}_A^{k+1} (B)/k! \right) e^{tA} f - \left(\sum_{k=0}^{\infty} t^k \operatorname{ad}_A^k (BA)/k! \right) e^{tA} f \\
&= e^{tA} A B f - \left(\sum_{k=0}^{\infty} t^k \operatorname{ad}_A^k (AB)/k! \right) e^{tA} f \\
&= A e^{tA} B f - A \left(\sum_{k=0}^{\infty} t^k \operatorname{ad}_A^k (B)/k! \right) e^{tA} f = A \Phi(t) f.
\end{aligned}$$

So the continuous function $u(t) := \Phi(t) f \in L^p$ satisfies the equation $\partial_t u(t) - A u(t) = 0$ with initial condition $u(0) = 0$. By the uniqueness of the solutions of this equation in L^p, we obtain that $u(t) = 0$, which is the desired Baker-Campbell-Hausdorff formula.

The indicated properties of $P_m(\theta) = P_m(L_0, L_m; \theta, x, \partial)$ are obtained directly from Lemma 4.4, as follows. We have $\operatorname{ad}_A^k (B) \in \mathcal{D}(m-k, k+2)$

and hence

$$P_m(\theta) := \sum_{k=0}^{m} \frac{\theta^k}{k!} \operatorname{ad}_A^k(B) \in \sum_{k=0}^{m} \mathcal{D}(m-k, k+2) \subset \mathcal{D}(m, m+2).$$

This completes the proof. $\square$

Lemma 4.6. *For a given multi-index $\alpha \in \mathfrak{A}_{k,\ell}$ with $k \le d = n$, let*

$$\mathcal{P}_\alpha(x, z, \partial) := \int_{\Sigma_k} \prod_{i=1}^{k} P_{\alpha_i}(L_0^z, L_{\alpha_i}^z; 1-\sigma_i, x, \partial) d\sigma,$$

where $P_{\alpha_i}(L_0^z, L_{\alpha_i}^z; 1-\sigma_i, x, \partial)$ is defined in Lemma 4.5. Then

$$\Lambda_{\alpha,z} = \mathcal{P}_\alpha(x, z, \partial) e^{L_0^z}$$

where the product is the composition of operators and $\mathcal{P}_\alpha$ is a differential operator of order $2k+\ell$ and polynomial degree $\le \ell = |\alpha| = \sum_{i=1}^{k} \alpha_i$. More precisely, we can write

$$\mathcal{P}_\alpha(x, z, \partial) = \sum_{|\beta| \le \ell} \sum_{|\gamma| \le \ell + 2k} a_{\beta,\gamma}(z)(x-z)^\beta \partial_x^\gamma, \tag{4.7}$$

with $a_{\beta,\gamma} \in \mathcal{C}_b^\infty(\mathbb{R}^N)$ and β and γ multi-indices.

Proof. The proof is a calculation based on the repeated application of Lemma 4.5 on $\Lambda_\alpha^{k,\ell}$. We fix $\alpha \in \mathfrak{A}_{k,\ell}$, and for simplicity we continue to denote $P_m(\theta) = P_m(L_0^z, L_m^z; \theta, x, \partial)$, when no confusion can arise. Then,

$$\begin{aligned}
\Lambda_{\alpha,z} &= \int_{\Sigma_k} e^{(1-\sigma_1)L_0^z} L_{\alpha_1} e^{(\sigma_1-\sigma_2)L_0^z} L_{\alpha_2} e^{(\sigma_2-\sigma_3)L_0^z} \cdots L_{\alpha_k} e^{\sigma_k L_0^z} d\sigma \\
&= \int_{\Sigma_k} P_{\alpha_1}(1-\sigma_1) e^{(1-\sigma_2)L_0^z} L_{\alpha_2} e^{(\sigma_2-\sigma_3)L_0^z} \cdots L_{\alpha_k} e^{\sigma_k L_0^z} d\sigma \\
&= \int_{\Sigma_k} P_{\alpha_1}(1-\sigma_1) P_{\alpha_2}(1-\sigma_2) e^{(1-\sigma_3)L_0^z} \cdots L_{\alpha_k} e^{\sigma_k L_0^z} d\sigma \\
&= \int_{\Sigma_k} P_{\alpha_1}(1-\sigma_1) P_{\alpha_2}(1-\sigma_2) \cdots P_{\alpha_k}(1-\sigma_k) e^{L_0^z} d\sigma \\
&= \int_{\Sigma_k} \prod_{i=1}^{k} P_{\alpha_i}(1-\sigma_i) e^{L_0^z} d\sigma \; = \left(\int_{\Sigma_k} \prod_{i=1}^{k} P_{\alpha_i}(1-\sigma_i) d\sigma \right) e^{L_0^z}.
\end{aligned}$$

The proof is complete. $\square$

Finally, for $\ell \le n$ we set

$$\mathcal{P}^\ell(x, z, \partial) := \sum_{\alpha \in \mathfrak{A}_\ell} \mathcal{P}_\alpha(x, z, \partial) = \sum_{k=1}^{\ell} \sum_{\alpha \in \mathfrak{A}_{k,\ell}} \int_{\Sigma_k} \prod_{i=1}^{k} P_{\alpha_i}(1-\sigma_i) d\sigma,$$

so that

$$\begin{aligned}\Lambda_z^\ell &= \sum_{k=1}^{\ell}\sum_{\alpha\in\mathfrak{A}_{k,\ell}}\Lambda_{\alpha,z} = \sum_{k=1}^{\ell}\sum_{\alpha\in\mathfrak{A}_{k,\ell}}\mathcal{P}_\alpha(x,z,\partial)e^{L_0^z}\\ &= \sum_{k=1}^{\ell}\sum_{\alpha\in\mathfrak{A}_{k,\ell}}\int_{\Sigma_k}\prod_{i=1}^{k}P_{\alpha_i}(L_0^z,L_{\alpha_i}^z;1-\sigma_i,x,\partial)d\sigma e^{L_0^z} = \mathcal{P}^\ell(x,z,\partial)e^{L_0^z}.\end{aligned}$$

A similar, but more complicated, representation holds also for $\Lambda_{\alpha,z}$ and for multi-indices $\alpha\in\mathfrak{A}_{n+1,\ell}$. Indeed,

$$\begin{aligned}&\Lambda_{\alpha,z} =\\ &= \int_{\Sigma_{n+1}} e^{(1-\sigma_1)L_0^z}L_{\alpha_1}e^{(\sigma_1-\sigma_2)L_0^z}L_{\alpha_2}\cdots e^{(\sigma_n-\sigma_{n+1})L_0^z}L_{\alpha_{n+1}}e^{\sigma_{n+1}L^{s,z}}d\sigma\\ &= \int_{\Sigma_{n+1}} P_{\alpha_1}(1-\sigma_1)e^{(1-\sigma_2)L_0^z}L_{\alpha_2}\cdots e^{(\sigma_n-\sigma_{n+1})L_0^z}\cdots L_{\alpha_{n+1}}e^{\sigma_{n+1}L^{s,z}}d\sigma\\ &= \int_{\Sigma_{n+1}} P_{\alpha_1}(1-\sigma_1)P_{\alpha_2}(1-\sigma_2)e^{(1-\sigma_3)L_0^z}\cdots L_{\alpha_{n+1}}e^{\sigma_{n+1}L^{s,z}}d\sigma\\ &= \int_{\Sigma_{n+1}} P_{\alpha_1}(1-\sigma_1)\cdots P_{\alpha_k}(1-\sigma_{n+1})e^{(1-\sigma_{n+1})L_0^z}e^{\sigma_{n+1}L^{s,z}}d\sigma.\end{aligned}$$

We are now in the position to state the main result of this section. Below, we set $\mathcal{P}^0=1$. Let us recall the error term

$$\mathbb{E}_{n,n}^{s,z} := \sum_{\ell=n+1}^{(n+1)^2} s^{\ell-n-1}\Lambda_z^\ell = \sum_{\ell=n+1}^{(n+1)^2}\sum_{k=1}^{n+1}\sum_{\alpha\in\mathfrak{A}_{k,\ell}} s^{\ell-n-1}\Lambda_{\alpha,z} \tag{4.8}$$

introduced in Equation (3.18). (There, we introduced $\mathbb{E}_{d,n}$, but such error term is independent of d, as long $d\geq n$, hence we can always assume that $d=n$.)

Theorem 4.7. *The perturbative expansion* (3.18) *of* $e^{L^{s,z}}$ *can be written in the form*

$$e^{L^{s,z}} = e^{L_0^z} + \sum_{\ell=1}^{n} s^\ell\mathcal{P}^\ell(x,z,\partial)e^{L_0^z} + s^{n+1}\mathbb{E}_{n,n}^{s,z},$$

where the differential operators $\mathcal{P}^\ell$ *are explicitly given by Lemmas 4.5 and 4.6.*

Proof. Starting with (3.18), we have

$$e^{L^{s,z}} = e^{L_0^z} + \sum_{\ell=1}^{n} \sum_{k=1}^{\ell} \sum_{\alpha \in \mathfrak{A}_{k,\ell}} s^\ell \Lambda_{\alpha,z} + s^{n+1} \mathbb{E}_{n,n}^{s,z}$$

$$= \sum_{\ell=0}^{n} s^\ell \Lambda_z^\ell + s^{n+1} \mathbb{E}_{n,n}^{s,z} = e^{L_0^z} + \sum_{\ell=1}^{n} s^\ell \mathcal{P}^\ell(x,z,\partial) e^{L_0^z} + s^{n+1} \mathbb{E}_{n,n}^{s,z}.$$

This completes the proof. □

Recall that $e^{L_0^z}(x,y)$ is explicit given in equation (3.12), since z is arbitrary, but fixed, and it agrees with the function $G^0(z;x,y)$ defined by equation (1.7) in the Introduction.

Corollary 4.8. *If $|\alpha| = \ell \leq n$, then the kernel of each operator $\Lambda_{\alpha,z}$ appearing in the perturbative expansion* (3.18) *is explicitly given by:*

$$\mathfrak{P}^\ell(z,x,y) G(z;x,y),$$

where the function $\mathfrak{P}^\ell$ are of the form

$$\mathfrak{P}^\ell(z,x,y) = \sum a_{\alpha,\beta}(z)(x-z)^\alpha (x-y)^\beta,$$

with $|\alpha| \leq \ell$, $\beta \leq 3\ell$, $a_{\alpha,\beta} \in \mathcal{C}_b^\infty(\mathbb{R}^N)$.

Proof. We observe that $e^{tL_0^z}$ is a convolution operator, since z is fixed, therefore

$$\left(\mathcal{P}_\alpha(x,z,\partial)\, e^{L_0^z}\right)(x,y) = \mathcal{P}_\alpha(x,z,\partial) \left(e^{L_0^z}(x,y)\right).$$

Then, the result follows from formula (1.7) for $e^{L_0^z}(x,y)$, formula (4.7) for $\mathcal{P}_\alpha(x,z,\partial)$, and the fact that $\mathcal{P}^\ell$ is a sum of such operators as α varies over $\mathfrak{A}_\ell$. (See also Lemma 5.1 in the next section, Section 5.) □

5. Error estimates

In this final section, we prove all the bounds necessary to justify the error estimate in the asymptotic expansion of Theorem 1.1. *Throughout this section, n will denote the order in the Taylor expansion of the coefficients of L, which may differ from the approximation order as defined in equation* (3.18). *Such approximation order will be denoted by μ, as in the statement of Theorem 1.1.* Recall that the definition of the operators $\Lambda_{\alpha,z}$ depends, in principle, on n. However, if $\alpha \in \mathfrak{A}_{k,\ell}$ and n is large ($n \geq k$, $n \geq \alpha_j$) the operator $\Lambda_{\alpha,z}$ no longer depends on n (in which case it does not depend on s either). This observation, together with the fact that n is fixed, justifies omitting n from the notation for $\Lambda_{\alpha,z}$. Moreover, the error terms $\mathbb{E}_{d,\nu}^{s,z}$ are independent of d, as long as $d \geq \nu$, which will always be the case, so we shall write $\mathbb{E}_{\nu,\nu}^{s,z} = \mathbb{E}_{d,\nu}^{s,z}$.

Below, we will use such error terms for $\nu = \mu$ and $\nu = n$, with $n > \mu$ appropriately chosen.

We start from Lemma 3.10. All the terms appearing in that lemma are operators with smooth distribution kernels by Corollary 3.9. We recall that we denote by $T(x, y)$ the distribution kernel of an operator T with smooth kernel (so $T(x, y)$ is a smooth function such that $Tf(x) = \int_{\mathbb{R}^N} T(x, y)f(y)dy$). In terms of kernels, the formula of Theorem 4.7 takes the form

$$
\begin{aligned}
(5.1) \quad e^{L^{s,z}}(x,y) &= e^{L_0^z}(x,y) + \sum_{\ell=1}^{\nu} s^\ell \Lambda_z^\ell(x,y) + s^{\nu+1}\mathbb{E}_{\nu,\nu}^{s,z}(x,y) \\
&= \sum_{\ell=0}^{\nu} s^\ell \Lambda_z^\ell(x,y) + s^{\nu+1}\mathbb{E}_{\nu,\nu}^{s,z}(x,y),
\end{aligned}
$$

where again $\nu = \mu$ or $\nu = n$.

We recall that L_0^z is obtained from L by freezing the coefficients of the highest order derivatives of L at z and by discarding the lower order terms.

We now substitute $x = z + s^{-1}(x - z)$, $y = z + s^{-1}(y - z)$, and $z = z(x, y)$ in the Equation (5.1) above, for some function $z(x, y)$ to be specified later. Lemma 3.2 and Equation (5.1) then give

$$
\begin{aligned}
(5.2) \quad e^{s^2 L}(x,y) &= s^{-N} e^{L^{s,z}}(z + s^{-1}(x-z), z + s^{-1}(y-z)) \\
&= \sum_{\ell=0}^{\nu} s^\ell \Lambda_z^\ell(z + s^{-1}(x-z), z + s^{-1}(y-z)) \\
&\quad + s^{\nu+1}\mathbb{E}_{\nu,\nu}^{s,z}(z + s^{-1}(x-z), z + s^{-1}(y-z)),
\end{aligned}
$$

which is valid for any $\nu \leq n$, in particular for $\nu = \mu$ and for $\nu = n$.

Using the definition of the approximate Green function $\mathcal{G}_t^{[\mu,z]}(x, y)$, for $t = s^2$, in Equation (1.14), we then obtain

$$
(5.3) \quad e^{s^2 L}(x,y) = \mathcal{G}_{s^2}^{[\nu,z]}(x,y) + s^{\nu+1}\mathbb{E}_{\nu,\nu}^{s,z}(z + s^{-1}(x-z), z + s^{-1}(y-z)).
$$

The error term in the approximation defined by Equation (1.14) is consequently given by

$$
(5.4) \quad e^{s^2 L}(x,y) - \mathcal{G}_{s^2}^{[\nu,z]}(x,y) = s^{\nu+1}\mathbb{E}_{\nu,\nu}^{s,z}(z + s^{-1}(x-z), z + s^{-1}(y-z)),
$$

where $\mathbb{E}_{\nu,\nu}^{s,z}$ is as in Equation (3.18) with $s = \sqrt{t}$, and $z = z(x, y)$.

We next introduce the dilated error operator

$$
(5.5) \qquad \mathcal{E}_{s^2}^{[\nu,z]} f(x) = \int_{\mathbb{R}^N} \mathbb{E}_{\nu,\nu}^{s,z}(z + s^{-1}(x-z), z + s^{-1}(y-z)) f(y)dy.
$$

and define the approximation kernel $\mathcal{G}_{s^2}^{[\nu,z]}$ to be the operator with kernel $\mathcal{G}_{s^2}^{[\mu,z]}(x,y)$, so that

$$e^{tL} - \mathcal{G}_t^{[\nu,z]} = t^{(\nu+1)/2}\mathcal{E}_t^{[\nu,z]}. \tag{5.6}$$

We will use the above formula *only* for $\nu = \mu < n$, where n will be taken large enough.

Indeed, if $\mu < n$, then the error term can be written as,

$$\begin{aligned}(5.7)\quad & \mathbb{E}_{\mu,\mu}^{s,z}(z + s^{-1}(x-z), z + s^{-1}(y-z)) = \\ & \sum_{\ell=\mu+1}^{(n+1)^2} \sum_{k=1}^{\max\{\ell,n+1\}} \sum_{\alpha\in\mathfrak{A}_{k,\ell}} s^{\ell-\mu-1}\Lambda_{\alpha,z}(z + s^{-1}(x-z), z + s^{-1}(y-z)).\end{aligned}$$

(See Equation (1.15), for instance.) We will estimate $\mathbb{E}_{\mu,\mu}^{s,z} = \mathbb{E}_{n,\mu}^{s,z}$ by writing

$$\mathbb{E}_{\mu,\mu}^{s,z} = \sum_{\ell=\mu+1}^{n} s^{\ell-\mu-1} \sum_{k=\mu+1}^{\ell} \sum_{\alpha\in\mathfrak{A}_{k,\ell}} \Lambda_{\alpha,z} + s^{n+1-\mu}\mathbb{E}_{n,n}^{s,z}. \tag{5.8}$$

The point of this formula is that the error term $\mathbb{E}_{\mu,\mu}^{s,z}$ is independent of n, as long as $\mu \leq n$. However, splitting the error as done above will allow a better control on the error estimate of Theorem 1.1. In fact, we will show that each Λ_z^ℓ in the first sum, which does not depend on s, is a pseudodifferential operator, and its contribution to the overall error after the parabolic rescaling will be obtained in terms of a refined analysis on its symbol. This analysis, in turn, leads to some refined estimates *uniformly in s* on the norm of the operator between weighted Sobolev Spaces. On the other hand, we will obtain only rough estimates on the remander term $\mathbb{E}_{n,n}$, which will nevertheless be enough, due to the additional factor $s^{n+1-\mu}$. The main issue in treating the remainder is that some of its terms $\Lambda_{\alpha,z}$ implicitly depend on s, a fact which makes it difficult to show the remainder is also a pseudodifferential operator, at least in the usual Hörmader class. It may be possible to show that $\mathbb{E}_{n,n}$ is indeed a pseudodifferential operator employing more exotic symbol classes or amplitudes, but we do not need to pursue this point here, since we are able to prove the *sharp* estimates of Theorem 1.1 in any case.

We now proceed along these lines. The dilated error operator introduced in equation (5.5) can be rewritten in terms of approximation operators

$$\mathcal{L}_{s,\alpha}f(x) = s^{-N}\int_{\mathbb{R}^N} \Lambda_{\alpha,z}(z + s^{-1}(x-z), z + s^{-1}(y-z))f(y)dy, \tag{5.9}$$

as

$$(5.10)\qquad \mathcal{E}_{s^2}^{[\mu,z]} = \sum_{\ell=\mu+1}^{(n+1)^2} \sum_{k=1}^{\max\{\ell,n+1\}} \sum_{\alpha\in\mathfrak{A}_{k,\ell}} s^{\ell+N-\mu-1}\mathcal{L}_{s,\alpha}.$$

We therefore obtain

$$(5.11)\qquad \mathcal{E}_{t}^{[\mu,z]} = \sum_{\ell=\mu+1}^{n} s^{\ell-\mu-1} \sum_{k=\mu+1}^{\ell} \sum_{\alpha\in\mathfrak{A}_{k,\ell}} \mathcal{L}_{s,\alpha} + s^{n+1-\mu}\mathcal{E}_{t}^{[n,z]}.$$

To evaluate $\|\mathcal{E}_{s^2}^{[n,z]} f\|$ in a desired norm, it will then be enough to evaluate each operator norm $\|\mathcal{L}_{s,\alpha}\|$ (between suitable Sobolev spaces). As explained above, we shall derive a rough estimate for the terms with $\alpha \in \mathfrak{A}_{n+1,\ell}$ or some $\alpha_i = n+1$ (which corresponds to $\Lambda_{\alpha,z}$ depending on s). When $\Lambda_{\alpha,z}$ is independent of s (that is for $\alpha \in \mathfrak{A}_{k,\ell}$, $k \leq n$, $\alpha_i \leq n$), we shall derive some more precise estimates. We begin with these refined, more precise estimates.

5.1. **Precise estimates.** Recall that we denote by $\Lambda_{\alpha,z}(x,y)$ the distribution kernel of the operator $\Lambda_{\alpha,z}$ since it is a smooth function. Thus, for $\alpha \in \mathfrak{A}_{k,\ell}$, $k \leq n$, $\alpha_i \leq n$, $\Lambda_{\alpha,z}(x,y)$ does not depend on s. Let us fix a function $z(x,y)$, which will be specified later, and let $\mathcal{L}_{s,\alpha}$ be the operator with distribution kernel

$$s^{-N}\Lambda_{\alpha,z}(z + s^{-1}(x-z), z + s^{-1}(y-z)),$$

introduced above in Equation (5.9), where $z = z(x,y)$.

We will show below that in this range of α for a suitable choice of the function z, the operator $\mathcal{L}_{s,\alpha}$ is a pseudodifferential operator whose symbol is well behaved. We shall then use symbol calculus to derive the desired error estimates. We refer to [44] for all relevant properties of pseudodifferential operators. Below, we follow the usual convention and set $D = \frac{1}{i}\partial$, $(i = \sqrt{-1})$, where if not specified otherwise $\partial = \partial_x$.

We shall need the standard seminorms $p_{m,\alpha,\beta}$ given by

$$(5.12)\qquad p_{m,\alpha,\beta}(a) = \sup_{(x,\xi)\in\mathbb{R}^N\times\mathbb{R}^N} |\langle\xi\rangle^{|\beta|-m}\partial_x^{\alpha}\partial_\xi^{\beta} a(x,\xi)|.$$

Then the Hörmander class $S^m_{1,0} := S^m_{(1,0)}(\mathbb{R}^N \times \mathbb{R}^N)$, $m > -\infty$, is by definition the set of functions $a : \mathbb{R}^{2N} \to \mathbb{C}$ satisfying $p_{m,\alpha,\beta}(a) < \infty$. The space $S^{-\infty} = S^{-\infty}(\mathbb{R}^N \times \mathbb{R}^N)$ is defined by the same seminorms, but with $m \in \mathbb{Z}$ arbitrary.

We also denote by

$$(5.13)\qquad \mathcal{F}u(x) = \hat{u}(\xi) := \int_{\mathbb{R}^N} e^{-i\,\xi\cdot x} u(x)dx$$

the usual Fourier transform of u. For any symbol a in the Hörmander class $S^m_{1,0} := S^m_{1,0}(\mathbb{R}^N \times \mathbb{R}^N)$, we denote by $a(x, D)$ the operator

$$a(x, D)u(x) = (2\pi)^{-N} \int_{\mathbb{R}^N} e^{i\,x\cdot\xi} a(x, \xi)\hat{u}(\xi)d\xi, \tag{5.14}$$

defined for u in the Schwartz space $\mathcal{S}(\mathbb{R}^N)$. We will denote by $\mathcal{F}_2$ the Fourier transform in the second variable of a function of two variables. For $a \in S^{-\infty} := S^{-\infty}_{1,0}(\mathbb{R}^N \times \mathbb{R}^N)$, the operator $a(x, D)$ is smoothing with distribution kernel

$$a(x, D)(x, y) = (2\pi)^{-N} \int_{\mathbb{R}^N} e^{i\,(x-y)\cdot\xi} a(x, \xi)d\xi = (\mathcal{F}_2^{-1}a)(x, x - y).$$

Let K be a smooth function on $\mathbb{R}^N \times \mathbb{R}^N$. If the integral operator defined by K, which is smoothing, is in fact a pseudodifferential operator $a(x, D)$, then we can recover a from K by the formula $(\mathcal{F}_2^{-1}a)(x, y) = K(x, x - y)$, so

$$a(x, \xi) = \int_{\mathbb{R}^N} e^{-i\,\xi\cdot y} K(x, x - y)dy. \tag{5.15}$$

Recall next the function $G(z; x) = (4\pi)^{-N/2} \det(A(z))^{-1/2} e^{-x^T A(z)^{-1}x/4}$ introduced in Equation (1.7): Then the distribution kernel of $e^{L_0^z}$ is given by

$$e^{L_0^z}(x, y) = G(z; x - y), \tag{5.16}$$

and we have the following result.

Lemma 5.1. *Let $z \in \mathbb{R}^N$ be a parameter and let us consider the operator $T = (x - z)^\beta \partial_x^\gamma e^{L_0^z}$, where β and γ are multi-indices. Then the distribution kernel of T is given by*

$$T(x, y) = (x - z)^\beta (\partial_x^\gamma G)(z; x - y).$$

Proof. The Lemma follows from a direct computation. □

We will also need the following standard result.

Lemma 5.2. *(i) The Fourier transform in the second variable establishes an isomorphism $\mathcal{F}_2 : S^{-\infty} := S^{-\infty}(\mathbb{R}^N \times \mathbb{R}^N) \to S^{-\infty}$.*

(ii) Multiplication defines a continuous map $S^m_{(1,0)} \times S^{-\infty} \to S^{-\infty}$.

(iii) If $\{a_s\}_{s\in(0,1]}$ is uniformly bounded in $S^{-\infty}$ and $b_s(x, \xi) = a_s(x, s\xi)$, then the family $\{s^k b_s\}_{s\in(0,1]}$ is uniformly bounded in $S^{-k}_{1,0}$, $k \geq 0$.

Proof. This follows from a straightforward calculation. □

For our main result, we require some assumptions on the dilation center z.

Definition 5.3. *A function $z : \mathbb{R}^{2N} \to \mathbb{R}^N$ will be called* admissible *if*

(i) $z(x, x) = x$, for all $x \in \mathbb{R}^N$.
(ii) All derivatives of z are bounded.

A typical example is $z(x, y) = \lambda x + (1-\lambda)y$, for some fixed parameter λ. A simple application of the mean value theorem gives that $\langle z - x\rangle \leq C\langle y - x\rangle$ for some constant $C > 0$.

We are now ready to state and prove the main result of this subsection.

Theorem 5.4. *Let $\alpha \in \mathfrak{A}_{k,\ell}$, $k \leq n$, $\alpha \leq n$. Assume that $z : \mathbb{R}^{2N} \times \mathbb{R}^N$ is admissible. Then there exists a uniformly bounded family $\{a_s\}_{s\in(0,1]}$ in $S^{-\infty}$ such that, if $b_s(x, \xi) := a_s(x, s\xi)$, then*

$$\mathcal{L}_{s,\alpha} = b_s(x, D).$$

Proof. By Lemma 4.6, we have that $\Lambda_{\alpha,z}$ is a finite sum of terms of the form $\varphi(z)(x - z)^\beta \partial_x^\gamma e^{L_0^z}$ with $\varphi \in C_b^\infty$. Let then $k_z(x, y)$ be the distribution kernel of $a(z)(x - z)^\beta \partial_x^\gamma e^{L_0^z}$ and let

$$K_s(x, y) := s^{-N} k_z(z + s^{-1}(x - z), z + s^{-1}(y - z)), \quad z = z(x, y).$$

By abuse of notation, we shall denote also by K_s the integral operator defined by K_s. It is enough then to prove our theorem for K_s. Namely, it is enough to show that there exists a uniformly bounded family $\{a_s\}_{s\in(0,1]}$ in $S^{-\infty}$ such that

$$K_s = a_s(x, sD).$$

By lemma 5.1, we have that the distribution kernel of $\partial_x^\gamma e^{L_0^z}$ is of the form $\psi(z, x - y)$ and belong to $S^{-\infty}$ as a function of $x - y$ for z fixed. (This is consistend with the fact that for each fixed z, $\partial_x^\gamma e^{L_0^z}$ is a convolution operator.) More precisely $\psi(z, x)$ is $\mathcal{F}_2(i\,\xi)^\gamma e^{-\xi^T \cdot A(z)\cdot\xi}$. This observation implies

$$\begin{aligned} K_s(x, y) = \varphi(z(x, y))s^{-|\beta|-N}(x - z(x, y))^\beta \psi(z(x, y), s^{-1}(x - y)) =: \\ \varphi(z)s^{-|\beta|-N}(x - z)^\beta \psi(z, s^{-1}(x - y)), \quad z = z(x, y). \end{aligned}$$

We then let

$$b_s(x, \xi) = \int_{\mathbb{R}^N} e^{-i\,y\cdot\xi}\phi(z)s^{-|\beta|-N}(x - z)^\beta \psi(z, s^{-1}y)dy, \quad z = z(x, x - y).$$

Next, we observe that if we change variables from y to sy, we can write $b_s(x, \xi) = a_s(x, s\xi)$, where

$$a_s(x, \xi) = \int_{\mathbb{R}^N} e^{-i\,y\cdot\xi}\phi(z)s^{-|\beta|}(x - z)^\beta \psi(z, y)dy, \quad z = z(x, x - sy).$$

We need to show that a_s is a bounded family in $S^{-\infty}$. To this end, we observe that, since $\varphi \in C_b^\infty$ and the derivatives of z are all bounded, $\varphi(z) \in S^1_{1,0}$ as a function of y for each x. Similarly, for each $j = 1, \ldots, N$, $s^{-1}(x_j - z_j(x, x - sy)) \in S^1_{1,0}$ as a function of y for fixed x, and collectively they form bounded families for $s \in (0, 1]$. Lastly, from what already observed above, $\psi(z, y) \in S^{-\infty}$ as a function of y for each fixed x. Therefore, $a_s \in S^{-\infty}$ uniformly in s by Lemma 5.2. The proof is complete. $\square$

We now obtain the desired refined mapping property estimate by standard results on pseudodifferential operators. Below, $t = s^2$.

Theorem 5.5. *Let $\alpha \in \mathfrak{A}_{k,\ell}$, $k \leq n$, $\alpha_j \leq n$. Assume that $z : \mathbb{R}^{2N} \times \mathbb{R}^N$ is admissible. Then for any $1 < p < \infty$, any $r \in \mathbb{R}$,*

$$t^{k/2} \|\mathcal{L}_{s,\alpha}\|_{W^{r,p} \to W^{r+k,p}} \leq C_{k,r,p}, \tag{5.17}$$

for a constant $C_{k,r,p}$ independent of $t \in (0, 1]$.

5.2. **Rough estimates.** We now move to study the mapping properties of $\Lambda_{\alpha,z}$ when either $\alpha \in \mathfrak{A}_{n+1,\ell}$ or some $\alpha_i = n + 1$. In this case, the operators $\Lambda_{\alpha,z}$ depend on s also, although this dependence is not shown in the notation.

The mapping properties that we establish in this subsection will allow us to obtain corresponding mapping properties for the error operator $\mathbb{E}^{s,z}_{n,n}$, which is not immediately in the form of a pseudodifferential operator. Consequently, we are not able to derive bounds as those in Theorem 5.4 above. Nevertheless, the bounds we derive are sufficient to establish the *sharp* error estimates as $t \to 0^+$ in weighted Sobolev spaces for the overall approximation, given in Theorem 1.1. This result is achieved by choosing judiciously an n large enough.

As before we denote $W^{r,p}_a = W^{r,p}_{a,w}$ as before, where w is the center of the weight $\langle x \rangle_w = \langle x - w \rangle = \langle w - x \rangle$ used to define the exponentially weighted Sobolev spaces (see equation (2.4)). We shall also write $L^p_a = W^{0,p}_a$. The main result of this section is the following proposition.

Proposition 5.6. *Assume that $z : \mathbb{R}^{2N} \times \mathbb{R}^N$ is admissible. For any α, any $1 < p < \infty$, $k \in \mathbb{Z}_+$, $r \geq 0$, and $a \in \mathbb{R}$,*

$$s^k \|\mathcal{L}_{s,\alpha}\|_{L^p_a \to W^{k,p}_a} \leq C_{k,p}, \tag{5.18}$$

for a constant $C_{k,p}$ independent of $s \in (0, 1]$, of a in a bounded set, and independent of the center of the weight that defines the weighted Sobolev spaces $W^{k,p}_a$.

Proof. The proof is based on explicit kernel estimates and Riesz' lemma. By replacing the operator L with $e^{a\langle x-w\rangle} L e^{-a\langle x-w\rangle}$, where w is the center of the weight, we can assume that $a = 0$, as before.

As before, $\Lambda_{\alpha,z}(x,y)$ is the smooth distribution kernel of the operator $\Lambda_{\alpha,z}$. For any given point $v \in \mathbb{R}^N$, we denote by δ_v^β the distribution defined by $\delta_v^\beta(f) = \partial^\beta f(v)$ (we agree that $\delta_v^0(f) = f(v)$. Then

$$\partial_x^\beta \partial_y^{\beta'} \partial_z^{\beta''} \Lambda_{\alpha,z}(x,y) = \langle \delta_x^\beta \ , \ (\partial_z^{\beta''} \Lambda_{\alpha,z})(\delta_y^{\beta'}) \rangle, \tag{5.19}$$

where $\langle , \rangle$ is the usual duality pairing. Since all the coefficients (and their derivatives) of L are uniformly bounded, the derivative $\partial_z^\beta \Lambda_{\alpha,z}$ will satisfy the same mapping properties as $\Lambda_{\alpha,z}$. Furthermore, for each multi-index β, $\partial^\beta \delta_y \in H^{-q}(\mathbb{R}^N)$ for $q > N/2 + |\beta|$ and has norm independent of y.

In the rest of the proof, we use the weighted Sobolev spaces introduced in (2.4). We recall that the mapping properties between these spaces are uniform in term of the base point. We can therefore choose the weight center at x in estimating (5.19). We will write $H_a^s = W_{a,x}^{s,2}$. Then $\delta_y \in H_a^{-q}$ for all $a \in \mathbb{R}$, $q > N/2 + |\beta|$, with

$$\|\partial^\beta \delta_y\|_{H_a^{-q}} := \|e^{a<y-x>} \partial^\beta \delta_y\|_{H^{-q}} \leq C_{q,\alpha} e^{(a+\epsilon)\langle y-x\rangle}.$$

Next, we pick an $\epsilon > 0$ small enough. Replacing ϵ with ϵ/k, where k is such that $\alpha \in \mathfrak{U}_{k,\ell}$ in Corollary 3.9 yields

$$\|\partial_z^\beta \Lambda_{\alpha,z} \|_{H_{-a}^{-q} \to H_{-a-\epsilon/k}^{q}} \| \leq e^{\epsilon\langle x-z\rangle},$$

and hence

$$\begin{aligned} \left|\partial_x^\beta \partial_z^{\beta'} \partial_y^{\beta''} \Lambda_{\alpha,z}(x,y)\right| &= \left|\langle \partial^\beta \delta_x \, , \partial_z^{\beta'} \Lambda_{\alpha,z} \, \partial^{\beta''} \delta_y \rangle\right| \\ &\leq C \|\partial^\beta \delta_x\|_{H_{-a-\epsilon/k}^{-q}} \|\partial_z^{\beta'} \Lambda_{\alpha,z} \|_{H_{-a}^{-q} \to H_{-a-\epsilon/k}^{q}} \|\partial^{\beta''} \delta_y\|_{H_{-a}^{-q}} \\ &\leq C e^{\epsilon\langle x-z\rangle - (a+\epsilon)\langle y-x\rangle}, \end{aligned} \tag{5.20}$$

where $q > N/2 + \max(|\beta|, |\beta'|, |\beta''|)$.

We will employ the bounds above to estimate

$$\mathcal{L}_{s,\alpha}(x,y) = s^{-N} \Lambda_{\alpha,z}(z + s^{-1}(x-z), z + s^{-1}(y-z)), \quad z = z(x,y). \tag{5.21}$$

We first use the chain rule to conclude that, if γ is any multi-index, then $\partial_x^\gamma \mathcal{L}_{s,\alpha}(x,y)$ is a sum of terms of the form

$$s^{-j} \partial_x^\beta \partial_z^{\beta'} \partial_y^{\beta''} \Lambda_{\alpha,z}(z + s^{-1}(x-z), z + s^{-1}(y-z)) P,$$

for appropriate multi-indices β, β', and β'', with P a product of factors of the form $\partial^{\alpha'} z$ and $j \leq |\gamma|$. Our assumptions on z imply that p is bounded. Using also Equation (5.20), we obtain for ϵ sufficiently small,

$$(5.22)\quad \left|\partial_x^\gamma \mathcal{L}_{s,\alpha}(x,y)\right| \le Cs^{-N-|\gamma|}\ e^{\epsilon\langle s^{-1}(x-z)\rangle - a\langle s^{-1}(y-x)\rangle} \le Cs^{-N-|\gamma|}\ e^{-a\langle s^{-1}(y-x)\rangle/2}, \qquad z = z(x,y),$$

where the last inequality follows from $\langle x-z\rangle \le C\langle y-x\rangle$. From this inequality, we obtain after the change of variables $v = s^{-1}(y-x)$

$$\int_{\mathbb{R}^N} \left|\partial_x^\gamma \mathcal{L}_{s,\alpha}(x,y)\right| dy \le C_a s^{-|\gamma|}, \quad \forall x \in \mathbb{R}^N,$$

and

$$\int_{\mathbb{R}^N} \left|\partial_x^\gamma \mathcal{L}_{s,\alpha}(x,y)\right| dx \le C_a s^{-|\gamma|}, \quad \forall y \in \mathbb{R}^N,$$

These two estimates together with Riesz Lemma give that the map $f \to s^{|\gamma|}\partial_x^\gamma \mathcal{L}_{s,\alpha} f$ is bounded from L^p to L^p, which is enough to establish the result. □

This proposition, and the definition of $\mathbb{E}_{n,n}^{s,z}$ immediately imply the following lemma, where as usual $t = s^2$.

Lemma 5.7. *Assume that $z : \mathbb{R}^{2N} \times \mathbb{R}^N$ is admissible, then for each $r \in \mathbb{R}$, $q > 0$, we have*

$$\|\mathcal{E}_t^{[n,z]}\|_{W^{r,p}\to W^{r+q,p}} \le C_T\, t^{-(r+q)/2}, \qquad t \in (0,T].$$

Proof. Indeed, this follows from Proposition 5.6, Equation (5.10), and the continuous inclusion $W^{r,p} \hookrightarrow L^p$, $r \ge 0$. For r noninteger we also use interpolation. □

We note that in the above proposition we have an additional factor of $t^{-q/2}$ compared with the refined estimates of Theorem 5.5. This extra factor will not affect the final result, however, provided the order n of the Taylor expansion of L is chosen sufficiently large.

Then, the lemma leads to the following more precise estimate for the error operator $\mathcal{E}_t^{[\mu,z]}$.

Theorem 5.8. *Assume that $z : \mathbb{R}^{2N} \times \mathbb{R}^N$ is admissible, then we have*

$$\|\mathcal{E}_t^{[\mu,z]}\|_{W^{r,p}\to W^{r+k,p}} \le C_T\, t^{-k/2}, \qquad t \in (0,T].$$

Proof. Let us chose $n+1 \ge \mu + r$ and $t = s^2$, as usual. Then Theorems 5.5 and 5.8 applied to Equation (5.11) give

$$\|\mathcal{E}_t^{[\mu,z]}\|_{W^{r,p}\to W^{r+k,p}} \le \sum_{\ell=\mu+1}^{n} s^{\ell-\mu-1} \sum_{k=\mu+1}^{\ell} \sum_{\alpha\in\mathfrak{A}_{k,\ell}} \|\mathcal{L}_{\alpha,z}\|_{W^{r,p}\to W^{r+k,p}} + s^{n+1-\mu}\|\mathcal{E}_t^{[n,z]}\|_{W^{r,p}\to W^{r+k,p}} \le Cs^{-k}(1 + s^{n+1-\mu}s^{-r-k}) \le Cs^{-k}.$$

□

This completes the proof of Theorem 1.1.

From (1.14), we immediately obtain the following property on the principal part of the asymptotic expansion.

Corollary 5.9. *Assume that $z : \mathbb{R}^{2N} \times \mathbb{R}^N$ is admissible. For each $1 < p < \infty$, $r \in \mathbb{R}$, $\mu \geq 0$, and any $f \in W_a^{r,p}$ let us define*

$$\mathcal{G}_t^{[\mu,z]} f(x) := \int_{\mathbb{R}^N} \mathcal{G}_t^{[\mu,z]}(x,y) f(y)\, dy,$$

then $\mathcal{G}_t^{[\mu,z]} f \to f$ in $W_a^{r,p}$ for $t \to 0_+$.

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