Short-time asymptotics of heat kernels of hypoelliptic Laplacians on unimodular Lie groups

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Abstract

We consider the problem of computing heat kernel small-time asymptotics for hypoelliptic Laplacians associated to left-invariant sub-Riemannian structures on unimodular Lie groups of type I. We use the non-commutative Fourier transform of the Lie group together with perturbation theory for semigroups of operators in deriving these asymptotics. We illustrate our approach on the example of the Heisenberg group, and, as an application, we compute the short-time behaviour of the hypoelliptic heat kernel on the step 3 nilpotent Cartan and Engel groups, for which no closed-form expression for the hypoelliptic heat kernel is yet known.

Keywords: Sub-Riemannian geometry; Hypoelliptic heat kernel; Non-commutative harmonic analysis; Trotter–Kato product formula

1. Introduction

The relations between the local geometry on a Riemannian manifold and the short-time behaviour of the heat kernel of the elliptic Laplacian associated to the Riemannian structure were first studied in the seminal work of Varadhan [26]; it was shown there that the Riemannian distance between two points can be read off the short-time behaviour of the heat kernel centered at one of these points, in line with the intuitive notion that heat diffuses along geodesics. In recent
work, Neel et al. [23,24] have related the short-time asymptotic behaviour of the gradient and Hessian of the logarithm of the heat kernel to the cut locus of the Riemannian structure. Of equal interest is the relation between sub-Riemannian structures and the heat kernels they define. An important point of divergence with Riemannian geometry is that the Laplacians associated to sub-Riemannian structures are not elliptic, but only hypoelliptic. Despite this, numerous relations between short-time heat kernel behaviour and local geometrical structure that hold in the Riemannian case have been shown to hold also in the sub-Riemannian case (see [9,13]). As a result, knowledge of the short-time behaviour of heat kernels of hypoelliptic Laplacians can be of great help in understanding the local sub-Riemannian geometry and its associated geodesic structure.

One of the early heat kernel calculations for sub-Riemannian structures was made by Gaveau [16], and, independently, Hulanicki [19]; the sub-Riemannian structure they considered was that of the Heisenberg group, which is a step 2 nilpotent Lie group. Gaveau made use of probabilistic reasoning and Paul Levy’s area formula for Brownian motion in the plane, whereas Hulanicki used the Fourier transform with respect to the center of the Heisenberg group. Following this, Rothschild and Stein [25] introduced a nilpotentization scheme for computing parametrices for hypoelliptic operators expressed as sums of squares of vector fields on Lie groups. Since those early works, much effort has been made towards computing exact expressions for heat kernels of various sub-Riemannian structures, together with their short-time asymptotics [18,4,5,21,9,13,3,10,28,2]. Much of this effort however has been limited by the fact that the tools used for computing particular hypoelliptic heat kernels and their short-time behaviour have been specific to the particular sub-Riemannian structure being studied, with no particular relation to one another.

In recent work [1], Agrachev et al. have introduced a unified approach for computing heat kernels of hypoelliptic left-invariant sub-Riemannian structures on unimodular Lie groups of type I. This approach makes essential use of the non-commutative harmonic analysis of the Lie group and hinges on the observation that for left-invariant sub-Riemannian structures, the non-commutative Fourier transform “diagonalizes” the hypoelliptic heat equation, just as the ordinary Fourier transform diagonalizes the heat equation on the real line, yielding a family of operator equations indexed by the equivalence classes of unitary irreducible representations of the Lie group (a related idea using spherical harmonics on $S^2$ can be found in [7]); the heat kernel is then obtained by an “inverse Fourier transform” from the solutions of these operator equations. As elegant and unifying as this approach may be, it often leads to operator equations which cannot be solved in closed form, and consequently to heat kernel expressions involving functions which are not computable. Such is the case, for example, for the hypoelliptic heat kernel expressions obtained by Boscain et al. [6] for the case of sub-Riemannian structures on step 3 nilpotent Lie groups, where the exact same non-commutative harmonic analysis approach as in [1] has been used.

The main motivation for this paper is the observation that the non-commutative harmonic analysis approach proposed by Agrachev et al. in [1] may be used to compute hypoelliptic heat kernel short-time asymptotics, as opposed to the heat kernel itself, even in situations where the exact expression of the heat kernel is impossible to compute due to intractable operator equations. In other words, it may be possible to take a shortcut to the small-time behaviour directly from the harmonic analysis on the Lie group while bypassing the exact computation of the heat kernel altogether. The main goal of this paper is to illustrate precisely how such a shortcut can be taken, the key idea being to approximate the intractable operator equations resulting from the non-commutative Fourier transform by possibly more tractable operator equations in such a way as to preserve (to a given order) the principal part of the heat kernel. Our main result is the following:
Theorem 1. For \( G \) a unimodular Lie group of type I, let \( (G, \Delta, g) \) be a left-invariant sub-Riemannian manifold satisfying the list \((L)\) of assumptions detailed in Section 3.3. Denote by \( \Delta_{sr} \) the associated hypoelliptic Laplacian and by \( \hat{\Delta}_{sr} \) its Generalized Fourier Transform, with \( \lambda \) indexing the elements of the dual \( \hat{G} \), and suppose that each acts on the Hilbert space \( \mathcal{H}_\lambda = L^2(\Omega_\lambda) \). Then, the operators of the semigroup \( e^{t\hat{\Delta}_{sr}} \) are integral operators having the following expression in small-time:

\[
\left[ e^{t\hat{\Delta}_{sr}} f \right](s) = \int_{\Omega_\lambda} \left[ k^\lambda(s, r) + t \lim_{n \to \infty} K^\lambda_{t/n}(s, r) \right] f( r) \, dr + \mathcal{O}(t^2) f(s),
\]

(1)

where the functions \( k^\lambda_t \) and \( K^\lambda_{t/n} \) are as defined in \((L)\), and where by \( \mathcal{O}(t^2) f \) we mean an operator \( D_t \) acting on \( f \), such that \( \|D_t f\|_1 \leq M t^2 \|f\|_1 \) for a constant \( M \) and for \( t \) small enough.

We give an application example of Theorem 1 by computing the short-time asymptotic behaviour of the hypoelliptic heat kernel on the Heisenberg group; the domain of validity of the small-time asymptotic behaviour we obtain coincides with the complement of the cut locus of the origin. We then apply Theorem 1 to computing the short-time asymptotic behaviour of the hypoelliptic heat kernel on the step 3 nilpotent Cartan and Engel groups; it is to be noted that for these groups, no closed-form expression for the hypoelliptic heat kernel is as of yet known. Our results for these groups are the following:

Theorem 2. The expression in small-time of the hypoelliptic heat kernel \( p_t(x_1, x_2, x_3, x_4) \) on the Engel group is given by

\[
p_t(x_1, x_2, x_3, x_4) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{1}{4t} x_1^2\right) \int_{\mathbb{R}^* \times \mathbb{R}} \exp\left(i \left( -\frac{\mu}{2\lambda} x_2 + \lambda x_4 \right) \right) \times \left[ \int_{\mathbb{R}} \exp\left( i \left( -\lambda x_3 r + \frac{\lambda}{2} x_2 r^2 \right) \right) e^{-t P_4(r, x_1)} \, dr \right] \, d\lambda \, d\mu + \mathcal{O}(t^{3/2}),
\]

(2)

where

\[
P_4(r, x_1) = \frac{\mu^2}{4\lambda^2} - \frac{\mu}{6} \left( (r + x_1)^2 + r^2 + (r + x_1)r \right) + \frac{\lambda^2}{20} \left( (r + x_1)^4 + r^4 + (r + x_1)^2 r^2 + (r + x_1)^3 r + (r + x_1)r^3 \right).
\]

Theorem 3. The expression in small-time of the hypoelliptic heat kernel \( p_t(x_1, x_2, x_3, x_4, x_5) \) on the Cartan group is given by

\[
p_t(x_1, x_2, x_3, x_4, x_5) = \frac{\sqrt{\lambda^2 + \mu^2}}{\sqrt{4\pi t}} \exp\left( -\frac{1}{4t} \frac{\left( \lambda x_1 + \mu x_2 \right)^2}{\lambda^2 + \mu^2} \right) \times \int_{\mathbb{R}} \int_{\lambda^2 + \mu^2 \neq 0} \int_{\mathbb{R}} \exp(i A^\lambda_{x_1, \mu, x_2}(r) \exp(-t P_4(r, x_1, x_2)) \, dr \, d\lambda \, d\mu \, dv + \mathcal{O}(t^{3/2}),
\]

(3)
with \( x = (x_1, x_2, x_3, x_4, x_5) \), and where the expression for \( A^\lambda_{\mu, \nu}^x \) is given in Proposition 5, and

\[
P_4(r, x_1, x_2) = \frac{\nu^2}{4(\lambda^2 + \mu^2)} + \frac{\nu}{6}(\lambda^2 + \mu^2)(\hat{r}^2 + r^2 + \hat{r}r) + \frac{(\lambda^2 + \mu^2)^3}{20}(\hat{r}^4 + r^4 + \hat{r}^2r^2 + \hat{r}^3r + \hat{r}^3),
\]

with \( \hat{r} = r + \frac{\lambda x_1 + \mu x_2}{\lambda^2 + \mu^2} \).

This paper is organized as follows: in Section 2 we review the classic concepts of sub-Riemannian geometry and we detail the construction of a natural left-invariant sub-Riemannian structure on Lie groups. We also recall the main results of [1], and in particular the explicit formula for the computation of the associated hypoelliptic heat kernel. We present our approach to computing heat kernel short-time asymptotics in Section 3; we first recall a few properties of semigroups and the Trotter–Kato product formula before proving our main theorem and restricting it to a particular case in Corollary 2. We illustrate the application of these results on the Heisenberg group in Section 4; this is followed with the computation of the small-time asymptotics of the heat kernel for the Cartan and Engel groups in Section 5.

2. Sub-Riemannian structures on Lie groups and non-commutative harmonic analysis

2.1. Sub-Riemannian geometry

We start with a few definitions:

**Definition 1.** Let \( M \) be a smooth manifold of dimension \( n \). A smooth distribution \( \mathcal{A} \) of constant rank \( m \leq n \) on \( M \) is a smooth map that to each point of \( M \) associates a subspace \( \mathcal{A}_q \) of dimension \( m \) of \( T_q M \).

The distribution \( \mathcal{A} \) is called bracket generating (also called non-holonomic, or verifying Hörmander’s condition) if at each point, the vector fields of \( \mathcal{A} \), together with a finite number of iterated Lie brackets, span the whole tangent space:

\[
\text{span}\{[X_1, [X_2, \ldots [X_{k-1}, X_k]]] (q) \mid X \in \mathcal{A}\} = T_q M,
\]

where \( \mathcal{A} = \{X \in \text{Vec}(M) \mid X(q) \in \mathcal{A}_q, \forall q \in M\} \).

We call \( \mathcal{A} \) the horizontal distribution, and \( \mathcal{A} \) the set of horizontal vector fields.

The absolutely continuous curves in \( M \) having tangent vector at almost every point in that distribution, i.e. absolutely continuous curves \( t \mapsto \gamma(t) \) such that, for almost all \( t \), \( \dot{\gamma}(t) \in \mathcal{A}_{\gamma(t)} \), are called horizontal curves.

We can now define a sub-Riemannian manifold:

**Definition 2.** A sub-Riemannian manifold is a triple \((M, \mathcal{A}, g)\), where \( M \) is a smooth manifold, \( \mathcal{A} \) a smooth bracket-generating distribution, endowed with a positive-definite, non-degenerate metric \( g \). This metric is called the sub-Riemannian metric or also the metric of Carnot–Carathéodory.
Just as in Riemannian geometry, such a metric enables us to define the length of a horizontal curve \( \gamma : [0, T] \rightarrow M \):

\[
l(\gamma) = \int_{0}^{T} \sqrt{g_{\gamma(t)}(\dot{\gamma}(t), \dot{\gamma}(t))} \, dt.
\]

(4)

We also recall the definition of a regular sub-Riemannian manifold \((M, \mathbf{\Lambda}, g)\). Let us introduce the notation:

\[
\mathbf{\Lambda}_{1} := \mathbf{\Lambda}, \quad \mathbf{\Lambda}_{n+1} = \mathbf{\Lambda}_{n} + [\mathbf{\Lambda}_{n}, \mathbf{\Lambda}] \quad \forall n \geq 1,
\]

which means that at every point \( q \in M \):

\[
\mathbf{\Lambda}_{n+1}(q) := \mathbf{\Lambda}_{n}(q) + [\mathbf{\Lambda}_{n}, \mathbf{\Lambda}](q) \\
= \{ X(q) + [Y, Z](q) \mid X(p), Y(p) \in \mathbf{\Lambda}_{n}(p), Z(p) \in \mathbf{\Lambda}(p), \forall p \in M \}.
\]

**Definition 3.** Let \((M, \mathbf{\Lambda}, g)\) be a sub-Riemannian manifold, and consider the sequence \(\mathbf{\Lambda}_{n}\) as defined above. We say that this sub-Riemannian manifold is regular if for every \( n \geq 1 \), the dimension of \( \mathbf{\Lambda}_{n}(q) \) is the same for every point \( q \in M \).

A key result in sub-Riemannian geometry is the following theorem of Chow [22]:

**Theorem 4.** Any two points in a connected sub-Riemannian manifold \((M, \mathbf{\Lambda}, g)\) can be joined by a horizontal curve.

Chow’s theorem, together with the sub-Riemannian metric on \( M \), enables us to define a sub-Riemannian distance on \( M \) as follows:

\[
d(x, y) := \inf \left( \int_{0}^{T} \sqrt{g_{\gamma(t)}(\dot{\gamma}(t), \dot{\gamma}(t))} \, dt \right), \quad \forall x, y \in M,
\]

(5)

where the infimum is taken over all horizontal curves \( \gamma \) such that \( \gamma(0) = x \) and \( \gamma(T) = y \).

We now detail the construction of natural sub-Riemannian structures on Lie groups:

**Definition 4.** Let \( G \) be a Lie group, with Lie algebra \( \mathfrak{L} \), and let \( \mathfrak{P} \) be a subset of \( \mathfrak{L} \) that verifies the bracket-generating condition:

\[
\text{Lie} \mathfrak{P} := \text{span}\{ p_1, [p_2, \ldots, [p_{n-1}, p_n]] \mid p_i \in \mathfrak{P} \} = \mathfrak{L}.
\]

Endow \( \mathfrak{P} \) with a positive-definite quadratic form \( \langle \cdot, \cdot \rangle \). We can therefore define a sub-Riemannian structure on \( G \) in the following way:
1. We define the distribution as: $$\Delta(g) := gP.$$ 
2. We define a quadratic form $g$ on the distribution: 
$$g_{\Delta}(v_1, v_2) := (g^{-1}v_1, g^{-1}v_2), \quad \text{for } v_1, v_2 \in \Delta(g).$$ 

With this construction, we will say that $(G, \Delta, g)$ is a left-invariant sub-Riemannian manifold.

It is important to notice that left-invariant sub-Riemannian manifolds $(G, \Delta, g)$ are always regular, which is clear from their construction.

Let now $(G, \Delta, g)$ be a left-invariant sub-Riemannian manifold, and let $(p_i)_{i=1}^m$ be an orthonormal frame for the subspace $\Delta(e)$ of the tangent space $T_e(G)$ to $G$ at the identity $e$. It follows from left-invariance of the sub-Riemannian structure that the family $(X_i)_{i=1}^m$ of smooth left-invariant vector fields on $G$ defined at each $g \in G$ by $X_i(g) = g \cdot p_i$ ($i = 1, \ldots, m$) is such that at each point $g \in G$, the family $(X_i(g))_{i=1}^m$ forms an orthonormal frame for the subspace $\Delta(g)$ of the tangent space $T_g(G)$ to $G$ at $g$. With the vector fields $(X_i)_{i=1}^m$ thus defined, the operator $\Delta_{sr}$ defined by

$$\Delta_{sr} = \sum_{i=1}^m L_{X_i}^2$$

is a left invariant second-order differential operator on $G$. Furthermore, it is not elliptic unless $m = n$, but is hypoelliptic as a result of Hörmander’s theorem, since the vector fields $(X_i)_{i=1}^m$ bracket-generate the tangent space to $G$ at each point by assumption on the distribution $\Delta$ and the fact that the $(X_i)_{i=1}^m$ form a frame for $\Delta$ at each point of $G$. It is important to note that if $(X_1')_{i=1}^m$ is another family of smooth left-invariant vector fields on $G$ such that at each $g \in G$ the vectors $(X_1'(g))_{i=1}^m$ form an orthonormal frame for the subspace $\Delta(g)$, then

$$\sum_{i=1}^m L_{X_i}^2 = \sum_{i=1}^m L_{X_1'}^2.$$

This leads naturally to the following definition:

Definition 5. Let $(G, \Delta, g)$ be a left-invariant sub-Riemannian manifold of rank $m$ and let $X_1, X_2, \ldots, X_m$ be left-invariant $C^\infty$ sections of the distribution $\Delta$ such that at each point $g \in G$ the vectors $(X_i(g))_{i=1}^m$ form an orthonormal frame for $\Delta(g)$ with respect to the sub-Riemannian metric at $g$. The left-invariant second order differential operator $\Delta_{sr}$ defined by

$$\Delta_{sr} = \sum_{i=1}^m L_{X_i}^2$$

is called the hypoelliptic Laplacian (or simply sub-Laplacian) associated to the left-invariant sub-Riemannian structure $(G, \Delta, g)$.

It is worth pointing out that for left-invariant sub-Riemannian structures defined on unimodular Lie groups, the hypoelliptic Laplacian can be constructed intrinsically, i.e. without resorting to any vector field (see Sections 2.2 and 2.3 in [1], also [8] and [22]).
Associated to the operator $\Delta_{sr}$ is the partial differential equation

$$\frac{\partial}{\partial t}\phi(t, g) = \Delta_{sr}\phi(t, g), \quad t > 0, \quad g \in G,$$

$$\lim_{t \to 0^+} \phi(t, \cdot) = \delta_e$$

($\delta_e$ denoting the Dirac distribution at the identity element $e$ of $G$) which we call the hypoelliptic heat equation. Note that as the vector fields $X_i$ are left-invariant, and by definition of the hypoelliptic Laplacian, for each $t > 0$ there exists a right-convolution kernel $p_t$ such that:

$$e^{t\Delta_{sr}}\phi_0(g) = \phi_0 \ast p_t(g), \quad t > 0,$$

where $\phi(0, g) = \phi_0(g)$ is the initial condition [27]. This fundamental solution $(t, g) \mapsto p_t(g)$ is called the hypoelliptic heat kernel.

### 2.2. Formula for the hypoelliptic heat kernel

The main idea proposed in [1] for a unified method of computation for the hypoelliptic heat kernel is the use of Generalized Fourier Analysis, otherwise known as non-commutative harmonic analysis. This theory has long been used to solve partial differential equations, and is for example the classic approach for solving the heat equation on Euclidean spaces. The key idea is that the Generalized Fourier Transform decomposes the right-regular representation, and that if $X$ is a left-invariant vector field, it is a differential operator associated to a semigroup of right-translations.

Let $G$ be a unimodular Lie group of type I (see for instance [11] for the definition of type I Lie groups), and recall that its dual $\hat{G}$ is the set of equivalence classes of unitary irreducible representations of $G$. We will denote by $\lambda$ an element of $\hat{G}$ and by $X^\lambda$ a representative of this equivalence class. $X^\lambda$ is therefore a homomorphism from $G$ to $U(H^\lambda)$, the set of unitary operators acting on the Hilbert space $H^\lambda$.

We define the Generalized Fourier Transform (GFT) of a function in the following way:

**Definition 6.** Let $G$ be a unimodular Lie group of type I, and $f \in L^1(G, \mathbb{C})$. The Generalized Fourier Transform of $f$ is the map $\hat{f}$ (or $F(f)$) that associates to each element $\lambda$ of the dual the linear operator on $H^\lambda$:

$$\hat{f}(\lambda) = \int_G f(g)X^\lambda(g^{-1})\,dg. \quad (6)$$

It can be shown that for all $\lambda \in \hat{G}$, $\hat{f}(\lambda)$ is a Hilbert–Schmidt operator on $H^\lambda$ and in particular is a bounded operator. We will denote by $\text{HS}^\lambda$ the set of Hilbert–Schmidt operators on $H^\lambda$.

The following proposition gives us the well known Plancherel formula and the inverse Generalized Fourier Transform:

**Proposition 1.** Let $G$ be a unimodular Lie group of type I. Then there exists on $\hat{G}$ a positive measure $dP(\lambda)$ called the Plancherel measure, such that for every $f \in L^1(G, \mathbb{C}) \cap L^2(G, \mathbb{C})$, we have:
\begin{equation}
\int_G |f(g)|^2 d\mu(g) = \int_{\hat{G}} \text{Tr}(\hat{f}(\lambda) \circ \hat{f}(\lambda)^*) dP(\lambda), \tag{7}
\end{equation}

\begin{equation}
f(g) = \int_{\hat{G}} \text{Tr}(\hat{f}(\lambda) \circ \hat{X}(g)) dP(\lambda). \tag{8}
\end{equation}

The definition of the generalized Fourier transform of a left-invariant vector field follows in a natural way from that of a function:

**Definition 7.** Let $G$ be a unimodular Lie group of type I, and $X$ a left-invariant vector field on $G$. The Generalized Fourier Transform of $X$ is defined as:

\[
\hat{X} = \mathcal{F}L_X \mathcal{F}^{-1}.
\]  \tag{9}

Clearly, $\hat{X}$ acts on the Hilbert–Schmidt operators $\hat{f}(\lambda)$, for $\lambda \in \hat{G}$. From [1] we have the following useful proposition.

**Proposition 2.** Let $G$ be a unimodular Lie group of type I with Lie algebra $L$, $X$ a left-invariant vector field on $G$ and $\hat{X}$ its Generalized Fourier Transform. Define by $dX^\lambda$ the differential of the representation $X^\lambda$:

\[
dX^\lambda(X) := \left. \frac{d}{dt} \right|_{t=0} X^\lambda(e^{tP}),
\]

where $X = gp$ ($p \in L$, $g \in G$). We have that $\hat{X}$ splits into the Hilbert sum of operators $\hat{X}^\lambda$, each of which acts on $\text{HS}^\lambda$. Moreover:

\[
\hat{X}^\lambda \Xi = dX^\lambda(X) \circ \Xi, \quad \forall \Xi \in \text{HS}^\lambda,
\]  \tag{10}

which means that $\hat{X}^\lambda$ acts as a left translation over $\text{HS}^\lambda$.

Let $\Delta_{sr}$ be the hypoelliptic Laplacian associated to a left-invariant sub-Riemannian manifold $(G, \Delta, g)$, and $\hat{\Delta}_{sr}$ its Generalized Fourier Transform. Denote by $(t, g) \mapsto p_t(g)$ the hypoelliptic heat kernel. The main result of [1] is the following theorem.

**Theorem 5.** Let $G$ be a unimodular Lie group of type I, and $(G, \Delta, g)$ a left-invariant sub-Riemannian manifold generated by the orthonormal basis $\{p_1, \ldots, p_m\}$. Our intrinsic hypoelliptic Laplacian is therefore $\Delta_{sr} = \sum_{i=1}^m L_{X_i}^2$, where $X_i = gp_i$. Let $\{X^\lambda\}_{\lambda \in \hat{G}}$ be the set of non-equivalent irreducible unitary representations of the group $G$, each acting on the Hilbert space $\mathcal{H}^\lambda$, and $dP(\lambda)$ the Plancherel measure on $\hat{G}$. We have the following:

(i) The Generalized Fourier Transform of $\Delta_{sr}$, $\hat{\Delta}_{sr} = \mathcal{F}\Delta_{sr}\mathcal{F}^{-1}$, splits into the Hilbert sum of operators $\hat{\Delta}_{sr}^\lambda$, each one of which leaves $\mathcal{H}^\lambda$ invariant:

\[
\hat{\Delta}_{sr} = \int_{\hat{G}} \hat{\Delta}_{sr}^\lambda, \quad \text{where} \quad \hat{\Delta}_{sr}^\lambda = \sum_{i=1}^m (\hat{X}_i^\lambda)^2.
\]
(ii) The operator $\hat{\Delta}_{sr}^\lambda$ is self-adjoint and is the infinitesimal generator of a contraction semigroup $e^{t\hat{\Delta}_{sr}^\lambda}$ over $\mathcal{HS}^\lambda$, i.e., $e^{t\hat{\Delta}_{sr}^\lambda} \Xi^\lambda_0$ is the solution for $t > 0$ to the operator equation $\partial_t \Xi^\lambda(t) = \hat{\Delta}_{sr}^\lambda \Xi^\lambda(t)$ in $\mathcal{HS}^\lambda$, with initial condition $\Xi^\lambda(0) = \Xi^\lambda_0$.

(iii) The hypoelliptic heat kernel is given by

$$p_t(g) = \int_{\hat{G}} \text{Tr}(e^{t\hat{\Delta}_{sr}^\lambda} X^\lambda(g)) \, dP(\lambda), \quad t > 0.$$  

In the case where for each $t > 0$ and each $\lambda \in \hat{G}$, $e^{t\hat{\Delta}_{sr}^\lambda}$ is an integral operator with integral kernel $Q_t^\lambda(\cdot, \cdot)$, we have the following corollary:

**Corollary 1.** Under the hypotheses of Theorem 5, if for all $\lambda \in \hat{G}$ we have $\mathcal{H}^\lambda = L^2(X^\lambda, d\theta^\lambda)$ for some measure space $(X^\lambda, d\theta^\lambda)$, and

$$[e^{t\hat{\Delta}_{sr}^\lambda} f^\lambda](\theta) = \int_{X^\lambda} f^\lambda(\bar{\theta}) Q_t^\lambda(\theta, \bar{\theta}) \, d\bar{\theta}$$

then

$$p_t(g) = \int_{\hat{G}} \int_{X^\lambda} X^\lambda(g) Q_t^\lambda(\theta, \bar{\theta})|_{\theta = \bar{\theta}} \, d\bar{\theta} \, dP(\lambda).$$  

In the next section we will focus on the semigroup $e^{t\hat{\Delta}_{sr}^\lambda}$ generated by the Fourier transformed hypoelliptic Laplacian, and for which, by formula (11), we need an expression in order to compute the heat kernel. In the case where this semigroup is intractable but where $\hat{\Delta}_{sr}^\lambda$ is the formal sum of two operators, we suggest an approach to approximate it with a simpler semigroup while preserving the short-time behaviour.

### 3. Short-time behaviour of the hypoelliptic heat kernel

#### 3.1. Semigroups of operators

We first recall the definition of a strongly continuous semigroup [14].

**Definition 8.** Let $(T(t))_{t \geq 0}$ be a family of bounded linear operators on a Banach space $X$, indexed by $t \in \mathbb{R}^+$. We will say that $(T(t))_{t \geq 0}$ is a strongly continuous semigroup of operators if the following conditions are verified:

1. $T(t)T(s) = T(t+s)$, $\forall t, s \in \mathbb{R}^+$,
2. $T(0) = \text{Id}$,
3. The map:

$$\mathbb{R}^+ \to X,$$

$$t \mapsto T(t)x$$

is continuous $\forall x \in X$. 

The generator of a semigroup $T(t)$ is the operator $A$ defined by
\[ Ax := \lim_{t \to 0} \frac{T(t)x - x}{t}, \]
for all $x \in X$ for which this limit exists; the domain of this operator is naturally defined as
\[ D(A) = \left\{ x \in X \mid \lim_{t \to 0} \frac{T(t)x - x}{t} \text{ exists} \right\}. \]

Consistent with the notation adopted for Theorem 5 and Corollary 1, we will denote the semigroup $(T(t))_{t \geq 0}$ generated by the operator $A$ by $e^{tA}$.

We now recall certain notions of functional analysis that will be used in the next section. Let $A$ be a linear, non-necessarily bounded operator on a Hilbert space $H$ with inner product $(\cdot, \cdot)$, and let $D(A)$ be the domain of $A$, i.e. the subspace of $H$ on which $A$ is defined.

**Definition 9.** We say that the operator $A$ is positive if:
\[ (Au, u) \geq 0, \quad \forall u \in D(A). \]
(We can also say that $-A$ is dissipative). We say that $A$ is symmetric if:
\[ (Au, v) = (u, Av), \quad \forall u, v \in D(A), \]
which means that $D(A) \subset D(A^*)$ and that $A$ and $A^*$ agree on $D(A)$. When $D(A) = D(A^*)$ (and therefore $A = A^*$), we will say that $A$ is self-adjoint.

Finally we say that $A$ is essentially self-adjoint if $A$ is closable and $\tilde{A} = A^*$, or equivalently if $A$ has a unique self-adjoint extension.

### 3.2. Trotter product formula

We now consider the case where an arbitrary operator $C$ can be expressed as the sum of two operators:
\[ C := A + B. \]

The following well-known theorem relates the semigroup generated by $C$ to those generated by $A$ and $B$ (see [14]):

**Theorem 6 (Trotter product formula).** Let $(T(t))_{t \geq 0}$ and $(S(t))_{t \geq 0}$ be strongly continuous semigroups on a Banach space $X$ satisfying the stability condition
\[ \left\| T(t/n)S(t/n) \right\|^n \leq Me^{w^t}, \quad \forall t \geq 0, \ n \in \mathbb{N}, \quad (13) \]
and for constants $M \geq 1$, $w \in \mathbb{R}$. Consider the sum $A + B$ on $D := D(A) \cap D(B)$ of the generators $(A, D(A))$ of $(T(t))_{t \geq 0}$ and $(B, D(B))$ of $(S(t))_{t \geq 0}$, and assume that $D$ and $(\lambda_0 - A - B)D$
are dense in \( X \) for some \( \lambda_0 \geq w \). Then: \( C := A + B \) generates a strongly continuous semigroup \((U(t))_{t \geq 0}\) given by the Trotter product formula

\[
U(t)x = \lim_{n \to \infty} [T(t/n)S(t/n)]^n x, \quad (14)
\]

with uniform convergence for \( t \) in compact intervals.

There exists another very useful version of the Trotter product formula, for the case of non-negative self-adjoint operators. It is often referred to as Kato’s strong Trotter product formula, and is proved in [20]:

**Theorem 7.** (See Kato [20].) Let \( A, B \) be non-negative self-adjoint operators on a Hilbert space \( H \). Let \( D' = D(A^{1/2}) \cap D(B^{1/2}) \), \( H' \) the closure of \( D' \), and \( P' \) the orthogonal projection of \( H \) onto \( H' \). We define the form sum of \( A, B \):

\[
C' = A + B
\]

as the self-adjoint operator in \( H' \) associated with the non-negative, closed quadratic form:

\[
u \mapsto \|A^{1/2}u\|^2 + \|B^{1/2}u\|^2
\]

which is densely defined in \( H' \). Then:

\[
\lim_{n \to \infty} \left[ e^{-(t/n)A}e^{-(t/n)B} \right]^n = e^{-tC'} P', \quad t > 0,
\]

the convergence being uniform in \( t \in [0, T] \) for any \( t > 0 \) when applied to \( u \in H' \), and in \( t \in [T_0, T] \) for any \( 0 < T_0 < T \) when applied to \( u \perp H' \).

Note that if \( D(A^{1/2}) \cap D(B^{1/2}) \) is dense in \( H \), then \( H' = H \) and \( P' \) is the identity operator; hence, in that particular case, Eq. (15) yields Eq. (14).

### 3.3. Short-time behaviour of semigroups associated to sums of operators

Although the limit \( \lim_{n \to \infty} [T(t/n)S(t/n)]^n \) appearing in Theorems 6 and 7, that is, the semigroup generated by \( C \), is often difficult to compute, a principal part for it can nevertheless be obtained. This is the subject of our proposition.

**Proposition 3.** Let \((S(t))_{t \geq 0}\) and \((T(t))_{t \geq 0}\) be two strongly continuous contraction semigroups on a Banach space \( L^p(\Omega) \) or \( C_0(\Omega) \), for \( \Omega \) a locally compact space, and \( 1 \leq p < \infty \). Suppose that these semigroups verify the conditions of Theorem 6, or of Theorem 7 with the additional assumption that \( H' = H \). Denote by \((A, D(A))\) and \((B, D(B))\) the respective infinitesimal generators of our two semigroups, and by \( C \) the formal sum of those operators, which we consider on \( D = D(A) \cap D(B) \). Assume that \( B, S(t) \) and \( T(t) \) are such that for any compact \( K \subset \Omega \), there exists a constant \( \alpha_K \) such that for all \( f \in C^K_\infty(\Omega) \) with support in \( K \), and every operator \( E \)
that is a composition of the operators $B, T(t)$ and $S(t)$: $\|Ef\|_1 \leq \alpha_k^k \|f\|_1$, where $k$ is the number of times the operator $B$ appears in $E$. Then $C$ generates a strongly continuous semigroup $(U(t))_{t \geq 0}$, which has the following short-time asymptotic:

$$U(t) f = T(t) f + \lim_{n \to \infty} \frac{t}{n} \left[ T(\frac{t}{n})^n B + T(\frac{t}{n})^{n-1} BT(\frac{t}{n}) + \cdots + T(\frac{t}{n}) BT(\frac{t}{n})^{n-1} \right] f + O(t^2) f,$$

where by $O(t^2) f$ we mean an operator $D_t$ acting on $f$, such that $\|D_t f\|_1 \leq Mt^2 \|f\|_1$ for a constant $M$ and for $t$ small enough.

It will be sufficient to prove Eq. (16) for functions $f \in C^\infty_c(\Omega)$, since $C^\infty_c(\Omega)$ is dense in both $C_0(\Omega)$ and $L^p(\Omega)$, $1 \leq p < \infty$. We will need a version of Taylor’s theorem with remainder for strongly continuous semigroups of operators (for more details see Sections 11.6–11.8 in [17]).

**Theorem 8.** Let $(T(t))_{t \geq 0}$ be a strongly continuous semigroup of bounded linear operators on a Banach space $X$, with corresponding infinitesimal generator $A$. Then for all $x \in D(A^n)$, and for all $t > 0$,

$$T(t)x = \sum_{k=0}^{m-1} \frac{t^k}{k!} A^k x + \frac{1}{(m-1)!} \int_0^t (t-s)^{m-1} T(s) A^m x \, ds, \quad \forall m \geq 1, \forall x \in X. \quad (17)$$

Notice that if $(T(t))_{t \geq 0}$ is a multiplication semigroup on $L^p(\mathbb{R})$, i.e. there is a function $p$ such that $[T(t)f](s) = e^{p(s)} f(s)$, with infinitesimal generator $A$: $[Af](s) = p(s) f(s)$, then Theorem 8 is nothing other than the classic Taylor’s theorem for $n$ times differentiable functions, with remainder in integral form.

We can use the mean value theorem to transform the remainder to a more convenient form. We have, $\forall f \in C^\infty_c(\Omega)$, and $\forall x \in D(A^n)$:

$$\frac{1}{(m-1)!} \int_0^t (t-s)^{m-1} T(s) A^m f(x) \, ds = \frac{1}{m!} t^m g(\xi, x)$$

$$= \frac{1}{m!} t^m T(\xi) A^m f(x), \quad \text{for a } \xi \in [0, t].$$

Note that $\xi$ is actually a function of $x$.

For $m = 2$, we therefore obtain $\forall f \in C^\infty_c(\Omega)$, and $\forall x \in D(A^n)$:

$$[T(t)f]x = f(x) + tAf(x) + \frac{t^2}{2} T(\xi) A^2 f(x), \quad \text{for a } \xi \in [0, t]. \quad (18)$$

We are now ready to prove Proposition 3.
Proof. Consider strongly continuous semigroups \((T(t))\) and \((S(t))\) that verify the assumptions of the theorem. Applying Trotter’s Product formula (Theorem 6), we obtain that the semigroup \((U(t))\) generated by the sum of the operators \(A\) and \(B\) verifies:

\[
U(t)f = \lim_{n \to \infty} \left[ T(t/n) S(t/n) \right]^n f, \quad \forall f \in C^\infty_C(\Omega).
\]

Applying Theorem 8 to our second semigroup \(S(t)\), with \(m = 2\), yields:

\[
S(t/n)f = f + \frac{t}{n} B f + \frac{1}{2} \left( \frac{t}{n} \right)^2 S(\xi_n) B^2 f, \quad \text{for a } \xi_n \in [0, t/n].
\]

Therefore, combining our two expressions, we obtain:

\[
U(t)f = \lim_{n \to \infty} \left[ T(t/n) \left[ I + (t/n)B + \frac{1}{2}(t/n)^2 S(\xi_n) B^2 \right] \right]^n f.
\]

Denote by \(K\) the compact support of a function \(f \in C^\infty_C(\Omega)\). Let us take a closer look at the composition of operators:

\[
\left( T(t/n) \left[ I + (t/n)B + \frac{1}{2}(t/n)^2 S(\xi_n) B^2 \right] \right)^n.
\]

We wish to express the resulting operator in the following form:

\[
D_0 + t D_1 + t^2 D_2 + \cdots + t^{2n} D_{2n},
\]

where the \(D_i, i \in \{0, \ldots, 2n\}\), are operators on the space of functions on which our original semigroups act, where \(D_0\) and \(D_1\) give the first two terms of Eq. (16) and with the remaining terms verifying:

\[
\left\| \lim_{n \to \infty} \left[ t^2 D_2 + \cdots + t^{2n} D_{2n} \right] f \right\|_1 \leqslant t^2 M \| f \|_1,
\]

for a constant \(M\), with \(t\) small enough and \(f \in C^\infty_C(\Omega)\) in our function space. We have in a straightforward way that \(D_0\) and \(D_1\) are given by:

\[
D_0 = T(t/n)^n, \quad D_1 = (1/n) \left[ T(t/n) BT(t/n)^{n-1} + \cdots + T(t/n)^n B \right].
\]

Notice that by using the Trotter product formula with \(S(t) \equiv \text{Id}, \forall t \geq 0\), we get that:

\[
\lim_{n \to \infty} T(t/n)^n f = T(t)f.
\]

Taking the limit \(n \to \infty\) in the expression therefore gives us the two first terms of Eq. (16).

For the remaining terms we will only need an upper bound, and we prove in Appendix A that:

\[
\| D_k f \|_1 \leqslant a_K^k \| f \|_1, \quad k \in \{0, 1, 2, \ldots, 2n\},
\]

for \(f \in C^\infty_C(\Omega)\) with support in a compact set \(K\). Using this we obtain:
\[\left\| \lim_{n \to \infty} \left[ t^2 D_2 + \cdots + t^{2n} D_{2n} \right] f \right\|_1 \leq \lim_{n \to \infty} \left[ t^2 \tilde{\alpha}_K^2 + \cdots + t^{2n} \tilde{\alpha}_K^{2n} \right] \| f \|_1 \]
\[= t^2 \sum_{k=0}^{\infty} (t \tilde{\alpha}_K)^k \| f \|_1 \]
\[= t^2 M \| f \|_1 \]

when \( t \) is small enough so that \( t \tilde{\alpha}_K \leq 1 \), and where \( M \) is the value of that infinite series. This concludes the proof of the proposition.

We now wish to bring back these technical results into the context of sub-Riemannian geometry. Consider a left-invariant sub-Riemannian manifold \((G, \Delta, g)\), and as usual denote by \(\Delta_{sr}\) the associated hypoelliptic Laplacian and by \(\hat{\Delta}_{sr}^\lambda\) its Generalized Fourier Transform, where \(\lambda\) indexes the elements of the dual \(\hat{G}\). We define a list \((L)\) of assumptions on this left-invariant sub-Riemannian manifold:

**Assumption 1.** For each \(\lambda\), the Transformed hypoelliptic Laplacian decomposes as a sum of two operators:

\[\hat{\Delta}_{sr}^\lambda = A^\lambda + B^\lambda.\]

**Assumption 2.** The operators \(A^\lambda\) and \(B^\lambda\) generate strongly semigroups \((T^\lambda(t))_{t \geq 0}\) and \((S^\lambda(t))_{t \geq 0}\) that verify the conditions of Proposition 3.

**Assumption 3.** For each \(t \geq 0\), \(T^\lambda(t)\) is an integral operator with kernel \(k^\lambda_t(s, r)\):

\[\left[ T^\lambda(t) f \right](s) = \int_{\Omega_\lambda} k^\lambda_t(s, r) f(r) \, dr.\]

**Assumption 4.** There exists an integrable function \(K^\lambda_{t/n}(s, r)\), uniformly bounded in \(s\) by an integrable function \(G^\lambda_t(s, r)\) for all \(n \geq 1\), such that:

\[(t/n) \left[ T^\lambda(t/n)^n B^\lambda + T^\lambda(t/n)^n B^\lambda T^\lambda(t/n) + \cdots + T^\lambda(t/n) B^\lambda T^\lambda(t/n)^{n-1} \right] f(s)\]
\[= t \int_{\Omega_\lambda} K^\lambda_{t/n}(s, r) f(r) \, dr.\]

We are now ready to prove Theorem 1:

**Proof.** Let \(G\) be a unimodular Lie group of type I, and \((G, \Delta, g)\) a left-invariant sub-Riemannian manifold verifying the conditions stated above as well as all the assumptions of \((L)\). From the Assumptions 1 and 2, we deduce that for every \(\lambda \in \hat{G}\), the short-time asymptotic of the semigroup generated by the operator \(\hat{\Delta}_{sr}\) is given by Eq. (16) of Proposition 3. The first term of Eq. (1) is a direct consequence of Assumption 3, whereas Assumption 4 enables us to use the Dominated Convergence Theorem in order to obtain the second term. \(\Box\)
Theorem 1 gives the following expression for the short-time behaviour of the semigroup generated by the transformed sub-Laplacian:

\[
\left[ e^{t \hat{\Delta}_{\lambda}^{\mathcal{K}}} f \right](s) = \int_{\Omega_{\lambda}} \left[ k^\lambda_t(s, r) + t \lim_{n \to \infty} K^\lambda_{t/n}(s, r) \right] f(r) \, dr + \mathcal{O}(t^2) f(s). \tag{19}
\]

To compute the corresponding integral kernel, consider a sequence of functions \( f_n \) with \( L^1 \) norm equal to 1, and such that \( \lim_{n \to \infty} f_n = \delta_r \) where \( \delta_r \) denotes the Dirac distribution at the point \( r \). Letting the operator \( e^{t \hat{\Delta}_{\lambda}^{\mathcal{K}}} \) act on this sequence and letting \( n \) go to \( \infty \), we obtain the value of the integral kernel of this operator at the point \( r \):

\[
Q^\lambda_t(s, r) = \tilde{Q}^\lambda_t(s, r) + \mathcal{O}(t^2), \tag{20}
\]

where

\[
\tilde{Q}^\lambda_t(s, r) = k^\lambda_t(s, r) + t \lim_{n \to \infty} K^\lambda_{t/n}(s, r). \tag{21}
\]

In Eq. (20), \( \mathcal{O}(t^2) \) denotes a function or distribution such that when integrated against a test function, it is an operator of order \( \mathcal{O}(t^2) \) as defined in Theorem 1. It follows from Corollary 1 that

\[
p_t(g) = \int_{\hat{G}} \int_{X^\lambda} \mathcal{X}^\lambda(g) \left[ \tilde{Q}^\lambda_t(s, r) + \mathcal{O}(t^2) \right] \bigg|_{s=r} \, dr \, dP(\lambda). \tag{22}
\]

It would be tempting to separate this integral into two, in order to have an expression of the form:

\[
p_t(g) = \int_{\hat{G}} \int_{X^\lambda} \mathcal{X}^\lambda(g) \tilde{Q}^\lambda_t(s, r) \big|_{s=r} \, dr \, dP(\lambda) + \int_{\hat{G}} \int_{X^\lambda} \mathcal{X}^\lambda(g) \mathcal{O}(t^2) \bigg|_{s=r} \, dr \, dP(\lambda),
\]

\[
\text{approximate heat kernel} \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad.
We now specialize our main theorem to the case where for each \( \lambda \) in the dual \( \hat{G} \), \( \mathcal{H}^\lambda \) is the Hilbert space \( L^2(\mathbb{R}) \), \( A^\lambda \) is the one-dimensional Laplacian:

\[
[A^\lambda f](x) = [\Delta f](x) = \frac{d^2}{dx^2} f(x),
\]

and \( B^\lambda \) is the multiplication operator:

\[
[B^\lambda f](x) = q^\lambda(x) f(x),
\]

where \( q^\lambda(x) \) is a negative polynomial depending on the parameter \( \lambda \), and for which there exists a polynomial \( p^\lambda(x) \) such that we can write:

\[
q^\lambda(x) = -p^\lambda(x)^2.
\]

Writing \( q^\lambda(x) \) in expanded form yields

\[
q^\lambda(x) = -\left[a_{2m}^\lambda x^{2m} + a_{2m-1}^\lambda x^{2m-1} + \cdots + a_1^\lambda x^1 + a_0^\lambda\right],
\]

where \( m \) is the degree of the polynomial \( p^\lambda(x) \), and \( a_{2m}^\lambda \) and \( a_0^\lambda \) are positive constants. We have:

**Corollary 2.** Let \( (G, \Delta, g) \) be a left-invariant sub-Riemannian manifold, with \( G \) a unimodular Lie group of type I. Denote by \( \Delta_{sr} \) the associated hypoelliptic Laplacian, and by \( \hat{\Delta}_{sr}^\lambda \) its Generalized Fourier Transform, where \( \lambda \) indexes the elements of the dual \( \hat{G} \). Assume that for all \( \lambda \), \( \hat{\Delta}_{sr}^\lambda = A^\lambda + B^\lambda \), for operators \( A^\lambda \) and \( B^\lambda \) in the form described above. Then, the conditions of Theorem 1 are verified, and the semigroup generated by the transformed hypoelliptic Laplacian has the following expression in small-time:

\[
[e^{t \hat{\Delta}_{sr}^\lambda} f](s) = \int \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{1}{4t}(s-r)^2\right) \left(1 - a_0^\lambda t - \sum_{k=1}^{2m} \frac{a_k^\lambda}{k+1} \sum_{i=0}^{k} s^{i,k-i}\right) f(r) \, dr
\]

\[
+ \left[ O(t^{3/2}) f \right](s), \quad \forall f \in C^\infty_c(\mathbb{R}).
\]

**Proof.** As our proof is independent of the element \( \lambda \) of the dual of \( G \), as well as to simplify the notation, we will consider \( \lambda \) fixed and we drop the indexing of the operators, functions and constants defined above. We first want to show that the operators \(-A\) and \(-B\) verify the assumptions of Theorem 7. To this end, we define the operators \( A' := -A = -\Delta \) and \( B' := -B \) on \( L^2(\mathbb{R}) \). Notice that the operators \( A' \) and \( B' \) are non-negative and symmetric. Indeed, for \( f, g \in C^\infty_c(\mathbb{R}) \):

\[
(-\Delta, g) = \int \Delta f(x) g(x) \, dx = \int \nabla f(x) \nabla g(x) \, dx = -\int f(x) \Delta g(x) \, dx = (f, -\Delta g),
\]

\[
(-\Delta, f) = \int -\Delta f(x) f(x) \, dx = \int |\nabla f(x)|^2 \, dx \geq 0.
\]
and the same is clearly true for the multiplication operator \( B' \) by a positive function. As a result, both \( A' \) and \( B' \) have a canonical self-adjoint extension, called the Friedrichs extension (for a detailed exposition of this notion, see Section II.5 of [27]). We can identify the two operators with their Friedrichs extension, and henceforth assume that they are self-adjoint. It follows that the corresponding semigroups verify the conditions of Theorem 7. We now compute the domains \( D(A'^{1/2}) \) and \( D(B'^{1/2}) \). We have that for \( f \in C^\infty_c(\mathbb{R}) \):

\[
\begin{align*}
(A'^{1/2} f, A'^{1/2} f) &= (A' f, f) = \int_\mathbb{R} |\nabla f(x)|^2 \, dx, \\
(B'^{1/2} f, B'^{1/2} f) &= (B' f, f) = \int_\mathbb{R} p(x)|f(x)|^2 \, dx
\end{align*}
\]

hence \( D(A'^{1/2}) = \{ f \in L^2(\mathbb{R}) \mid \nabla f \in L^2(\mathbb{R}) \} = H^1(\mathbb{R}) \) and similarly we find that \( D(B'^{1/2}) = \{ f \in L^2(\mathbb{R}) \mid pf \in L^2(\mathbb{R}) \} \). Hence we have \( C^\infty_c(\mathbb{R}) \subseteq D(A'^{1/2}) \cap D(B'^{1/2}) \), and as \( C^\infty_c(\mathbb{R}) \) is dense in \( L^2(\mathbb{R}) \) so is \( D' = D(A'^{1/2}) \cap D(B'^{1/2}) \). Therefore the closure \( H' \) of \( D' \) is equal to \( L^2(\mathbb{R}) \), and \( P' \) is just the identity operator. The semigroup associated to the 1-dimensional Euclidean Laplacian is the convolution semigroup given by

\[
T(t) f(s) = (4\pi t)^{-1/2} \int_{-\infty}^\infty e^{-\frac{(s-r)^2}{4t}} f(r) \, dr
\]  

(26)

and the semigroup associated with the multiplication operator \( B \) is given by

\[
S(t) f(s) = e^{-tp(s)^2} f(s).
\]  

(27)

We therefore have that \( S(t) \) and \( T(t) \) are contraction semigroups, and as \( B \) is a multiplication operator, then considering any function \( f \in C^\infty_c(\mathbb{R}) \) with support in a compact \( K \), there exists a constant \( \alpha_K \) such that any operator \( E \) which is a composition of operators \( S(t), T(t) \) and \( B \) verifies \( \| Ef \|_1 \leq \alpha_K \| f \|_1 \), where \( k \) is the number of times the operator \( B \) appears in \( E \) (in this case \( \alpha_K \) will in fact be the maximum of the function \( q \) on the compact set \( K \)). All the hypotheses of Proposition 3 are verified, and we only have to verify the additional conditions of Theorem 1.

We need to compute the sum:

\[
S_{t/n}(s_0) := \frac{t}{n} \left[ T(t/n)^n B + T(t/n)^{n-1} BT(t/n) + \cdots + T(t/n)BT(t/n)^{n-1} \right] f(s_0)
\]

which is in our case:

\[
S_{t/n}(s_0) = \frac{t}{n} \left( \frac{4\pi t}{n} \right)^{-n/2} \int_{\mathbb{R}^n} \cdots \int_{\mathbb{R}^n} \exp \left[ -\frac{n}{4t} (s_0 - s_1)^2 + (s_1 - s_2)^2 + \cdots + (s_{n-1} - s_n)^2 \right] \\
\times \left[ -p(s_1)^2 - p(s_2)^2 - \cdots - p(s_n)^2 \right] f(s_n) \, ds_n \, ds_{n-1} \cdots ds_1
\]

\[
= - \int_{-\infty}^{\infty} K_{n,t/n}(s_0, s_n) f(s_n) \, ds_n
\]
where
\[
K_{n,t/n}(s_0, s_n) = \frac{t}{n} \left( \frac{4\pi t}{n} \right)^{-n/2} \int_{\mathbb{R}^{n-1}} \prod_{s=1}^{n} \exp \left[ -\frac{n}{4t} \left( (s_0 - s_1)^2 + (s_1 - s_2)^2 + \cdots + (s_{n-1} - s_n)^2 \right) \right] 
\times \left[ p(s_1)^2 + p(s_2)^2 + \cdots + p(s_n)^2 \right] ds_{n-1} \ldots ds_1.
\]

In this last expression of the function $S_{t/n}$, Fubini’s theorem can be used to exchange the order of integration, which is justified as the integrand is the pointwise multiplication of a Schwartz function and a function in $L^2$. By the Cauchy–Schwarz inequality, the resulting function is in $L^1$.

The following lemma on the computation of $n$-dimensional Gaussian integral with linear term will be our main tool for most of the calculations of this paper:

**Lemma 1.** If $A$ is a symmetric positive-definite $n \times n$ matrix, and $\vec{b}$ an $n \times 1$ vector, the following equality is true:

\[
\int_{\mathbb{R}^n} \prod_{s=1}^{n} \exp \left( -\frac{1}{2} \vec{x}^T A \vec{x} + \vec{b}^T \vec{x} \right) d\vec{x} = \sqrt{\frac{(2\pi)^n}{\det A}} \exp (\vec{b}^T A^{-1} \vec{b}).
\]

Using the previous lemma, we can find a bound on our integral kernel; more precisely, $\forall n \in \mathbb{N}$:

\[
0 \leq K_{n,t/n}(s_0, s_n) \leq \left( \frac{4\pi t}{n} \right)^{-n/2} \int_{\mathbb{R}^{n-1}} \prod_{s=1}^{n} \exp \left[ -\frac{n}{4t} \left( (s_0 - s_1)^2 + (s_1 - s_2)^2 + \cdots + (s_{n-1} - s_n)^2 \right) \right] ds_{n-1} \ldots ds_1 
\]

\[
= \frac{1}{4\pi t} \exp \left[ -\frac{1}{2} (s_0 - s_n)^2 \right]
\]

(see Appendix B.1 for the explicit calculations). Therefore, we can use the Dominated Convergence Theorem and exchange the limit and the integral, to finally get:

\[
\lim_{n \to \infty} S_{t/n}(s_0) = \int_{-\infty}^{\infty} \left[ \lim_{n \to \infty} K_{n,t/n}(s_0, s_n) \right] f(s_n) ds_n \tag{28}
\]

We also have verified all the conditions of Theorem 1, and all that remains is the computation of the limit of the integral kernel $K_{n,t/n}(s_0, s_n)$ as $n \to \infty$,

\[
K_{n,t/n}(s_0, s_n) = \frac{t}{n} \left( \frac{4\pi t}{n} \right)^{-n/2} \exp \left[ -\frac{n}{4t} \left( s_0^2 + s_n^2 \right) \right]
\]
\[
\times \int_{\mathbb{R}^{n-1}} \cdots \int \exp \left[ -\frac{n}{2t} \left( s_1^2 + s_2^2 + \cdots + s_{n-1}^2 - s_0 s_1 - s_1 s_2 - \cdots - s_{n-1} s_n \right) \right] \\
\times \left[ \sum_{k=0}^{2m} a_k \sum_{i=1}^{n-1} s_i^k + p(s_n)^2 \right] ds_{n-1} \cdots ds_1.
\]

Since the terms in \( s_n \) or in \( a_0 \) can be taken out of the integral, we compute the following integrals:

\[
I_0(s_0, s_n) = \int_{\mathbb{R}^{n-1}} \cdots \int \exp \left[ -\frac{n}{2t} \left( \sum_{j=1}^{n-1} s_j^2 - s_0 s_1 - \cdots - s_{n-1} s_n \right) \right] ds_{n-1} \cdots ds_1,
\]

\[
I_{i,k}(s_0, s_n) = \int_{\mathbb{R}^{n-1}} \cdots \int \exp \left[ -\frac{n}{2t} \left( \sum_{j=1}^{n-1} s_j^2 - s_0 s_1 - \cdots - s_{n-1} s_n \right) \right] s_i^k ds_{n-1} \cdots ds_1,
\]

where \( i \in \{1, \ldots, n-1\}, k \in \{1, \ldots, 2m\} \).

**Proposition 4.** For \( i \in \{1, 2, \ldots, n-1\} \), the previous integrals are equal to:

\[
I_0(s_0, s_n) = \left( \frac{t}{n} \right)^{(n-1)/2} 2^{n-1} \pi^{(n-1)/2} \left( \frac{1}{4t} \left[ (n-1)s_0^2 + (n-1)s_n^2 + 2s_0 s_n \right] \right). \tag{29}
\]

\[
I_{i,k}(s_0, s_n) = I_0(s_0, s_n) \cdot \sum_{j=0}^{k} \frac{k!}{(k-j)! (j/2)!} \left( \frac{t}{n} \right)^{j/2} \left( \frac{1}{n} \right)^{j/2} \left( \frac{(n-i)s_0 + is_n}{n} \right)^{k-j}. \tag{30}
\]

**Proof.** See Appendix B. \( \square \)

All that is left to obtain Eq. (25) is to compute the sums over \( i \) of the integrals \( I_{i,k}(s_0, s_n) \); for these calculations, see Appendix C.

This completes the proof of the corollary.

4. Example of the Heisenberg group

In this section, we illustrate the main steps of the analysis developed in Section 3 on the canonical example of the Heisenberg group. The Heisenberg group has been studied extensively [22] and is the simplest non-trivial example of a left-invariant sub-Riemannian manifold. Furthermore, it is a step 2, 3-dimensional nilpotent Lie group, and its dual is well-known [11]. Its heat kernel has also been computed explicitly multiple times [16,19]. These properties will lead to simple calculations, as well as to a final approximation which can be compared to the exact formula.
4.1. The Heisenberg group $H_1$

The Heisenberg group is a unimodular Lie group and consists of the $3 \times 3$ upper-triangular matrices of the form

$$H_1 = \left\{ \begin{pmatrix} 1 & x & z + \frac{1}{2}xy \\ 0 & 1 & y \\ 0 & 0 & 1 \end{pmatrix} \bigg| x, y, z \in \mathbb{R} \right\},$$

with the usual matrix multiplication. We can identify the Heisenberg group with $\mathbb{R}^3$ in the following way:

$$(x, y, z) \sim \begin{pmatrix} 1 & x & z + \frac{1}{2}xy \\ 0 & 1 & y \\ 0 & 0 & 1 \end{pmatrix},$$

with the resulting multiplication law:

$$(a, b, c) \cdot (x, y, z) = \begin{pmatrix} 1 & x & z + \frac{1}{2}xy \\ 0 & 1 & y \\ 0 & 0 & 1 \end{pmatrix}.$$ (33)

We denote the identity element $(0, 0, 0)$ of $H_1$ by $\mathbf{0}$. We consider the rank 2 left-invariant sub-Riemannian structure on $H_1$ defined by the left-invariant vector fields

$$X_1 = \partial/\partial x - \frac{y}{2} \partial/\partial z,$$

$$X_2 = \partial/\partial y + \frac{x}{2} \partial/\partial z.$$

The hypoelliptic Laplacian is then given by:

$$\Delta_{sr} = X_1^2 + X_2^2,$$ (34)

with the vector fields $X_i$ identified with their Lie derivatives $L_{X_i}$.

4.2. Dual of $H_1$

The dual $\hat{H}_1$ of $H_1$ is given by [11]:

$$\hat{H}_1 = \mathbb{R}^2 \cup \{ \pi_\lambda : \lambda \neq 0 \},$$

with the one-dimensional representations $\chi_{a,b}(x, y, z) = e^{i(ax+by)}$ indexed by $\mathbb{R}^2$, and the representations $\pi_\lambda$, $\lambda \neq 0$, acting on the Hilbert space $L^2(\mathbb{R})$ in the following way:

$$[\pi_\lambda(x, y, z)\phi](\theta) = e^{2\pi i\lambda(z+xy/2-y\theta)}\phi(\theta - x).$$
The Plancherel measure has support on the set \( \{ \pi_{\lambda} \}_{\lambda \in \mathbb{R}^*} \) and is given on that set by \( |\lambda| \, d\lambda \) [11]. Moreover, for every \( \lambda \in \mathbb{R}^* \) and \( f \in \mathcal{S}(H_1) \), we have that \( \pi_{\lambda}(f) \) is a Hilbert–Schmidt operator:

\[
\int_{\mathbb{R}^*} \| \pi_{\lambda}(f) \|_{H_1}^2 |\lambda| \, d\lambda = \int_{H_1} |f(h)|^2 \, dh.
\]  

(36)

4.3. The Generalized Fourier Transform of the hypoelliptic Laplacian on \( H_1 \)

To compute the Generalized Fourier Transform of the hypoelliptic Laplacian on \( H_1 \), we need only compute the operators \( \hat{X}_{i}^\lambda \), where \( \lambda \in \mathbb{R}^* \) indexes the representations \( \pi_{\lambda} \).

Note that from Proposition 2, we can identity \( \hat{X}_{i}^\lambda \) with the operator \( d \pi_{\lambda}(X_i) \) on the representation space \( L^2(\mathbb{R}) \) of \( \pi_{\lambda} \), for \( i = 1, 2 \). Letting \( p_1 = X_1(0) \) and \( p_2 = X_2(0) \), we compute, for \( \psi \in L^2(\mathbb{R}) \),

\[
[\hat{X}_{1}^\lambda \psi](\theta) = \frac{d}{dt} \Big|_{t=0} \left[ \pi_{\lambda}(e^{tp_1}) \psi \right](\theta) = \frac{d}{d\theta} \psi(\theta),
\]

and

\[
[\hat{X}_{2}^\lambda \psi](\theta) = \frac{d}{dt} \Big|_{t=0} \left[ \pi_{\lambda}(e^{tp_2}) \psi \right](\theta) = -i\lambda \theta \psi(\theta).
\]

The Generalized Fourier Transform of the hypoelliptic Laplacian on \( H_1 \) is then:

\[
[\hat{\Delta}_{sr}^\lambda \psi](\theta) = \left[ \frac{d^2}{d\theta^2} - \lambda^2 \theta^2 \right] \psi(\theta).
\]

(37)

4.4. Approximation of the semigroups \( e^{t\hat{\Delta}_{sr}^\lambda} \)

We now follow the approach developed in Section 3 to find an approximation in small-time of the semigroups \( e^{t\hat{\Delta}_{sr}^\lambda} \). We begin by separating the operator \( \hat{\Delta}_{sr}^\lambda \) in the most natural way:

\[
\hat{\Delta}_{sr}^\lambda = A^\lambda + B^\lambda,
\]

where \( A^\lambda \psi(\theta) = \frac{d^2}{d\theta^2} \psi(\theta) \) and \( B^\lambda \psi(\theta) = -\lambda^2 \theta^2 \psi(\theta) \). Applying Corollary 2 with \( a_0^\lambda = a_1^\lambda = 0 \), and \( a_2^\lambda = \lambda^2 \) yields the following expression for the operator \( e^{t\hat{\Delta}_{sr}^\lambda} \):

\[
\left[ e^{t\hat{\Delta}_{sr}^\lambda} f \right](s) = \int_{\mathbb{R}} \frac{1}{\sqrt{4\pi t}} \exp \left( -\frac{1}{4t}(s-r)^2 \right) \left( 1 - i\frac{\lambda^2}{3} (s^2 + sr + r^2) \right) f(r) \, dr \\
+ \left[ \mathcal{O} (r^{3/2}) f \right](s).
\]
The integral kernel of the operator $e^{t\hat{\Delta}_{\lambda}}$ is therefore given by

$$Q_t^\lambda(s, r) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{1}{4t}(s - r)^2\right) \left(1 - t \frac{\lambda^2}{3} (s^2 + sr + r^2)\right) + O(t^{3/2}), \quad (38)$$

which, since $\frac{1}{\sqrt{4\pi t}} \exp(-\frac{1}{4t}(s - r)^2) = O(t^{-1/2})$ and $O(t^{-1/2})O(t^2) = O(t^{3/2})$ we can equivalently write as

$$Q_t^\lambda(s, r) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{1}{4t}(s - r)^2\right) \left(1 - t \frac{\lambda^2}{3} (s^2 + sr + r^2)\right) + O(t^2). \quad (39)$$

4.5. Small-time behaviour of the hypoelliptic heat kernel on $H_1$

Combining now this expression with Corollary 1, we can formally compute for an element $g = (x, y, z) \in H_1$:

$$p_t(g) = \int_{\hat{\gamma}} \int_{\mathbb{R}} \pi_\lambda(g) Q_t^\lambda(s, r)|_{s=r} \, dr \, dP(\lambda)$$

$$= \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right) \int_{\mathbb{R}^*} e^{i\lambda(z + \frac{iy}{2})} \int_{\mathbb{R}} e^{-i\lambda y r} \left(1 - t \frac{\lambda^2}{3} (3r^2 - 3xr + x^2) + O(t^2)\right) |\lambda| \, dr \, d\lambda.$$

The change of variables $(r - \frac{1}{2}x) \mapsto r$, gives the simpler expression

$$p_t(g) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right) \int_{\mathbb{R}^*} e^{i\lambda z} \int_{\mathbb{R}} e^{-i\lambda y r} \left(1 - t \frac{\lambda^2}{12} x^2 - t \lambda^2 r^2 + O(t^2)\right) |\lambda| \, dr \, d\lambda.$$

Note now that the equality:

$$1 - t \frac{\lambda^2}{12} x^2 - t \lambda^2 r^2 = \exp\left(-t\lambda^2\left(\frac{x^2}{12} + r^2\right)\right) + O(t^2) \quad (40)$$

would suggest the choice of

$$R_t^\lambda(g, r) = \exp\left(-t\lambda^2\left(\frac{x^2}{12} + r^2\right)\right)$$

in order to obtain a small-time approximation to $p_t$ (see discussion following the proof of Theorem 1). This yields

$$p_t(g) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right) \int_{\mathbb{R}^*} e^{i\lambda z} \int_{\mathbb{R}} e^{-i\lambda y r} \left[\exp\left(-t\lambda^2\left(\frac{x^2}{12} + r^2\right)\right) + O(t^2)\right] |\lambda| \, dr \, d\lambda.$$
Furthermore, \( \forall t > 0 \), the function

\[
g = (x, y, z) \mapsto \tilde{p}_t(g)
\]

is defined and \( C^\infty \) only on \( H_1 \setminus \{ x = 0 \} \) (due to the integrand being rapidly decreasing in that region). Since, by hypoellipticity of \( \Delta_{sr} \), \( p_t \) is \( C^\infty \) on \( H_1 \), it follows that we can write \( p_t \) as the sum

\[
p_t = \tilde{p}_t + r_t,
\]

where \( r_t = p_t - \tilde{p}_t \) is necessarily also \( C^\infty \) on \( H_1 \setminus \{ x = 0 \} \). A computation yields:

\[
\tilde{p}_t(g) = \frac{\sqrt{3\pi}}{t^{3/2}|x|} \exp \left( -\frac{x^2 + y^2}{4t} \right) \exp \left( -\frac{3z^2}{2tx} \right),
\]

whereas the remainder term can be simplified, using the equalities \( t^2 \mathcal{O}(1) = \mathcal{O}(t^2) \) and \( \mathcal{O}(t^{-1/2})\mathcal{O}(t^2) = \mathcal{O}(t^{3/2}) \) to yield:

\[
r_t(g) = \frac{1}{\sqrt{4\pi t}} \exp \left( -\frac{x^2}{4t} \right) \int_{\mathbb{R}^*} e^{i\lambda z} \int_{\mathbb{R}} e^{-i\lambda yr} \mathcal{O}(r^2) |\lambda| \, dr \, d\lambda.
\]

\[
= \mathcal{O}(t^{3/2}).
\]

It is important to note that the short-time estimate \( \tilde{p}_t \) of the hypoelliptic heat kernel \( p_t \) obtained on \( H_1 \setminus \{ x = 0 \} \) is not symmetric in \( x \) and \( y \) and hence does not reflect the \( SO(2) \) symmetry of \( \Delta_{sr} \). To remedy this, we could start instead from the equality

\[
1 - t \frac{\lambda^2}{12} x^2 - t \lambda^2 r^2 = \exp \left( -t \frac{\lambda^2 x^2}{12} - \frac{3t \lambda^2}{t^2 \lambda^2 + 3} r^2 \right) + \mathcal{O}(t^3);
\]

we obtain \( p_t = \tilde{p}_t + r_t \), with

\[
\tilde{p}_t(g) = \frac{1}{2t} \exp \left( -\frac{x^2 + y^2}{4t} \right) \int_{\mathbb{R}^*} e^{i\lambda z} \sqrt{1 + \frac{t^2 \lambda^2}{3} \exp \left( -t \frac{\lambda^2 x^2 + y^2}{12} \right)} \, d\lambda
\]

\[
= \frac{1}{t^2} \exp \left( -\frac{x^2 + y^2}{4t} \right) \int_{\mathbb{R}^*} \exp \left( -\frac{(x^2 + y^2)\tau^2}{3t} \right) \sqrt{1 + \frac{4\tau^2}{3} \cos \left( \frac{2\pi z}{t} \right)} \, d\tau.
\]

This last expression has the \( SO(2) \) symmetry of the hypoelliptic Laplacian and is defined and \( C^\infty \) on \( H_1 \setminus \{ x^2 + y^2 = 0 \} \). This estimate is therefore valid on a larger domain than the previous one. It is interesting to note that this domain is in fact the complement of the cut locus of the origin.
(see for example [16]). Note finally, for comparison, that the exact expression of the hypoelliptic heat kernel on $H_1$ is given by [1]:

$$p_t(g) = \frac{1}{(2\pi t)^2} \int_{\mathbb{R}} \frac{2\tau}{\sinh(2\tau)} \exp \left( \frac{-\tau(x^2 + y^2)}{2t \tanh(2\tau)} \right) \cos \left( \frac{2\tau z}{t} \right) d\tau.$$ \hspace{1cm} (42)

5. Application to the Engel and Cartan groups: the quartic oscillator

We now apply Theorem 1 to the study of the hypoelliptic heat kernel on the Engel and the Cartan groups, thereby continuing the work in [6]. We first recall the structure of those groups:

5.1. Structure of the Lie groups

Denote the Engel group by $G_4$. Its Lie algebra $L_4 = \text{span}\{l_1, l_2, l_3, l_4\}$ has generators verifying the following bracket relations:

$$[l_1, l_2] = l_3, \quad [l_1, l_3] = l_4, \quad [l_2, l_3] = [l_3, l_4] = [l_1, l_4] = [l_2, l_4] = 0.$$ 

This Lie algebra is therefore nilpotent of step 3, and through the exponential map we obtain a step 3 nilpotent Lie group. We endow $G_4$ with a left-invariant sub-Riemannian structure generated by the subset $p = \text{span}\{l_1, l_2\}$, which is clearly bracket-generating. It is easily seen that the resulting distribution is regular and has growth vector $(2, 3, 4)$. $G_4$ can be represented in matrix notation, and can be identified with $\mathbb{R}^4$, but we will not detail this in the present paper (see for example [6]). Since it is nilpotent it is unimodular, and we can therefore use Theorem 5. We will recall the necessary steps leading to the computation of short-time behaviour of the heat kernel.

Similarly, denote by $G_5$ the Cartan group, which is defined to be the free nilpotent group with Lie algebra $L_5 = \text{span}\{l_1, l_2, l_3, l_4, l_5\}$, with generators verifying the following bracket relations:

$$[l_1, l_2] = l_3, \quad [l_1, l_3] = l_4, \quad [l_2, l_3] = l_5,$$ 

all the other brackets being equal to 0. It is easy to see that $G_5$ is step 3 nilpotent. In a similar fashion as for $G_4$, we know that the distribution generated by $p = \text{span}\{l_1, l_2\}$ is regular, and has growth vector $(2, 3, 5)$. Also, $G_5$ is isomorphic to $\mathbb{R}^5$ on which we define a new operation, but we will not make this isomorphism explicit here (see [6]).

The following proposition describes the dual of both the Engel and the Cartan groups, and is due to Dixmier [12].

**Proposition 5.** (See Dixmier [12].)

1. The dual space of the group $G_4$ is $\hat{G}_4 = \{ \mathcal{X}^{\lambda, \mu} \mid \lambda \neq 0, \mu \in \mathbb{R} \}$ where each representation $\mathcal{X}^{\lambda, \mu}$ acts on the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$ endowed with the standard inner product $\langle f_1, f_2 \rangle := \int_{\mathbb{R}} f_1(\theta) \overline{f_2(\theta)} d\theta$ and acts in the following way:
\[ \mathcal{H} \to \mathcal{H}, \]
\[ X^{\lambda, \mu}(x_1, x_2, x_3, x_4) : \phi(\theta) \mapsto \exp \left( i \left( -\frac{\mu}{2\lambda} x_1 + \lambda x_4 - \lambda x_3 \theta + \frac{\lambda}{2} x_2 \theta^2 \right) \right) \phi(\theta + x_1). \]

The Plancherel measure on \( G_4 \) is the Lebesgue measure on \( \mathbb{R}^2 \): \( dP(\lambda, \mu) = d\lambda \, d\mu \).

2. The dual space of the group \( G_5 \) is \( \hat{G}_5 = \{ X^{\lambda, \mu, \nu} : \lambda^2 + \mu^2 \neq 0, \nu \in \mathbb{R} \} \), where the representations \( X^{\lambda, \mu, \nu} \) all have representation space \( \mathcal{H} = L^2(\mathbb{R}) \), and act in the following way:

\[ \mathcal{H} \to \mathcal{H}, \]
\[ X^{\lambda, \mu, \nu}(x_1, x_2, x_3, x_4, x_5) : \phi(\theta) \mapsto \exp \left( i A^{\lambda, \mu, \nu}_{x_1, x_2, x_3, x_4, x_5}(\theta) \right) \phi \left( \theta + \frac{\lambda x_1 + \mu x_2}{\lambda^2 + \mu^2} \right), \]

with
\[
A^{\lambda, \mu, \nu}_{x_1, x_2, x_3, x_4, x_5}(\theta) = -\frac{1}{2} \frac{\nu}{\lambda^2 + \mu^2} (\mu x_1 - \lambda x_2) + \lambda x_4 + \mu x_5
- \frac{1}{6} \frac{\mu}{\lambda^2 + \mu^2} \left( \lambda^2 x_3^2 + 3 \lambda \mu x_1 x_2 + 3 \mu^2 x_1 x_2^2 - \lambda \mu x_3^2 \right)
+ (\lambda^2 + \mu^2) x_3 \theta + \mu x_1 x_2 \theta + \lambda \mu (x_1^2 - x_2^2) \theta
+ \frac{1}{2} (\lambda^2 + \mu^2) (\mu x_1 - \lambda x_2) \theta^2.
\]

The Plancherel measure on \( G_5 \) is the Lebesgue measure on \( \mathbb{R}^3 \): \( dP(\lambda, \mu, \nu) = d\lambda \, d\mu \, dv \).

5.2. Principal part for the hypoelliptic heat kernel

For both groups, we consider the sub-Laplacian \( \Delta_{sr} = X_1^2 + X_2^2 \). In the case of the Engel group, we have:

\[
X_1(x) = \frac{\partial}{\partial x_1} \quad \implies \quad [dX_1^{\lambda, \mu} \phi](\theta) = \frac{d}{d\theta} \phi(\theta),
\]
\[
X_2(x) = \frac{\partial}{\partial x_2} - x_1 \frac{\partial}{\partial x_3} + \frac{x_1^2}{2} \frac{\partial}{\partial x_3} \quad \implies \quad [dX_2^{\lambda, \mu} \phi](\theta) = \left( -\frac{i}{2} \frac{\mu}{\lambda} + \frac{i}{2} \lambda \theta^2 \right) \phi(\theta),
\]

where \( x = (x_1, x_2, x_3, x_4) \). We therefore obtain the General Fourier transform of our sub-Laplacian:

\[
\hat{\Delta}_{sr}^{\lambda, \mu} f(\theta) = \left( \frac{d^2}{d\theta^2} - \frac{1}{4} \left( \lambda \theta^2 - \frac{\mu}{\lambda} \right)^2 \right) f(\theta).
\]

(43)

This operator is the Laplacian with quartic potential (also called the quartic oscillator), and its associated evolution equation is, to our knowledge, not solvable. We will now give a proof of Theorem 2, which consists in an expression in small-time of the fundamental solution of the heat equation associated to \( \Delta_{sr} \).
Proof. The Engel group endowed with the sub-Riemannian structure we defined is a left-invariant sub-Riemannian manifold verifying the conditions of Corollary 2, with \((\lambda, \mu)\) indexing the elements of the dual and:

\[
m = 2, \quad a_0^{\lambda, \mu} = \left(\frac{\mu}{2\lambda}\right)^2, \quad a_2^{\lambda, \mu} = -\frac{\mu}{2}, \quad a_4^{\lambda, \mu} = \frac{\lambda^2}{4}, \quad a_1^{\lambda, \mu} = a_3^{\lambda, \mu} = 0.
\]

Let us denote by \(Q_t^{\lambda, \mu}(s, r)\) the integral kernel of the operator \(e^{t\tilde{\Delta}^{\lambda, \mu}_t}\), for which as we said no expression is known, but of which Corollary 2 gives us the behaviour in short-time:

\[
\left[e^{t\tilde{\Delta}^{\lambda, \mu}_t} f\right](s) = \int_\mathbb{R} \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{1}{4t}(s-r)^2\right) f(r) \, dr + \mathcal{O}(t^2) f(s).
\]

Let us now consider a sequence of functions \(f_n\) with \(L^1\) norm constant and equal to 1, and such that \(\lim_{n \to \infty} f_n = \delta_r\) where \(\delta_r\) denotes the Dirac distribution at the point \(r\). Letting the operator \(e^{t\tilde{\Delta}^{\lambda, \mu}_t}\) act on this sequence and letting \(n\) go to \(\infty\), we find the value of the integral kernel at the point \(r\):

\[
Q_t^{\lambda, \mu}(s, r) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{1}{4t}(s-r)^2\right) \times \left(1 - t\left(\frac{\mu}{2\lambda}\right)^2 + t\frac{\mu}{3}\left(s^2 + sr + r^2\right) - t\frac{\lambda^2}{5}\left(s^4 + s^3r + s^2r^2 + sr^3 + r^4\right)\right) f(r) \, dr + \mathcal{O}(t^2) f(s).
\]

Let us now consider a sequence of functions \(f_n\) with \(L^1\) norm constant and equal to 1, and such that \(\lim_{n \to \infty} f_n = \delta_r\) where \(\delta_r\) denotes the Dirac distribution at the point \(r\). Letting the operator \(e^{t\tilde{\Delta}^{\lambda, \mu}_t}\) act on this sequence and letting \(n\) go to \(\infty\), we find the value of the integral kernel at the point \(r\):

\[
Q_t^{\lambda, \mu}(s, r) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{1}{4t}(s-r)^2\right) \times \left(1 - t\left(\frac{\mu}{2\lambda}\right)^2 + t\frac{\mu}{6}\left(s^2 + sr + r^2\right) - t\frac{\lambda^2}{20}\left(s^4 + s^3r + s^2r^2 + sr^3 + r^4\right)\right) f(r) \, dr + \mathcal{O}(t^2).
\]

We can now combine this expression with Corollary 1 to obtain:

\[
\rho_t(x_1, x_2, x_3, x_4) = \int_{\mathbb{R}^* \times \mathbb{R} \times \mathbb{R} \times \mathbb{R}} \mathcal{F}^{\lambda, \mu}(x_1, x_2, x_3, x_4) Q_t^{\lambda, \mu}(s, r)|_{s=r} \, dr \, d\lambda \, d\mu
\]

\[
= \int_{\mathbb{R}^* \times \mathbb{R} \times \mathbb{R} \times \mathbb{R}} \exp\left(i\left(-\frac{\mu}{2\lambda}x_2 + \lambda x_4 - \lambda x_3 s + \frac{\lambda}{2}x_2 s^2\right)\right) Q_t^{\lambda, \mu}(s + x_1, r)|_{s=r} \, dr \, d\lambda \, d\mu
\]
\[
\begin{align*}
&= \int_{\mathbb{R}^* \times \mathbb{R} \times \mathbb{R}} \exp \left( i \left( -\frac{\mu}{2\lambda} x_2 + \lambda x_4 - \lambda x_3 r + \frac{\lambda}{2} x_2 r^2 \right) \right) \\
&\quad \times \left[ \frac{1}{\sqrt{4\pi t}} \exp \left( -\frac{1}{4t} x_1^2 \right) \left( 1 - t \frac{\mu^2}{4\lambda^2} + \frac{\mu}{6} t (r + x_1)^2 + r^2 + (r + x_1) r \right) \\
&\quad - \frac{\lambda^2}{20} t (r + x_1)^4 + r^4 + (r + x_1)^2 r^2 + (r + x_1)^3 r + (r + x_1) r^3 \right) + O(t^2) \right] dr \ d\lambda \ d\mu \\
&= \frac{1}{\sqrt{4\pi t}} \exp \left( -\frac{1}{4t} x_1^2 \right) \int_{\mathbb{R}^* \times \mathbb{R} \times \mathbb{R}} \exp \left( i \left( -\frac{\mu}{2\lambda} x_2 + \lambda x_4 - \lambda x_3 r + \frac{\lambda}{2} x_2 r^2 \right) \right) \\
&\quad \times \left( 1 - t P_4(r, x_1) + O(t^2) \right) dr \ d\lambda \ d\mu,
\end{align*}
\]

where \( P_4(r, x_1) \) denotes the degree 4 polynomial

\[
\begin{align*}
\frac{\mu^2}{4\lambda^2} - \frac{\mu}{6} (r + x_1)^2 + r^2 + (r + x_1) r \\
+ \frac{\lambda^2}{20} (r + x_1)^4 + r^4 + (r + x_1)^2 r^2 + (r + x_1)^3 r + (r + x_1) r^3.
\end{align*}
\]

It is important to notice that the coefficient of \( r^4 \) in the expansion of \( P_4(r, x_1) \) is always positive. Using the equality

\[
1 - t P_4(r, x_1) = e^{-t P_4(r, x_1)} + O(t^2)
\]

(see again the discussion following the proof of Theorem 1), we can separate the heat kernel in the following way:

\[
\begin{align*}
p_t(x_1, x_2, x_3, x_4) &= \frac{1}{\sqrt{4\pi t}} \exp \left( -\frac{1}{4t} x_1^2 \right) \int_{\mathbb{R}^* \times \mathbb{R}} \exp \left( i \left( -\frac{\mu}{2\lambda} x_2 + \lambda x_4 \right) \right) \\
&\quad \times \left[ \int_{\mathbb{R}} \exp \left( i \left( -\lambda x_3 r + \frac{\lambda}{2} x_2 r^2 \right) \right) e^{-t P_4(r, x_1)} \ dr \right] d\lambda \ d\mu \\
&\quad + \frac{1}{\sqrt{4\pi t}} \exp \left( -\frac{1}{4t} x_1^2 \right) \int_{\mathbb{R}^* \times \mathbb{R}} \exp \left( i \left( -\frac{\mu}{2\lambda} x_2 + \lambda x_4 \right) \right) \\
&\quad \times \left[ \int_{\mathbb{R}} \exp \left( i \left( -\lambda x_3 r + \frac{\lambda}{2} x_2 r^2 \right) \right) O(t^2) \ dr \right] d\lambda \ d\mu.
\end{align*}
\]

By construction the first term is a well-defined \( C^\infty \) function on the subset of \( \mathcal{G}_4 \) on which the integrals converge, but as its computation necessitates the use of special functions, we will leave it in this form. Moreover, the second term is by default a well-defined \( C^\infty \) function on the same domain, and using the same tools as in the case of the Heisenberg group we can show that it is in fact a function of order \( O(t^{3/2}) \).
The estimate we obtain is:

\[
\tilde{p}_t(x_1, x_2, x_3, x_4) = \frac{1}{\sqrt{4\pi t}} \exp\left( -\frac{1}{4t} x_1^2 \right) \int_{\mathbb{R}^4} \exp\left( i \left( -\frac{\mu}{2\lambda} x_2 + \lambda x_4 \right) \right) \\
\times \left[ \int_{\mathbb{R}} \exp\left( i \left( -\lambda x_3 r + \frac{\lambda}{2} x_2 r^2 \right) \right) e^{-tP_4(r,x_1)} \, dr \right] d\lambda d\mu.
\]

In the case of the Cartan group, we can show (see [6]) that the Generalized Fourier Transform of the hypoelliptic Laplacian is:

\[
\hat{\Delta}_{\nu}^{\lambda,\mu,\nu} \psi(s) = \frac{1}{\lambda^2 + \mu^2} \frac{d^2 \psi(\theta)}{d\theta^2} - \frac{(\nu + (\lambda^2 + \mu^2)^2 \theta)^2}{4(\lambda^2 + \mu^2)} \psi(\theta),
\]

which yields the transformed heat equation:

\[
\frac{\partial}{\partial s} \psi(\theta) = \frac{1}{\lambda^2 + \mu^2} \frac{d^2 \psi(\theta)}{d\theta^2} - \left( \frac{\lambda^2 + \mu^2}{2} \theta^2 + \nu \right)^2.
\]

We now give a proof of Theorem 3, which is very similar to the one of Theorem 2:

**Proof.** Using Corollary 2, this time with:

\[
m = 2, \quad a^{\lambda,\mu,\nu}_0 = \frac{\nu^2}{4}, \quad a^{\lambda,\mu,\nu}_2 = \frac{\nu(\lambda^2 + \mu^2)}{2},
\]

\[
a^{\lambda,\mu,\nu}_4 = \frac{(\lambda^2 + \mu^2)^2}{4}, \quad a^{\lambda,\mu,\nu}_1 = a^{\lambda,\mu,\nu}_3 = 0,
\]

and using the same sequence \(f_n\) that goes to the Dirac distribution with constant \(L^1\) norm equal to 1 as \(n\) goes to \(\infty\), we compute the small-time behaviour of the integral kernel \(Q^{\lambda,\mu,\nu}_\tau(\theta, r)\) of the operator \(e^{t\Delta^{\lambda,\mu,\nu}_\tau}\):

\[
Q^{\lambda,\mu,\nu}_\tau(s, r) = \frac{1}{\sqrt{4\pi \tau}} \exp\left( -\frac{1}{4\tau} (s - r)^2 \right) \left( 1 - \tau \frac{\nu^2}{4} - \frac{\tau}{3} \frac{\nu(\lambda^2 + \mu^2)^2}{2} (s^2 + r^2 + sr) \right.
\]

\[
- \frac{\tau}{5} \frac{(\lambda^2 + \mu^2)^4}{4} (s^4 + r^4 + s^2r^2 + s^3r + sr^3) + \mathcal{O}(\tau^{3/2})
\]

\[
= \frac{1}{\sqrt{4\pi \tau}} \exp\left( -\frac{1}{4\tau} (s - r)^2 \right) \left( 1 - \tau \frac{\nu^2}{4} - \frac{\tau}{3} \frac{\nu(\lambda^2 + \mu^2)^2}{2} (s^2 + r^2 + sr) \right.
\]

\[
- \frac{\tau}{5} \frac{(\lambda^2 + \mu^2)^4}{4} (s^4 + r^4 + s^2r^2 + s^3r + sr^3) + \mathcal{O}(\tau^2)
\].
Putting this together with Corollary 1, and using the notation $x = (x_1, x_2, x_3, x_4, x_5)$, we obtain

$$p_t(x) = \int_{\mathbb{R}} \int_{\lambda^2 + \mu^2 \neq 0} \int_{\mathbb{R}} \exp(i A_{x}^{\lambda, \mu, v}(s)) Q_{x}^{\lambda, \mu, v}\left(s + \frac{\lambda x_1 + \mu x_2}{\lambda^2 + \mu^2}, r\right) dr \, d\lambda \, d\mu \, dv$$

$$= \sqrt{\frac{\lambda^2 + \mu^2}{4\pi t}} \exp\left(-\frac{1}{4t} \frac{(\lambda x_1 + \mu x_2)^2}{\lambda^2 + \mu^2}\right)$$

$$\times \int_{\mathbb{R}} \int_{\lambda^2 + \mu^2 \neq 0} \int_{\mathbb{R}} \exp(i A_{x}^{\lambda, \mu, v}(r))(1 - t P_4(r, x_1, x_2) + \mathcal{O}(t^2)) \, dr \, d\lambda \, d\mu \, dv,$$

where we define

$$P_4(r, x_1, x_2) = \frac{\nu^2}{4(\lambda^2 + \mu^2)} + \frac{\nu}{6} (\lambda^2 + \mu^2) (\hat{r}^2 + r^2 + \hat{r} r)$$

$$+ \frac{(\lambda^2 + \mu^2)^3}{20} (\hat{r}^4 + r^4 + \hat{r}^2 r^2 + \hat{r}^3 r + \hat{r}^4),$$

with $\hat{r} = r + \frac{\lambda x_1 + \mu x_2}{\lambda^2 + \mu^2}$. Finally, we use the equality

$$1 - t P_4(r, x_1, x_2) = \exp(-t P_4(r, x_1, x_2)) + \mathcal{O}(t^2).$$

Using the fact that the coefficient of $r^4$ in $P_4(r, x_1, x_2)$ is always positive, we obtain a separable expression for $p_t(x)$, where the estimate is the one given in Eq. (3), and the error term is of order $\mathcal{O}(t^{3/2})$. This concludes the proof of the theorem. □

6. Conclusion

We have presented an approach to computing short-time asymptotics of heat kernels of hypoelliptic Laplacians on unimodular Lie groups of type I. This approach uses the noncommutative Fourier transform on the Lie group in order to transform the hypoelliptic heat equation on the Lie group into a family of operator equations indexed by the unitary irreducible representations of the Lie group. These operator equations are then perturbed in order to obtain computable small-time approximations of the heat kernel. We have detailed this approach for the case of the Heisenberg group, and we have applied it as well to computing small-time asymptotic approximations of the hypoelliptic heat kernel on the Cartan and Engel groups. The small-time approximation we have obtained in the Heisenberg case suggests a strong relation between the small-time behaviour and the cut locus of the origin. This would suggest that the small-time behaviour could be used in order to extract information about the cut locus.

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Appendix A. Upper bounds on the operators $D_k$

We will want to study the operators $D_k$, $k \geq 2$, in a combinatorial way, and for this purpose let us go back to the composition of operators:

$$T(t/n) \cdot \left[I + (t/n)B + \frac{1}{2}(t/n)^2S(\xi_n)B^2\right] \cdot \cdots \cdot T(t/n) \cdot \left[I + (t/n)B + \frac{1}{2}(t/n)^2S(\xi_n)B^2\right],$$

and recall that we defined the operator $D_k$ as the factor in $t^k$ obtained when expanding this expression. Let us start by noticing that the term $D_2$ is obtained by summing the operators that result either from choosing the term in $t^2$ in one of the $n$ factors and the identity operator in the remaining ones, or by choosing the term in $t$ in two factors and the identity operator for the remaining ones. The result is the operator:

$$D_2 = \frac{1}{2n^2} \left[ T(t/n)S(\xi_n)B^2T(t/n)^n - 1 + T(t/n)^2S(\xi_n)B^2T(t/n)^n - 2 + \cdots + T(t/n)^nS(\xi_n)B^2T(t/n)^n - 1 \right] + \frac{1}{n^2} \left[ T(t/n)BT(t/n)BT(t/n)^n - 2 + \cdots + T(t/n)^n - 1 BT(t/n)B \right].$$

We can see that there are $n$ operators of the first kind, corresponding to the $n$ choices of the factor in which we pick the term of degree 2, and $\left(\begin{array}{c} n \n \end{array}\right)$ of the second kind. Moreover, notice that each one of these operators is a composition of the operators $S(t)$, $T(t)$ and $B$, where the operator $B$ appears twice. Using the hypothesis of Proposition 3, we obtain:

$$\|D_2 f\|_1 \leq \frac{1}{n^2} N(2) \alpha_K^2 \|f\|_1,$$

where $N(2) = n + \left(\begin{array}{c} n \n \end{array}\right)$. $N(k)$ can in fact be viewed as the number of ways to obtain a final sum of $k$ when picking a number in $n$ different jars, each containing the numbers 0, 1 and 2. It is important to note that $N(2) \leq n^2$. Continuing in the same fashion, we find that:

$$\|D_k f\|_1 \leq \frac{1}{n^k} N(k) \alpha_K^k \|f\|_1, \quad k \in \{0, 1, 2, \ldots, 2n\}.$$

The general expression for $N(k)$ varies for $k$ even or odd. For $k = 2s$, and supposing first that $k \leq n$, we have:

$$N(k) = \left(\begin{array}{c} n \n s \end{array}\right) + \left(\begin{array}{c} n \n s - 1 \end{array}\right) \left(\begin{array}{c} n - 1 \n 2 \end{array}\right) + \cdots + \left(\begin{array}{c} n \n 1 \end{array}\right) \left(\begin{array}{c} n - 1 \n 2s - 2 \end{array}\right) + \left(\begin{array}{c} n \n 2s \end{array}\right).$$

Similarly, for $k = 2s + 1$ and also supposing that $k \leq n$, we have the expression:

$$N(k) = \left(\begin{array}{c} n \n s \end{array}\right) \left(\begin{array}{c} n - 1 \n 1 \end{array}\right) + \left(\begin{array}{c} n \n s - 1 \end{array}\right) \left(\begin{array}{c} n - 1 \n 3 \end{array}\right) + \cdots + \left(\begin{array}{c} n \n 1 \end{array}\right) \left(\begin{array}{c} n - 1 \n 2s - 1 \end{array}\right) + \left(\begin{array}{c} n \n 2s + 1 \end{array}\right).$$

In both cases, if $k > n$, $N(k)$ will consist only of some of the first terms of the expression.
We want to prove using induction that \( N(k) \leq n^k \). We have shown that it is true for \( k = 2 \), and let us now assume that it is true for \( k = 2s \). If \( k + 1 \leq n \), using the identity: \( \binom{n}{k} = n \binom{n-1}{k-1} \), we have:

\[
N(k + 1) = \binom{n}{s} (n - 1) + \binom{n}{s - 1} (n - 1) + \cdots + \binom{n}{1} (n - 1) + \binom{n}{2s + 1} \leq nN(k) \leq n^{k+1}.
\]

If we now assume that it is true for \( k = 2s + 1 \) and that \( k + 1 \leq n \), we obtain that:

\[
N(k + 1) = \binom{n}{s + 1} + \binom{n}{s} (n - 1) + \cdots + \binom{n}{1} (n - 1) + \binom{n}{2s + 2} \leq \binom{n}{(k + 1)/2} + n^{k+1} \leq n^{k+1},
\]

for \( k \geq 3 \). In the case where \( k + 1 > n \), then \( N(k + 1) \) will have either the same number of terms as \( N(k) \), or will have one less term. In both scenarios, using the same identity as above together with the assumption that \( N(k) \leq n^k \) will lead to \( N(k + 1) \leq n^{k+1} \).

This finishes to prove that for all \( k \in \{0,1,\ldots,2n\} \), \( N(k) \leq n^k \), and hence that \( \|D(k)f\|_1 \leq \alpha^k_n \|f\|_1 \).

**Appendix B. Proof of Proposition 4**

**B.1. Calculation of \( I_0 \)**

Recall that we defined:

\[
I_0(s_0, s_n) = \int_{\mathbb{R}^{n-1}} \cdots \int_{\mathbb{R}^{n-1}} \exp \left[ -\frac{n}{2t} \left( \sum_{i=1}^{n-1} s_i^2 - s_0 s_1 - s_1 s_2 - \cdots - s_{n-1} s_n \right) \right] ds_{n-1} \cdots ds_1.
\]

Using a change of variables \( \sqrt{\frac{t}{n}} s_i =: u_i , i = 0, \ldots, n \), we obtain an integral independent of \( \frac{t}{n} \):

\[
I_0(u_0, u_n) = \left( \frac{1}{n} \right)^{(n-1)/2} \int_{\mathbb{R}^{n-1}} \cdots \int_{\mathbb{R}^{n-1}} \exp \left[ -\frac{1}{2} \left( \sum_{i=1}^{n-1} u_i^2 - u_0 u_1 - u_1 u_2 - \cdots - u_{n-1} u_n \right) \right] du_{n-1} \cdots du_1.
\]
This \((n - 1)\)-dimensional integral is of the form
\[
\int_{\mathbb{R}^k} \cdots \int \exp\left(-\frac{1}{2} \tilde{x}^T A \tilde{x} + \tilde{b}^T \tilde{x}\right) d\tilde{x},
\]
with \(k = n - 1\), \(\tilde{x} = \tilde{u}\), \(A\) the following clearly positive-definite \((n - 1) \times (n - 1)\) matrix:
\[
A = \begin{bmatrix}
1 & -\frac{1}{2} & 0 & \cdots & 0 \\
-\frac{1}{2} & 1 & -\frac{1}{2} & \cdots & 0 \\
0 & -\frac{1}{2} & 1 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & -\frac{1}{2} & 1
\end{bmatrix}
\]
and \(\tilde{b}\) the following vector of length \((n - 1)\):
\[
\tilde{b}^T = \frac{1}{2} [u_0, 0, \ldots, 0, u_n].
\]

We can therefore use Lemma 1, for which we first need to compute the determinant of \(A\) and its inverse. Denote by \(A_k\) the \(k \times k\) matrices in the same form as \(A\), by \(D_k\) its determinant and by \(A_k^{-1}\) its inverse. Using induction we find that \(D_k = (k + 1)/2^k\), and that:
\[
A_k^{-1} = \frac{2}{k + 1} \begin{bmatrix}
k & k - 1 & k - 2 & k - 3 & \cdots & 2 & 1 \\
k - 1 & 2(k - 1) & 2(k - 2) & 2(k - 3) & \cdots & 4 & 2 \\
k - 2 & 2(k - 2) & 3(k - 2) & 3(k - 3) & \cdots & 6 & 3 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
2 & 4 & 6 & 8 & \cdots & (k - 1)2 & k - 1 \\
1 & 2 & 3 & 4 & \cdots & k - 1 & k
\end{bmatrix}.
\]

We therefore have all we need to use Lemma 1. We obtain:
\[
I_0(u_0, u_n) = \left(\frac{n}{t}\right)^{(n-1)/2} \sqrt{\frac{(2\pi)^{n-1}}{\det(A)}} \exp\left(\frac{1}{2} \tilde{b}^T A^{-1} \tilde{b}\right)
\]
\[
= \left(\frac{n}{t}\right)^{(n-1)/2} \sqrt{\frac{(2\pi)^{n-1}}{\det(A_{n-1})}} \exp\left(\frac{1}{2} \tilde{b}^T A_{n-1}^{-1} \tilde{b}\right)
\]
\[
= \left(\frac{n}{t}\right)^{(n-1)/2} \frac{2^{n-1} \pi^{(n-1)/2}}{\sqrt{n}} \exp\left(\frac{1}{4n} \left[ (n - 1)u_0^2 + (n - 1)u_n^2 + 2u_0u_n \right]\right)
\]
and hence by substituting in our original variables we obtain the desired result:
\[
I_0(s_0, s_n) = \left(\frac{n}{t}\right)^{(n-1)/2} \frac{2^{n-1} \pi^{(n-1)/2}}{\sqrt{n}} \exp\left(\frac{1}{4t} \left[ (n - 1)s_0^2 + (n - 1)s_n^2 + 2s_0s_n \right] \right).
\]
B.2. Calculation of the integrals $I_{i,k}$

Recall that we had defined those integrals as:

$$I_{i,k}(s_0, s_n) = \int_{\mathbb{R}^{n-1}} \cdots \int_{\mathbb{R}^{n-1}} \exp \left[ -\frac{n}{2t} \left( \sum_{j=1}^{n-1} s_j^2 - s_0 s_1 - \cdots - s_{n-1} s_n \right) \right] s_i^k \, ds_{n-1} \cdots ds_1,$$

for $i \in \{1, 2, \ldots, n-1\}$, $k \in \{1, 2, \ldots, 2m\}$, and that we want to prove that they are equal to:

$$I_{i,k}(s_0, s_n) = I_0 \cdot \sum_{j=0}^{k} \frac{k!}{(k-j)!} \frac{1}{(j/2)!} \left( \frac{t}{n} \right)^{j/2} \left( \frac{1}{n} \right)^{j/2} \left( (n-i)s_0 + is_n \right)^{k-j}.$$

Those integrals will involve an integration by parts step, which will always be of the form of the following lemma:

**Lemma 2.** For $d, e \in \mathbb{R}^+$,

$$\int_{-\infty}^{\infty} \exp(-d w^2 + ew) w^m \, dw = \exp(\frac{e^2}{4d}) \sqrt{\frac{\pi}{d}} \sum_{k=0}^{m} \frac{(m)!}{(m-k)!} \frac{1}{(k/2)!} \frac{1}{2^k} d^{-k/2} \left( \frac{e}{2d} \right)^{m-k}. \quad (B.1)$$

**Proof.** Straightforward by using a change of variable and the binomial theorem. \qed

Performing the change of variables $u_i := (\sqrt{n/t}) s_i$ as in the previous section, we obtain that

$$I_{i,k}(u_0, u_n) = \left( \frac{t}{n} \right)^{(n-1)/2} \left( \frac{t}{n} \right)^{k/2} \int_{\mathbb{R}^{n-1}} \cdots \int_{\mathbb{R}^{n-1}} \exp \left[ -\frac{1}{2} \left( \sum_{i=1}^{n-1} u_i^2 - u_0 u_1 - \cdots - u_{n-1} u_n \right) \right] u_i^k \, du_{n-1} \cdots du_1.$$

We can separate this integral to get:

$$I_{i,k}(u_0, u_n) = \left( \frac{t}{n} \right)^{(n-1)/2} \left( \frac{t}{n} \right)^{k/2} \int_{\mathbb{R}} \exp \left( -\frac{1}{2} u_i^2 \right) u_i^k \, du_i \times \left[ \int_{\mathbb{R}^{n-2}} \cdots \int_{\mathbb{R}^{n-2}} \exp \left( -\frac{1}{2} \sum_{j=1}^{n-1} u_j^2 - u_0 u_1 - \cdots - u_{n-1} u_n \right) \, du_{n-1} \cdots du_{i+1} \, du_{i-1} \cdots du_1 \right] du_i,$$

$$\underbrace{J_{i,k}}.$$
We can see that the \((n-2)\)-dimensional integral \(J_{i,k}\) defined above resembles \(I_0\) computed above. Indeed, it is also of the form

\[
\int \cdots \int_{\mathbb{R}^l} \exp\left(-\frac{1}{2} \vec{x}^T A \vec{x} + \vec{b}^T \vec{x}\right) \, d\vec{x},
\]

this time with \(l = n - 2\), \(\vec{x}^T = [u_1, \ldots, u_{i-1}, u_{i+1}, \ldots, u_{n-1}]\), \(A\) the following \((n-2) \times (n-2)\)-dimensional matrix:

\[
A = \begin{bmatrix}
A_{i-1} & 0 \\
0 & A_{n-i-1}
\end{bmatrix}
\]

and \(\vec{b}\) the following vector of length \(n - 2\),

\[
\vec{b}^T = \frac{1}{2} [u_0, 0, \ldots, 0, u_i, u_i, 0, \ldots, 0, u_n].
\]

We can now use Lemma 1. Notice that our matrix \(A\) is block-diagonal with first block \(A_{i-1}\) and second block \(A_{n-i-1}\), using the same notation for the matrices \(A_k\) as in Appendix B.1. By using our previous work on those matrices we get:

\[
\det(A) = \det(A_{i-1}) \cdot \det(A_{n-i-1}) = \frac{2^{i-1}}{i} \cdot \frac{2^{n-i-1}}{n-i} = \frac{2^{n-2}}{i(n-i)}
\]

and

\[
A^{-1} = \begin{bmatrix}
A_{i-1}^{-1} & 0 \\
0 & A_{n-i-1}^{-1}
\end{bmatrix}
\]

We are ready to apply Lemma 1. We obtain:

\[
J_{i,k} = \frac{2^{n-2} \pi^{(n-2)/2}}{\sqrt{i(n-i)}} \cdot \exp\left[\frac{i-1}{4i} u_0^2 + \frac{n-i-1}{4(n-i)} u_n^2 + \left(\frac{u_0}{2i} + \frac{u_n}{2(n-i)}\right) u_i\right]
\]

\[
+ \left(\frac{i-1}{4i} + \frac{n-i-1}{4(n-i)}\right) u_i^2
\]

Using this in our expression for \(I_{i,k}\):

\[
I_{i,k}(u_0, u_n) = \left(\frac{t}{n}\right)^{(n-1)/2} \cdot \left(\frac{t}{n}\right)^{k/2} \cdot \frac{2^{n-2} \pi^{(n-2)/2}}{\sqrt{i(n-i)}} \cdot \exp\left[\frac{i-1}{4i} u_0^2 + \frac{n-i-1}{4(n-i)} u_n^2\right]
\]

\[
\times \int_{\mathbb{R}} \exp\left[-u_i^2 \left(\frac{1}{2} - \left(\frac{i-1}{4i} + \frac{n-i-1}{4(n-i)}\right)\right) + \left(\frac{(n-i)u_0 + iu_n}{2i(n-i)}\right) u_i\right] u_i^k \, du_i.
\]
Now this last integral is exactly of the form of Lemma 2, with, in the same notation:

\[ d = \frac{1}{2} - \left( \frac{i - 1}{4i} + \frac{n - i - 1}{4(n - i)} \right) = \frac{n}{4i(n - i)}, \]

\[ e = \frac{(n - i)u_0 + iu_n}{2i(n - i)}. \]

Therefore, applying Lemma 2 and rearranging we get the formula for \( I_{i,k} \):

\[
I_{i,k}(u_0, u_n) = \left( \frac{t}{n} \right)^{(n-1)/2} \cdot \frac{2^{n-1} \pi^{(n-1)/2}}{\sqrt{n}} \cdot \left( \frac{t}{n} \right)^{k/2} \times \exp \left[ \frac{1}{4n} \left( (n - 1)u_0^2 + (n - 1)u_n^2 + 2u_0u_n \right) \right] \\
\times \sum_{j=0}^{k} \frac{k!}{(k-j)! (j/2)!} \frac{1}{2^{j/2}} \left( \frac{4i(n - i)}{n} \right)^{j/2} \left( \frac{(n - i)u_0 + iu_n}{n} \right)^{k-j}
\]

\[ = I_0 \cdot \left( \frac{t}{n} \right)^{k/2} \cdot \sum_{j=0}^{k} \frac{k!}{(k-j)! (j/2)!} \frac{1}{2^{j/2}} \left( \frac{4i(n - i)}{n} \right)^{j/2} \left( \frac{(n - i)u_0 + iu_n}{n} \right)^{k-j}. \]

Returning to our original variables we finally obtain the formula for \( I_{i,k}(s_0, s_n) \), given in Proposition 4.

Appendix C. End of the proof of Corollary 2

Recall that we obtained the expression:

\[
K_{n,t/n}(s_0, s_n) = \frac{t}{n} \left( \frac{4\pi t}{n} \right)^{-n/2} \exp \left[ -\frac{n}{4t} \left( s_0^2 + s_n^2 \right) \right] \\
\times \left[ \frac{1}{p} (s_n)^2 + (n - 1)a_0 \right] I_0(s_0, s_n) + \sum_{k=1}^{2m} \sum_{i=1}^{n-1} d_k \sum_{i=1}^{n-1} I_{i,k}(s_0, s_n).
\]

Hence, putting this together with the results from Proposition 4, we find:

\[
\lim_{n \to \infty} K_{n,t/n}(s_0, s_n) = \lim_{n \to \infty} \frac{t}{n} \left( \frac{4\pi t}{n} \right)^{-n/2} \exp \left[ -\frac{n}{4t} \left( s_0^2 + s_n^2 \right) \right] \\
\times \left( \frac{t}{n} \right)^{(n-1)/2} \frac{2^{n-1} \pi^{(n-1)/2}}{\sqrt{n}} \exp \left( \frac{1}{4t} \left[ (n - 1) s_0^2 + (n - 1) s_n^2 + 2s_0 s_n \right] \right).
\]
\[
\times \left[ (n - 1)a_0 + p(s_n)^2 + \sum_{k=1}^{2m} a_k \sum_{i=1}^{n-1} \left( \frac{(n - i)s_0 + is_n}{n} \right)^k \right] + O(t)
\]
\[
= \lim_{n \to \infty} \frac{t}{n} \sqrt{\frac{4}{\pi t}} \exp \left[ -\frac{1}{4t} (s_0 - s_n)^2 \right] \times \left[ (n - 1)a_0 + p(s_n)^2 + \sum_{k=1}^{2m} a_k \sum_{i=1}^{n-1} \left( \frac{(n - i)s_0 + is_n}{n} \right)^k \right] + O(t^{3/2}).
\]

Here we used the fact that \( \exp[-\frac{1}{4t} (s_0 - s_n)^2] \) can be made as small as we want for \( t \) small enough, and therefore is a function of order \( O(1) \). We are then able to say that
\[
\frac{1}{\sqrt{4\pi t}} \exp \left[ -\frac{1}{4t} (s_0 - s_n)^2 \right] = O(t^{-1/2}),
\]
and to use the equality \( tO(t^{-1/2})O(t) = O(t^{3/2}) \) to obtain our final bound on the error term. To compute the sums in the previous expression, we will need the proposition.

**Proposition 6 (Faulhaber’s formula).**

\[
\sum_{k=1}^{n} k^p = \frac{1}{p+1} \sum_{i=1}^{p+1} (-1)^{s_p} B_{p+1-i} n^i,
\]

where \( B_i \) is the \( i \)th Bernoulli number.

Notice that as \( B_0 = 1 \), \( \sum_{k=1}^{n} k^p \) is a polynomial in \( n \) of degree \( p + 1 \), where the coefficient of the highest order term is \( \frac{1}{p+1} \). We have:

\[
\sum_{i=1}^{n-1} [(n - i)s_0 + is_n]^k = \sum_{i=1}^{n-1} \sum_{j=0}^{k} \binom{k}{j} s_0^i s_n^{k-j} (n - i)^j i^{k-j}
\]

\[
= \sum_{j=0}^{k} \binom{k}{j} s_0^j s_n^{k-j} \sum_{i=1}^{n-1} (n - i)^j i^{k-j}
\]

\[
= \sum_{j=0}^{k} \binom{k}{j} s_0^j s_n^{k-j} \sum_{i=1}^{n-1} \sum_{l=0}^{j} \binom{j}{l} (-1)^{j-l} i^{j-l} i^{l} i^{k-j}
\]

\[
= \sum_{j=0}^{k} \binom{k}{j} s_0^j s_n^{k-j} \sum_{i=1}^{n-1} \sum_{l=0}^{j} \binom{j}{l} (-1)^{j-l} i^{j-l} i^{l} i^{k-l}.
\]

This term \( n^l \sum_{i=1}^{n-1} i^{k-l} \) is, by Faulhaber’s formula, equal to a polynomial in \( n \) of degree \( k + 1 \), where the term of degree \( k + 1 \) has a coefficient \( \frac{1}{k+1} \). Notice that we had a factor of \( \frac{1}{n^{k+1}} \) multiplying this term, so when taking the limit the only term that remains is \( \frac{1}{k+1} \). Explicitly:
lim_{n \to \infty} K_{n,t/n}(s_0, s_n)

= t \lim_{n \to \infty} \frac{1}{\sqrt{4\pi t}} \exp\left( -\frac{1}{4t} (s_0 - s_n)^2 \right)
\times \left[ \frac{n-1}{n} a_0 + \sum_{k=1}^{2m} a_k \sum_{j=0}^{k} \binom{k}{j} s_0^j s_n^{k-j} \sum_{l=0}^{j} \binom{j}{l} (-1)^{j-l} \frac{1}{k-l+1} \right] + O(t^2)

= \frac{1}{\sqrt{4\pi t}} \exp\left( -\frac{t}{4t} (s_0 - s_n)^2 \right) \left[ a_0 t + \sum_{k=1}^{2m} a_k t \sum_{j=0}^{k} s_0^j s_n^{k-j} \frac{1}{k+1} \right] + O(t^2).

In this last expression we used the equality:

\sum_{l=0}^{j} \binom{k}{j} \binom{j}{l} (-1)^{j-l} \frac{1}{k-l+1} = \frac{1}{k+1},

which can be deduced from:

\sum_{i=0}^{k} (-1)^i \binom{k}{i} \frac{1}{i-\beta} = \frac{k! \Gamma(-\beta)}{\Gamma(k+1-\beta)}

(see [15]).

References