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GLOBAL HEAT KERNELS FOR PARABOLIC HOMOGENEOUS HÖRMANDER OPERATORS

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ABSTRACT

The aim of this paper is to prove the existence and several selected properties of a global fundamental Heat kernel Γ for the parabolic operators $\mathcal{H} = \sum_{j=1}^{m} X_j^2 - \partial_t$, where $X_1, \ldots, X_m$ are smooth vector fields on $\mathbb{R}^n$ satisfying Hörmander's rank condition, and enjoying a suitable homogeneity assumption with respect to a family of non-isotropic dilations. The proof of the existence of Γ is based on a (algebraic) global lifting technique, together with a representation of Γ in terms of the integral (performed over the lifting variables) of the Heat kernel for the Heat operator associated with a suitable sub-Laplacian on a homogeneous Carnot group. Among the features of Γ we prove: homogeneity and symmetry properties; summability properties; its vanishing at infinity; the uniqueness of the bounded solutions of the related Cauchy problem; reproduction and density properties; an integral representation for the higher-order derivatives.

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1. Introduction

Given a certain class of Hörmander PDOs (Partial Differential Operators, here and throughout), the availability of some 'explicit' integral representation formulas for an associated global fundamental solution Γ and for its derivatives in terms of well-behaved kernels defined on richer higher dimensional structures (such as homogeneous Carnot groups) can lead to global pointwise estimates of Γ and of its derivatives. This can be achieved only through profound results on the underlying geometry of Hörmander operators; see, e.g., the recent investigation [9]. A considerable amount of work needs to be accomplished in order to obtain both the existence of a global Γ and of well-behaved representation formulas, as shown in [7].

The aim of the present study is to accomplish this work for a class of Heat-type evolution PDOs not contained in the stationary case faced in [7]. As the approach in the latter paper proved fruitful, we shall try to adapt some ideas therein contained to the evolutive case; with respect to the stationary case, this programme is complicated by the preliminary need for a Gaussian behavior of the lifted Heat kernels (see, e.g., [25, 35, 34, 40]). The parabolic setting features interesting problems, such as the study of the initial Cauchy problem, and the richer properties of the associated potentials.

The results established in the present work provide a starting point to obtain Gaussian pointwise estimates of the Heat kernel herein constructed and of its X-derivatives (of arbitrary order); see the recent paper [11].

The aim of this paper is to prove, via a construction as explicit as possible, the existence of a well-behaved global fundamental solution Γ (also referred to as a Heat kernel) for the (degenerate) evolution Heat-type PDOs $\mathcal{H}$ of the form

$$\mathcal{H} = \sum_{j=1}^{m} X_j^2 - \frac{\partial}{\partial t} \quad \text{on } \mathbb{R}^{1+n} = \mathbb{R}_t \times \mathbb{R}^n_x, \tag{1.1}$$

where $X_1, \ldots, X_m$ are smooth vector fields on $\mathbb{R}^n_x$ satisfying Hörmander's rank condition in space $\mathbb{R}^n_x$, and enjoying a suitable homogeneity assumption w.r.t. a family of non-isotropic dilations, which we shall describe subsequently. Our approach is two-fold: it relies on a (algebraic) global 'lifting' procedure, and on an integral 'saturation' technique. Roughly put, we construct a lifting operator $\widetilde{\mathcal{H}}$

for $\mathcal{H}$ of the form

$$(1.2)\qquad \widetilde{\mathcal{H}} = \sum_{j=1}^{m} (X_j(x) + R_j(x,\xi))^2 - \frac{\partial}{\partial t} \quad \text{on } \mathbb{R}^{1+n+p} = \mathbb{R}_t \times \mathbb{R}^n_x \times \mathbb{R}^p_\xi,$$

where $R_1(x,\xi), \dots, R_m(x,\xi)$ are vector fields operating only in the variables $\xi = (\xi_1, \dots, \xi_p)$ (with coefficients possibly depending on $(x,\xi) \in \mathbb{R}^n \times \mathbb{R}^p$), in such a way that the existence of a global (i.e., defined throughout $\mathbb{R}^{1+n+p}$) fundamental solution $\widetilde{\Gamma}$ for $\widetilde{\mathcal{H}}$ be ensured. Then, we want to redeem a fundamental solution Γ for $\mathcal{H}$ by integrating $\widetilde{\Gamma}$ over the lifting variables $\xi \in \mathbb{R}^p$; to this end, it is necessary to know that $\widetilde{\Gamma}$ be globally integrable w.r.t. $\xi \in \mathbb{R}^p$, which is one of the crucial points of our approach. We refer to this integration procedure as a 'saturation' argument.

In the analysis of fundamental solutions for linear PDOs, the idea of passing through a lifting procedure and a saturation of the lifting variables is certainly not new, and it traces back to Rothschild and Stein's pivotal paper [37] (see also Nagel, Stein, Wainger [36]); however, Rothschild and Stein's lifting is a local tool, whereas, as we stressed, we need a global technique since we aim to obtain fundamental solutions defined on the whole space (and vanishing at infinity). Global integrability (at infinity) over the saturation variables is a non-trivial fact. We shall describe in a moment how we face these problems. Incidentally, we observe that in [37] only suitable parametrices of a fundamental solution are studied, which again reflects the local/approximation nature of the lifting in [37].

The basic idea of obtaining fundamental solutions for Heat-type operators via saturation arguments is very well described in the Euclidean setting. Indeed, it is well known that a global fundamental solution (with pole at the origin of $\mathbb{R}^{1+n}$) for the classical Heat operator $\mathcal{H}_n := \Delta_n - \partial/\partial t$ on $\mathbb{R}^{1+n}$ is given by (we use the notation χ_A for the indicator function of a set A)

$$\Gamma_n(t,x) = \chi_{(0,\infty)}(t)\, \frac{1}{(4\,\pi\, t)^{n/2}}\, \exp\left(- \frac{\sum_{j=1}^n x_j^2}{4\,t} \right), \quad (t,x) \in \mathbb{R} \times \mathbb{R}^n.$$

Then, if we consider the Heat operator $\mathcal{H}_{n+p}$ on $\mathbb{R}^{1+n+p}$ and if we integrate its fundamental solution Γ_{n+p} (with pole at the origin of $\mathbb{R}^{1+n+p}$) with respect to the last p variables, we obtain (upon the trivial fact $\int_{\mathbb{R}} \exp(-\frac{\xi^2}{4t})\,\mathrm{d}\xi = \sqrt{4\pi t}\,$)

$$\begin{aligned}\int_{\mathbb{R}^p} &\Gamma_{n+p}(t,x,\xi)\,\mathrm{d}\xi \\ &= \chi_{(0,\infty)}(t)\,\frac{1}{(4\pi\,t)^{(n+p)/2}}\,\exp\Big(-\frac{\sum_{j=1}^n x_j^2}{4\,t}\Big)\int_{\mathbb{R}^p}\exp\Big(-\frac{\sum_{j=1}^p \xi_j^2}{4\,t}\Big)\,\mathrm{d}\xi \\ &= \chi_{(0,\infty)}(t)\,\frac{1}{(4\,\pi\,t)^{n/2}}\,\exp\Big(-\frac{\sum_{j=1}^n x_j^2}{4\,t}\Big) = \Gamma_n(t,x).\end{aligned}$$

In other words, the Heat kernel Γ_n of $\mathcal{H}_n$ can be recovered by the Heat kernel Γ_{n+p} of $\mathcal{H}_{n+p}$ by a saturation technique:

$$\Gamma_n(t,x) = \int_{\mathbb{R}^p} \Gamma_{n+p}(t,x,\xi)\,\mathrm{d}\xi, \quad (t,x) \in \mathbb{R}\times\mathbb{R}^n.$$

A global lifting/saturation process may likely occur in other interesting cases (for non-elliptic operators): see, e.g., Bauer, Furutani and Iwasaki [2]; Calin, Chang, Furutani and Iwasaki [19, Sect. 10.3]; Beals, Gaveau, Greiner and Kannai [5]. Explicit formulas for some Heat kernels on nilpotent Lie groups can be found in: Agrachev, Boscain, Gauthier and Rossi [1]; Beals, Gaveau and Greiner [3, 4]; Boscain, Gauthier and Rossi [17]; Cygan [20]; Furutani [23]; Gaveau [24].

The same process was exploited in the paper [7], which provides some general structural assumptions showing when lifting/saturation can be successfully applied (see Theorem 2.3). We fix once and for all the definition of a lifting of a PDO P, while postponing the precise notion of a global fundamental solution Γ to Theorem 1.4; for the time being, by Γ we mean a function of two variables $(z;\zeta) \in \mathbb{R}^{1+n}\times\mathbb{R}^{1+n}$ (the first of which is called the 'pole') such that, for any fixed pole z, we have $P(\Gamma(z;\cdot)) = -\mathrm{Dir}_z$ in the weak sense of distributions (Dir_z is the Dirac mass at z).

In order to distinguish it from the local Rothschild and Stein's lifting technique, we define a simpler notion of the lifting of P as follows: if P is a smooth linear PDO on $\mathbb{R}^{1+n}_z$, we say that the PDO $\widetilde{P}$ defined on $\mathbb{R}^{1+n}_z \times \mathbb{R}^p_\xi$ is a lifting of P (or simply that $\widetilde{P}$ lifts P) if:

- $\widetilde{P}$ has smooth coefficients, possibly depending on $(z,\xi) \in \mathbb{R}^{1+n}\times\mathbb{R}^p$;
- for every fixed $f \in C^\infty(\mathbb{R}^{1+n}_z)$, one has

(1.3) $$\widetilde{P}(f\circ\pi)(z,\xi) = (Pf)(z), \quad \text{for every } (z,\xi)\in\mathbb{R}^{1+n}\times\mathbb{R}^p,$$

where $\pi(z,\xi) = z$ is the canonical projection of $\mathbb{R}^{1+n}\times\mathbb{R}^p$ onto $\mathbb{R}^{1+n}$.

For example, with this definition, $\widetilde{\mathcal{H}}$ in (1.2) is a lifting of $\mathcal{H}$ in (1.1).

In general, the idea of obtaining a fundamental solution Γ for P via a fundamental solution $\widetilde{\Gamma}$ for $\widetilde{P}$ by integration over the lifting $\mathbb{R}^p_\xi$-variables is natural but subtle, as we now describe. Let us start by writing down the definition of the distributional identity

$$\widetilde{P}\{(\zeta,\eta)\mapsto\widetilde{\Gamma}((z,\xi);(\zeta,\eta))\} = -\mathrm{Dir}_{(z,\xi)}, \tag{1.4}$$

by first conveniently freezing the variable ξ at $0\in\mathbb{R}^p$: this boils down to the identity (valid for every $\psi\in C_0^\infty(\mathbb{R}^{1+n+p})$ and every $(z,0)\in\mathbb{R}^{1+n+p}$)

$$\int_{\mathbb{R}^{1+n}}\mathrm{d}\zeta\int_{\mathbb{R}^p}\mathrm{d}\eta\,\widetilde{\Gamma}((z,0);(\zeta,\eta))\,\widetilde{P}^*(\psi(\zeta,\eta)) = -\psi(z,0). \tag{1.5}$$

Then, we aim to recover a fundamental solution Γ for P starting from identity (1.5) in the most direct way, if possible. To this end, it seems appropriate to define Γ by the inner η-integral in (1.5), that is

$$\Gamma(z;\zeta) := \int_{\mathbb{R}^p}\widetilde{\Gamma}((z,0);(\zeta,\eta))\,\mathrm{d}\eta \quad (\text{for } z\neq\zeta \text{ in } \mathbb{R}^{1+n}). \tag{1.6}$$

If in (1.5) we were allowed to take as a test function ψ any function of the form $\varphi(z)$ in $C_0^\infty(\mathbb{R}^{1+n})$, then (1.5) would easily prove that Γ is a fundamental solution of P, in view of the fact that $\widetilde{P}(\varphi\circ\pi) = P\varphi$. Unfortunately, a test function $\varphi(z)$ on $\mathbb{R}^{1+n}$ does not become a test function ψ on $\mathbb{R}^{1+n+p}$ by simply considering $\psi=\varphi\circ\pi$ (where π is the projection in (1.3)).

A more promising procedure (still based on (1.5)) is the "product-like" choice

$$\psi(z,\xi) = \varphi(z)\,\theta_j(\xi),$$

where $\theta_j\in C_0^\infty(\mathbb{R}^p_\xi)$ is such that $\theta_j\to 1$ as $j\to\infty$: indeed, one may formally let $j\to\infty$ in the following identity (resulting from (1.5) with this choice of ψ)

$$\int_{\mathbb{R}^{1+n}}\mathrm{d}\zeta\int_{\mathbb{R}^p}\mathrm{d}\eta\,\widetilde{\Gamma}((z,0);(\zeta,\eta))\,\widetilde{P}^*(\varphi(\zeta)\,\theta_j(\eta)) = -\varphi(z)\,\theta_j(0), \tag{1.7}$$

with the hope that, when $j\to\infty$ (by again exploiting the fact that $\widetilde{P}$ lifts P), this may lead to

$$\int_{\mathbb{R}^{1+n}}\left(\int_{\mathbb{R}^p}\widetilde{\Gamma}((z,0);(\zeta,\eta))\,\mathrm{d}\eta\right)P^*\varphi(\zeta)\,\mathrm{d}\zeta = -\varphi(z).$$

In the end, the latter identity would produce the fact that the function Γ in (1.6) is indeed a global fundamental solution for P.

In order to make this argument more than heuristic, it appears that some a priori assumptions must be conveniently made, namely:

- we need to know that Γ in (1.6) is well posed as a convergent integral; we also need to know some summability properties of Γ (implicit in the definition of a fundamental solution, see Section 2);
- some structural and growth assumptions on the formal adjoint of the "remainder" operator $R := \widetilde{P} - P$ (which operates on the lifting variables ξ only) should be conveniently made to rigorously pass to the limit in (1.7).

This discussion fully motivates the technical assumptions that we shall make in the saturation Theorem 2.3, postponed to the next section.

It is now time to describe in detail the assumptions on the vector fields X_j in (1.1). Let $X = \{X_1, \ldots, X_m\}$ be a set of smooth and linearly independent[1] vector fields on $\mathbb{R}^n$ satisfying the following assumptions:

(H.1) there exists a family of (non-isotropic) dilations $\{\delta_\lambda\}_{\lambda>0}$ of the form

$$\delta_\lambda : \mathbb{R}^n \longrightarrow \mathbb{R}^n, \quad \delta_\lambda(x) = (\lambda^{\sigma_1} x_1, \ldots, \lambda^{\sigma_n} x_n),$$

where $1 = \sigma_1 \leq \ldots \leq \sigma_n$ are integer numbers, such that $X_1, \ldots, X_m$ are δ_λ-homogeneous of degree 1, i.e.,

$$X_j(f \circ \delta_\lambda) = \lambda\,(X_j f) \circ \delta_\lambda, \quad \forall\, \lambda > 0,\ f \in C^\infty(\mathbb{R}^n),\ j = 1, \ldots, m;$$

(H.2) the set X satisfies Hörmander's rank condition at 0, i.e.,

$$\dim\{Y(0) : Y \in \mathrm{Lie}\{X\}\} = n.$$

By $\mathrm{Lie}\{X\}$ we mean the smallest Lie sub-algebra of the smooth vector fields $\mathcal{X}(\mathbb{R}^n)$ on $\mathbb{R}^n$ containing X. Here $\mathcal{X}(\mathbb{R}^n)$ is equipped with its obvious structures of vector space and of Lie algebra.

In the literature, the use of a dilation-invariance property as in assumption (H.1) has been already proved to be fruitful in order to establish 'global' properties for $\mathcal{L} = \sum_{j=1}^m X_j^2$ and for its parabolic counterpart $\mathcal{H} = \sum_{j=1}^m X_j^2 - \partial_t$; we refer, e.g., to the series of papers [26, 31, 30, 28, 29, 27] and to the references

[1] The linear independence of $X_1, \ldots, X_m$ is meant in the vector space $\mathcal{X}(\mathbb{R}^n)$ of the smooth vector fields on $\mathbb{R}^n$, and it must not be confused with the linear independence of the (tangent) vectors $X_1(x), \ldots, X_m(x)$; for example, the Grushin vector fields in $\mathbb{R}^2$ defined by $X_1 = \partial_{x_1}$ and $X_2 = x_1 \partial_{x_2}$ are linearly independent in $\mathcal{X}(\mathbb{R}^2)$, despite that the vectors of $\mathbb{R}^2$ given by $X_1(x) \equiv (1, 0)$ and $X_2(x) \equiv (0, x_1)$ are dependent when $x_1 = 0$.

therein. We also point out that, in the absence of a homogeneity property of the X_i's, another assumption leading to a 'global' analysis of $\mathcal{L}$ and $\mathcal{H}$ is the invariance of $X_1, \ldots, X_m$ with respect to a (Lie) group of translations (see, e.g., [12, 33, 32]); however, in our context we do not assume any left-invariance property on the vector fields in X (see Theorem 1.2 below).

Remark 1.1: It is not difficult to show that, since $X_1, \ldots, X_m$ are δ_λ-homogeneous of degree 1, the validity of Hörmander's rank condition at 0 implies the validity of the latter at any $x \in \mathbb{R}^n$, and that $n \leq \dim(\mathrm{Lie}\{X\}) < \infty$.

Thus, the Hörmander parabolic operator $\mathcal{H}$ in (1.1) is C^∞-hypoelliptic on every open subset of $\mathbb{R}^{1+n}$. Moreover, $\mathcal{H}$ satisfies the Weak Maximum Principle on every bounded open subset of $\mathbb{R}^{1+n}$: this follows from (H.1)–(H.2), as is proved in [8, Sect. 8.4].

The following result is relevant for our purposes, and it can be proved starting from [6, Thm. 1.4] and [7, Thm 3.1]. We refer to [15, §1.4] for the notions of sub-Laplacian and of homogeneous[2] Carnot group on $\mathbb{R}^N$.

Theorem 1.2: *Assume that $X = \{X_1, \ldots, X_m\}$ satisfies the above assumptions* (H.1) *and* (H.2). *Moreover, let $N = \dim(\mathrm{Lie}\{X\})$. Then the following facts hold:*

1. *If $N = n$, there exists a homogeneous Carnot group $\mathbb{G}$ (with underlying manifold $\mathbb{R}^n$ and the same dilations δ_λ as in* (H.1)*) such that X is a system of Lie-generators of* $\mathrm{Lie}(\mathbb{G})$*; hence $\mathcal{L} := \sum_{j=1}^m X_j^2$ is a sub-Laplacian on $\mathbb{G}$.*
2. *If $N > n$, there exist a homogeneous Carnot group $\mathbb{G}$ (with underlying manifold $\mathbb{R}^N$) and a system $\{Z_1, \ldots, Z_m\}$ of Lie-generators of* $\mathrm{Lie}(\mathbb{G})$ *such that Z_i is a lifting of X_i for every $i = 1, \ldots, m$ (in the previously defined sense); hence the sub-Laplacian $\sum_{j=1}^m Z_j^2$ is a lifting of $\mathcal{L}$.*

The demonstration of Theorem 1.2 is quite delicate: for example, the proof of (2) makes use of the global lifting method for homogeneous vector fields proved by Folland [22], a notable refinement of the local lifting technique introduced by Rothschild and Stein in [37] for Hörmander PDOs: a proof of (2) can be found in [7]. As for assertion (1) in Theorem 1.2, one argues as follows:

[2] Essentially, this is a triple $(\mathbb{R}^N, \star, D_\lambda)$ of a Lie group $(\mathbb{R}^N, \star)$ and a family of dilations D_λ which are group automorphisms.

Remark 1.3: Consider the following facts:

- $\mathrm{Lie}\{X\}$ is an n-dimensional Lie algebra of analytic vector fields in $\mathbb{R}^n$ (analyticity follows from the fact that the X_j's have polynomial component functions, due to (H.1));
- X is a Hörmander system, due to (H.1)–(H.2) (see Remark 1.1);
- any vector field $Y \in \mathrm{Lie}\{X\}$ is complete, i.e., the integral curves of Y are defined on the whole of $\mathbb{R}$ (this can be proved as a consequence of (H.1)).

Under these three conditions, Theorem 1.4 in [6] proves that $\mathrm{Lie}\{X\}$ coincides with the Lie algebra of a Lie group $\mathbb{G}$ on $\mathbb{R}^n$. As a matter of fact, under assumption (H.1), this Lie group $\mathbb{G}$ turns out to be a homogeneous Carnot group with dilations δ_λ (see, e.g., [8, Chapter 16]). Thus (1) follows.

All this being said, our aim in this paper is to prove that a saturation/lifting approach can be performed for the Heat type operators $\mathcal{H} = \sum_{j=1}^m X_j^2 - \partial_t$, where $X_1, \dots, X_m$ satisfy (H.1) and (H.2). To this end, it is enough to assume that $N > n$, since (by Theorem 1.2-(1)) the case $N = n$ is already known (see Folland, [21]). When $N > n$ we will obtain the existence of a global fundamental solution (also called Heat kernel) Γ for $\mathcal{H}$ obtained via the saturation formula (1.6), taking in this case the following special form

$$\Gamma(t, x; s, y) := \int_{\mathbb{R}^p} \Gamma_{\mathbb{G}}(t, x, 0; s, y, \eta)\, \mathrm{d}\eta,$$

where $\Gamma_{\mathbb{G}}$ is a fundamental solution for the Heat-type operator

$$\mathcal{H}_{\mathbb{G}} := \sum_{j=1}^m Z_j^2 - \frac{\partial}{\partial t}$$

on the Lie group $\mathbb{R} \times \mathbb{G}$ (here the Carnot group $\mathbb{G}$ and $Z_1, \dots, Z_m$ are the same as in Theorem 1.2). The existence of $\Gamma_{\mathbb{G}}$ was proved in [21] (see also [13]), where it was also shown that it takes a group-convolution form; this will lead to the even more profitable expression

$$\Gamma(t, x; s, y) = \int_{\mathbb{R}^p} \gamma_{\mathbb{G}}(s - t, (x, 0)^{-1} \star (y, \eta))\, \mathrm{d}\eta, \tag{1.8}$$

where $\gamma_{\mathbb{G}}$ is the fundamental solution of $\mathcal{H}_{\mathbb{G}}$ with pole at the origin, and $\star$ is the group law of the Carnot group in Theorem 1.2-(2). In showing that $\mathcal{H}$ satisfies the assumptions for the saturation procedure heuristically described above, one must also use the global Gaussian estimates of $\gamma_{\mathbb{G}}$ (see, e.g., Jerison and Sánchez-Calle [25]; Kusuoka, Stroock [35, 34]; Varopoulos, Saloff-Coste and Coulhon [40]).

Strictly speaking, formula (1.8) does not equip Γ with a translation-invariance property, as is shown by the Grushin-type example (see, e.g., [19])

$$G = \Big(\frac{\partial}{\partial x_1}\Big)^2 + \Big(x_1\,\frac{\partial}{\partial x_2}\Big)^2 - \frac{\partial}{\partial t}.$$

Nonetheless, (1.8) is a nicely "hybrid" expression of the fundamental solution of $\mathcal{H}$ as an integral of a translation-invariant kernel; this expression is indeed worthwhile since we shall derive from it plenty of properties of Γ, as is shown in the following theorem, our main result:

Theorem 1.4 (Existence and properties of the global Heat-kernels for homogeneous Hörmander PDOs): *Let X be a set of smooth vector fields on $\mathbb{R}^n$ satisfying assumptions* (H.1) *and* (H.2), *and let us assume that*

$$N = \dim(\mathrm{Lie}\{X\}) > n.$$

Let $\mathcal{H}$ be the Heat-type operator on $\mathbb{R}^{1+n}$ defined in (1.1), *and let us denote by $z = (t,x)$ the points of $\mathbb{R}^{1+n} = \mathbb{R}_t \times \mathbb{R}^n_x$. Then $\mathcal{H}$ admits a global fundamental solution $\Gamma(z;\zeta)$; this means that $\Gamma(z;\zeta)$ is defined for any couple of points $z,\zeta \in \mathbb{R}^{1+n}$ and it satisfies the following property: for any $z \in \mathbb{R}^{1+n}$ (the pole), $\Gamma(z;\cdot)$ is in $L^1_{\mathrm{loc}}(\mathbb{R}^{1+n})$ and*

$$\int_{\mathbb{R}^{1+n}} \Gamma(z;\zeta)\,\mathcal{H}^*\varphi(\zeta)\,\mathrm{d}\zeta = -\varphi(z), \quad \text{for every } \varphi \in C_0^\infty(\mathbb{R}^{1+n}),$$

where $\mathcal{H}^* = \sum_j X_j^2 + \partial/\partial t$ is the formal adjoint of $\mathcal{H} = \sum_j X_j^2 - \partial/\partial t$.

More precisely, we take as Γ the integral function

$$\Gamma(z;\zeta) = \Gamma(t,x;s,y) = \int_{\mathbb{R}^p} \gamma_{\mathbb{G}}(s-t,(x,0)^{-1}\star(y,\eta))\,\mathrm{d}\eta, \tag{1.9}$$

where $\gamma_{\mathbb{G}}$ is the unique fundamental solution, with pole at 0 and vanishing at infinity, of the Heat-type operator $\mathcal{H}_{\mathbb{G}} := \sum_{j=1}^m Z_j^2 - \partial/\partial t$ on $\mathbb{R}\times\mathbb{G}$ (which is a lifting of $\mathcal{H}$); the Carnot group $\mathbb{G} = (\mathbb{R}^N,\star)$ and the vector fields $Z_1,\dots,Z_m$ are as in Theorem 1.2-(2). The existence of $\gamma_{\mathbb{G}}$ is granted by [21].

Moreover, Γ in (1.9) *also enjoys the following list of properties:*

(i) $\Gamma \geq 0$ *and we have*

$$\Gamma(t,x;s,y) = 0 \quad \text{if and only if} \quad s \leq t.$$

(ii) *We have* $\Gamma(t,x;s,y)=\Gamma(-s,x;-t,y)$*, and* Γ *depends on* t *and* s *only through* $s-t$*:*

$$\Gamma(t,x;s,y)=\Gamma(0,x;s-t,y)=\Gamma(t-s,x;0,y).$$

Furthermore Γ *is symmetric in the space variables* x *and* y*, i.e.,*

$$\Gamma(t,x;s,y)=\Gamma(t,y;s,x).$$

(iii) *For every* $\lambda>0$ *we have*

$$\Gamma(\lambda^2 t,\delta_\lambda(x);\lambda^2 s,\delta_\lambda(y))=\lambda^{-q}\,\Gamma(t,x;s,y),\quad \text{where } q=\sum_{j=1}^m \sigma_j.$$

(iv) Γ *is smooth out of the diagonal of* $\mathbb{R}^{1+n}\times\mathbb{R}^{1+n}$*.*

(v) *For every compact set* $K\subseteq\mathbb{R}^{1+n}$*, we have*

$$\lim_{\|\zeta\|\to\infty}\big(\sup_{z\in K}\Gamma(z;\zeta)\big)=\lim_{\|\zeta\|\to\infty}\big(\sup_{z\in K}\Gamma(\zeta;z)\big)=0.$$

(vi) $\Gamma\in L^1_{\mathrm{loc}}(\mathbb{R}^{1+n}\times\mathbb{R}^{1+n})$ *and, for every fixed* $z\in\mathbb{R}^{1+n}$*, we have*

$$\Gamma(z;\cdot),\ \Gamma(\cdot;z)\in L^1_{\mathrm{loc}}(\mathbb{R}^{1+n}).$$

(vii) *For every fixed* $(t,x)\in\mathbb{R}^{1+n}$ *we have*

$$\int_{\mathbb{R}^n}\Gamma(t,x;s,y)\,\mathrm{d}y=1,\quad \text{for every } s>t.$$

(viii) *For every fixed* $\varphi\in C_0^\infty(\mathbb{R}^{1+n})$*, the map defined by the potential function*

$$\mathbb{R}^{1+n}\ni\zeta\mapsto\Lambda_\varphi(\zeta):=\int_{\mathbb{R}^{1+n}}\Gamma(z;\zeta)\,\varphi(z)\,\mathrm{d}z$$

is smooth, it vanishes at infinity and $\mathcal{H}(\Lambda_\varphi)=-\varphi$ *on* $\mathbb{R}^{1+n}$*.*

(ix) *If* $\varphi\in C(\mathbb{R}^n)$ *is bounded, then the potential-type function*

$$u(t,x):=\int_{\mathbb{R}^n}\Gamma(0,y;t,x)\,\varphi(y)\,\mathrm{d}y$$

defined for $(t,x)\in\Omega=(0,\infty)\times\mathbb{R}^n$ *is the unique bounded classical solution of the homogeneous Cauchy problem*

$$\begin{cases}\mathcal{H}u=0 & \text{in } \Omega,\\ u(0,x)=\varphi(x) & \text{for } x\in\mathbb{R}^n.\end{cases}$$

(x) *For every* $x,y\in\mathbb{R}^n$ *and every* $s,t>0$*, we have the reproduction formula*

$$\Gamma(0,y;t+s,x)=\int_{\mathbb{R}^n}\Gamma(0,w;t,x)\,\Gamma(0,y;s,w)\,\mathrm{d}w.$$

Finally, if we consider the function Γ^* *defined by*

$$\Gamma^*(t,x;s,y) := \Gamma(s,y;t,x), \quad \textit{for every } (t,x),(s,y) \in \mathbb{R}^{1+n},$$

then Γ^* *is a global fundamental solution for* $\mathcal{H}^* = \sum_{j=1}^m X_j^2 + \partial/\partial_t$*, satisfying dual statements of* (i)–(x).

We observe that there exists at most one fundamental solution Γ of $\mathcal{H}$ such that, for any fixed $z \in \mathbb{R}^{1+n}$, it holds that $\Gamma(z;\cdot)$ is continuous out of z, and

$$\lim_{\|\zeta\|\to\infty} \Gamma(z;\zeta) = 0$$

(see Remark 2.2-(c)). As a consequence (see properties (iv,v) above) the function Γ satisfying the properties of Theorem 1.4 is unique.

Remark 1.5: Many of the properties (i)–(x), albeit not unexpected, are based on quite technical arguments made possible by the very formula (1.9), which therefore proves to be fruitful. From a recent investigation with Marco Bramanti [9], it appears that, in the case of the stationary operator $\mathcal{L} = \sum_{j=1}^m X_j^2$, one can pass from the integral representation analogous to (1.9) to pointwise estimates of the fundamental solution (and of its derivatives) in terms of the Carnot–Carathéodory distance associated with $X_1, \dots, X_m$: this requires some work, also based on results by Nagel, Stein and Wainger [36], by Sánchez-Calle [38], and by Bramanti, Brandolini, Manfredini and Pedroni [18].

In the recent paper [11], we have exploited in a crucial way formula (1.9) (together with the aforementioned results on the geometry of Hörmander operators) to derive pointwise Gaussian estimates of the Heat kernel Γ. We also point out that the techniques of this paper are the starting point to prove uniform and global estimates for the fundamental solutions of the operators $\sum_{i,j} a_{i,j} X_i X_j - \partial/\partial t$, as the matrix $(a_{i,j})$ ranges over the $m \times m$ symmetric and positive-definite matrices satisfying a suitable (uniform) ellipticity condition, see [10]. In its turn, these uniform estimates are used in [10] to study the parametrices for non-constant $a_{i,j}$'s (see also [14]).

Our integral representation is also sufficiently helpful that it produces analogous representations for any higher order derivative, as this theorem shows:

Theorem 1.6 (Representation of the derivatives of Γ): *Let the assumptions of Theorem 1.4 hold (from which we inherit the notation), and let* Γ *be the fundamental solution of* $\mathcal{H}$ *in* (1.9).

Then, for any $\alpha, \beta \in \mathbb{N} \cup \{0\}$, any $h, k \geq 1$ and any choice of indexes $i_1, \dots, i_h, j_1, \dots, j_k$ in $\{1, \dots, m\}$, we have the following representation formulas (holding true for $(t, x) \neq (s, y)$ in $\mathbb{R}^{1+n}$), respectively concerning X-derivatives in the y-variable, in the x-variable, and in the mixed (x, y)-case:

$$\begin{aligned}&\Big(\frac{\partial}{\partial s}\Big)^{\alpha}\Big(\frac{\partial}{\partial t}\Big)^{\beta} X^y_{i_1}\cdots X^y_{i_h}\Gamma(t,x;s,y)\\ &\quad= (-1)^{\beta}\int_{\mathbb{R}^p}\Big(\Big(\frac{\partial}{\partial \tau}\Big)^{\alpha+\beta} Z_{i_1}\cdots Z_{i_h}\gamma_{\mathbb{G}}\Big)(s-t,(x,0)^{-1}\star(y,\eta))\,\mathrm{d}\eta;\end{aligned}\tag{1.10}$$

$$\begin{aligned}&\Big(\frac{\partial}{\partial s}\Big)^{\alpha}\Big(\frac{\partial}{\partial t}\Big)^{\beta} X^x_{j_1}\cdots X^x_{j_k}\Gamma(t,x;s,y)\\ &\quad= (-1)^{\beta}\int_{\mathbb{R}^p}\Big(\Big(\frac{\partial}{\partial \tau}\Big)^{\alpha+\beta} Z_{j_1}\cdots Z_{j_k}\gamma_{\mathbb{G}}\Big)(s-t,(y,0)^{-1}\star(x,\eta))\,\mathrm{d}\eta;\end{aligned}\tag{1.11}$$

$$\begin{aligned}&\Big(\frac{\partial}{\partial s}\Big)^{\alpha}\Big(\frac{\partial}{\partial t}\Big)^{\beta} X^x_{j_1}\cdots X^x_{j_k}X^y_{i_1}\cdots X^y_{i_h}\Gamma(t,x;s,y)\\ &\quad= (-1)^{\beta}\int_{\mathbb{R}^p}\Big(\Big(\frac{\partial}{\partial \tau}\Big)^{\alpha+\beta} Z_{j_1}\cdots Z_{j_k}((Z_{i_1}\cdots Z_{i_h}\gamma_{\mathbb{G}})\circ\widetilde{\iota})\Big)\\ &\qquad\qquad\times(s-t,(y,0)^{-1}\star(x,\eta))\,\mathrm{d}\eta\,.\end{aligned}\tag{1.12}$$

Here $\widetilde{\iota}: \mathbb{R}^{1+N} \to \mathbb{R}^{1+N}$ is the map defined by

$$\widetilde{\iota}(t,(x,\xi)) = (t,(x,\xi)^{-1}) \quad (\textit{with } t\in\mathbb{R},\ x\in\mathbb{R}^n,\ \xi\in\mathbb{R}^p),$$

and $(x, \xi)^{-1}$ is the inverse of (x, ξ) in the Lie group $\mathbb{G} = (\mathbb{R}^N, \star)$; moreover, $Z_1, \dots, Z_m$ are the lifting vector fields of $X_1, \dots, X_m$ as in Theorem 1.2.

Similarly to what was described in Remark 1.5, formulas (1.10)–(1.12) lead to global upper Gaussian estimates for the X-derivatives of arbitrary order of Γ, see [11].

The plan of the paper is now in order:

- in Section 2 we use Theorem 1.2 to prove the existence of Γ as in Theorem 1.4;
- in Section 3 we prove Theorem 1.6, furnishing the integral representation of the higher order derivatives of Γ;
- in Section 4 we briefly study the existence and the uniqueness of the solutions of the Cauchy problem for $\mathcal{H}$;
- in Section 5 we prove all the distinguished features of Γ in Theorem 1.4.

2. Existence of a global fundamental solution for $\mathcal{H}$

In the sequel, we tacitly inherit all the notations and assumptions in Theorem 1.4. In this section we shall prove the existence of a global fundamental solution for $\mathcal{H}$. To begin with, for the sake of clarity, we recall the definition of a (global) fundamental solution for a generic smooth linear PDO P.

Definition 2.1: On Euclidean space $\mathbb{R}^N$, we consider a linear PDO

$$P = \sum_{|\alpha|\leq d} a_\alpha(x)\, D_x^\alpha,$$

with smooth real-valued coefficients $a_\alpha(x)$ on $\mathbb{R}^N$. We say that a function

$$\Gamma : \{(x,y) \in \mathbb{R}^N \times \mathbb{R}^N : x \neq y\} \longrightarrow \mathbb{R}$$

is a (global) fundamental solution for P if it satisfies the following property: for every $x \in \mathbb{R}^n$, the function $\Gamma(x;\cdot)$ is locally integrable on $\mathbb{R}^N$ and

$$\text{(2.1)} \qquad \int_{\mathbb{R}^N} \Gamma(x;y)\, P^*\varphi(y)\,\mathrm{d}y = -\varphi(x) \quad \text{for every } \varphi \in C_0^\infty(\mathbb{R}^N,\mathbb{R}),$$

where P^* denotes the formal adjoint of P.

Remark 2.2: (a) The existence of a global fundamental solution for P is far from being obvious and it is, in general, a very delicate issue. In the particular case of C^∞-hypoelliptic linear PDOs P having a C^∞-hypoelliptic formal adjoint P^*, it is possible to prove the local existence of a fundamental solution on a suitable neighborhood of each point of $\mathbb{R}^N$ (see, e.g., [39]; see also [16]).

(b) Fundamental solutions are, in general, not unique since the addition of a P-harmonic function (that is, a smooth function h such that $Ph = 0$ in $\mathbb{R}^N$) to a fundamental solution produces another fundamental solution.

(c) Nonetheless, if P is C^∞-hypoelliptic and fulfills the Weak Maximum Principle on every bounded open set of $\mathbb{R}^N$, then there exists at most one fundamental solution Γ for P such that

$$\lim_{\|y\|\to\infty} \Gamma(x;y) = 0, \quad \text{for every } x \in \mathbb{R}^N.$$

Indeed, if Γ_1, Γ_2 are two such functions, then (for every fixed $x \in \mathbb{R}^N$) the map $u_x := \Gamma_1(x,\cdot) - \Gamma_2(x,\cdot)$ belongs to $L^1_{\mathrm{loc}}(\mathbb{R}^N)$ and it is a solution of $Pu_x = 0$ in the weak sense of distributions on $\mathbb{R}^N$; the hypoellipticity of P ensures that u_x is (a.e. equal to) a smooth function on $\mathbb{R}^N$ which vanishes at infinity by the assumptions on Γ_1, Γ_2; from the Weak Maximum Principle for P it is standard to obtain that $\Gamma_1 \equiv \Gamma_2$ (a.e.).

Next, as explained in Section 1, we need the following theorem. Despite its seemingly technical assumptions, this theorem is applicable in many interesting situations, as we shall discuss in Example 2.4.

THEOREM 2.3 (see [7, Theorem 2.5]): *Let P be a smooth linear PDO on $\mathbb{R}^N_z$, and let $\widetilde{P}$ be a lifting of P on $\mathbb{R}^N_z \times \mathbb{R}^p_\xi$ which satisfies the following structural assumptions:*

(S.1) *the formal adjoint R^* of $R := \widetilde{P} - P$ annihilates any $u \in C^2(\mathbb{R}^N_z \times \mathbb{R}^p_\xi)$ independent of ξ, i.e.,*

$$R^* = \sum_{\beta \neq 0} r^*_{\alpha,\beta}(z,\xi) \left(\frac{\partial}{\partial z}\right)^\alpha \left(\frac{\partial}{\partial \xi}\right)^\beta, \tag{2.2}$$

for (finitely many, possibly identically vanishing) smooth functions $r^*_{\alpha,\beta}(z,\xi)$;

(S.2) *there exists a sequence $\{\theta_j(\xi)\}_j$ in $C^\infty_0(\mathbb{R}^p, [0,1])$ such that*[3]

$$\{\theta_j = 1\} \uparrow \mathbb{R}^p \quad \text{as } j \uparrow \infty,$$

with the following property: for every compact set $K \subset \mathbb{R}^n$ and for any coefficient function $r^*_{\alpha,\beta}$ of R^* as in (2.2) one can find constants $C_{\alpha,\beta}(K)$ s.t.

$$\left| r^*_{\alpha,\beta}(z,\xi) \left(\frac{\partial}{\partial \xi}\right)^\beta \theta_j(\xi) \right| \leq C_{\alpha,\beta}(K),$$

uniformly for every $z \in K$, $\xi \in \mathbb{R}^p$ and $j \in \mathbb{N}$.

Assume that $\widetilde{P}$ admits a global fundamental solution $\widetilde{\Gamma} = \widetilde{\Gamma}((z,\xi);(\zeta,\eta))$ (with pole (z,ξ)) satisfying the following integrability assumptions:

(i) *for every fixed $z, \zeta \in \mathbb{R}^N$ with $z \neq \zeta$, we have that*

$$\eta \mapsto \widetilde{\Gamma}((z,0);(\zeta,\eta)) \quad \text{belongs to } L^1(\mathbb{R}^p),$$

(ii) *for every fixed $z \in \mathbb{R}^N$ and every compact set $K \subseteq \mathbb{R}^N$, we have that*

$$(\zeta,\eta) \mapsto \widetilde{\Gamma}((z,0);(\zeta,\eta)) \quad \text{belongs to } L^1(K \times \mathbb{R}^p).$$

Then the function Γ defined by (1.6) is a global fundamental solution for P on $\mathbb{R}^N$ with pole z.

---

[3] By this we mean that, denoting by Ω_j the set $\{\xi \in \mathbb{R}^p : \theta_j(\xi) = 1\}$, one has

$$\bigcup_{j \in \mathbb{N}} \Omega_j = \mathbb{R}^p \quad \text{and} \quad \Omega_j \subset \Omega_{j+1} \quad \text{for any } j \in \mathbb{N}.$$

Example 2.4: Theorem 2.3 can be applied in the following examples:

(1) The choices of lifting pairs $(P, \widetilde{P})$ given by

$$(\Delta_n, \Delta_{n+p}) \quad \text{and} \quad (\mathcal{H}_n, \mathcal{H}_{n+p})$$

trivially satisfy assumptions (S.1)–(S.2) and (i)–(ii) of Theorem 2.3.

(2) A less trivial example is given (as a very particular case of the PDOs in the present paper) by the "parabolic Grushin operator" on $\mathbb{R}^3_z \equiv \mathbb{R}_t \times \mathbb{R}^2_x$ (where $z = (t, x)$), i.e.,

$$G = \frac{\partial^2}{\partial x_1^2} + x_1^2 \frac{\partial^2}{\partial x_2^2} - \frac{\partial}{\partial t},$$

with a lifting given by

$$\widetilde{G} = \frac{\partial^2}{\partial x_1^2} + \Big(\frac{\partial}{\partial \xi} + x_1 \frac{\partial}{\partial x_2}\Big)^2 - \frac{\partial}{\partial t} \quad \text{on } \mathbb{R}_t \times \mathbb{R}^2_x \times \mathbb{R}_\xi.$$

As we shall see, for this last example not only (S.1)–(S.2) are satisfied, but there also exists a fundamental solution $\widetilde{\Gamma}$ for $\widetilde{G}$ satisfying hypotheses (i)–(ii) of Theorem 2.3. Therefore, we can infer that G admits a global fundamental solution given by the saturation function (1.6).

(3) More generally, in the paper [7] a meaningful case is described where Theorem 2.3 can always be applied: namely, any Hörmander sum of squares $P = \sum_{j=1}^m X_j^2$, where $X_1, \dots, X_m$ satisfy axioms (H.1)–(H.2), fulfils the assumptions of Theorem 2.3, thus admitting a global fundamental solution.

Now, we proceed as follows: first we use Theorem 1.2 to prove the existence of a lifting $\widetilde{\mathcal{H}}$ for $\mathcal{H}$ satisfying assumptions (S.1) and (S.2) of Theorem 2.3; then we show the existence of a fundamental solution $\widetilde{\Gamma}$ for $\widetilde{\mathcal{H}}$ fulfilling conditions (i) and (ii) of Theorem 2.3: the latter will then ensure the existence of a fundamental solution Γ for $\mathcal{H}$.

According to Theorem 1.2, given a family X of vector fields in $\mathbb{R}^n$ satisfying axioms (H.1)–(H.2), and setting $N = \dim(\mathrm{Lie}\{X\})$, it is possible to find a homogeneous Carnot group $\mathbb{G} = (\mathbb{R}^N, \star, D_\lambda)$ on $\mathbb{R}^N = \mathbb{R}^n_x \times \mathbb{R}^p_\xi$ (with m generators and nilpotent of step $r = \sigma_n$) and a system $\{Z_1, \dots, Z_m\}$ of Lie-generators of $\mathrm{Lie}(\mathbb{G})$ such that, for every $i = 1, \dots, m$, Z_i is a lifting of X_i. It can also be shown that the dilations $\{D_\lambda\}_{\lambda>0}$ on $\mathbb{G}$ take the form

$$D_\lambda(x, \xi) = (\delta_\lambda(x), \delta^*_\lambda(\xi)), \quad \text{for every } (x, \xi) \in \mathbb{R}^N = \mathbb{R}^n_x \times \mathbb{R}^p_\xi, \tag{2.3}$$

where δ^*_λ is another family of non-isotropic dilations on $\mathbb{R}^p$ which we write as

$$\delta^*_\lambda(\xi) = (\lambda^{\sigma^*_1}\xi_1, \dots, \lambda^{\sigma^*_p}\xi_p), \quad \xi \in \mathbb{R}^p. \tag{2.4}$$

Note that, at this stage, three homogeneous dimensions naturally arise:

$$q := \sum_{j=1}^n \sigma_j, \quad q^* := \sum_{j=1}^p \sigma^*_j, \quad Q = q + q^*, \tag{2.5}$$

which are, respectively, the homogeneous dimensions of

$$(\mathbb{R}^n, \delta_\lambda), \quad (\mathbb{R}^p, \delta^*_\lambda), \quad (\mathbb{R}^N, D_\lambda).$$

Accordingly, we fix the canonical homogeneous norms S, N, h on the spaces $\mathbb{R}^n, \mathbb{R}^p, \mathbb{R}^N$ respectively, defined by

$$S(x) := \sum_{j=1}^n |x_j|^{1/\sigma_j}, \quad N(\xi) := \sum_{j=1}^p |\xi_j|^{1/\sigma^*_j}, \quad h(x,\xi) := S(x) + N(\xi). \tag{2.6}$$

We note that, if d is any homogeneous norm on $\mathbb{G}$, then by [15, Proposition 5.1.4] we have

$$\vartheta^{-1} h(x,\xi) \le d(x,\xi) \le \vartheta h(x,\xi) \quad \forall\,(x,\xi) \in \mathbb{G}, \tag{2.7}$$

where $\vartheta = \vartheta(\mathbb{G}) \ge 1$ is a suitable constant.

Remark 2.5: For strictly technical reasons, following [7], we need to look at the following "convolution-like" map

$$F : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^p \longrightarrow \mathbb{R}^N, \quad F(x,y,\eta) := (x,0)^{-1} \star (y,\eta).$$

As in [15, Chapter 1.3]), one can prove that

$$\begin{aligned} F_1(x,y,\eta) &= y_1 - x_1, \\ F_i(x,y,\eta) &= y_i - x_i + p_i(x,y,\eta) \quad (i = 2,\dots,n), \\ F_{n+k}(x,y,\eta) &= \eta_k + q_k(x,y,\eta), \qquad (k = 1,\dots,p), \end{aligned} \tag{2.8}$$

where, p_i and q_k are polynomials with the following features:

- p_i only depends on those variables x_h, y_h and η_j such that $\sigma_h, \sigma^*_j < \sigma_i$;
- q_k only depends on those variables x_h, y_h and η_j such that $\sigma_h, \sigma^*_j < \sigma^*_k$;
- $p_i(0,y,\eta) = q_k(0,y,\eta) = 0$, for every $(y,\eta) \in \mathbb{R}^N$.

Let now $x, y \in \mathbb{R}^n$ be fixed. Since q_1 does not depend on $\eta_1, \dots, \eta_p$ and since, for every $k \in \{2, \dots, p\}$, q_k only depends on $\eta_1, \dots, \eta_{k-1}$, we see that the map

$$\Psi_{x,y} : \mathbb{R}^p \longrightarrow \mathbb{R}^p, \quad \Psi_{x,y}(\eta) := (F_{n+1}(x, y, \eta), \dots, F_{n+p}(x, y, \eta)) \tag{2.9}$$

defines a C^∞-diffeomorphism of $\mathbb{R}^p$, with polynomial components. Hence, in particular, $\Psi_{x,y}$ is a proper map, which is equivalent to saying that

$$\lim_{\|\eta\| \to \infty} \|\Psi_{x,y}(\eta)\| = \infty.$$

Furthermore, by (2.8), one has

$$\det(\mathcal{J}_{\Psi_{x,y}}(\eta)) = 1, \quad \text{for every } \eta \in \mathbb{R}^p.$$

The map $\Psi_{x,y}$ will be repeatedly used as a change of variable in integral estimates; indeed, one has

$$(x, 0)^{-1} \star (y, \Psi_{x,y}^{-1}(\eta')) = (F_1(x, y, \Psi_{x,y}^{-1}(\eta')), \dots, F_n(x, y, \Psi_{x,y}^{-1}(\eta')), \eta');$$

consequently, with the notation in (2.6), $\Psi_{x,y}$ enjoys the nice (technical) feature

$$h((x, 0)^{-1} \star (y, \Psi_{x,y}^{-1}(\eta'))) \geq N(\eta'). \tag{2.10}$$

Up to some constant, here h can be replaced by any homogeneous norm d on $\mathbb{G}$, see (2.7).

If $\mathcal{L}_{\mathbb{G}} = \sum_{j=1}^m Z_j^2$, it is straightforward to recognize that the Heat operator $\mathcal{H}_{\mathbb{G}} = \mathcal{L}_{\mathbb{G}} - \partial_t$ is a lifting of $\mathcal{H} = \mathcal{L} - \partial_t$ on $\mathbb{R}^{1+N} = \mathbb{R}_t \times \mathbb{R}^n_x \times \mathbb{R}^p_\xi$, that is,

$$\mathcal{H}_{\mathbb{G}}(u \circ \pi)(t, x, \xi) = (\mathcal{H}u)(t, x), \quad \forall\, t \in \mathbb{R},\, (x, \xi) \in \mathbb{R}^N,\, u \in C^2(\mathbb{R}^{1+n}),$$

where $\pi : \mathbb{R}^{1+N} \to \mathbb{R}^{1+n}$ is the canonical projection of $\mathbb{R}^{1+N}$ onto $\mathbb{R}^{1+n}$. Our aim is now to prove that the operator $\mathcal{H}_{\mathbb{G}}$, as a lifting of $\mathcal{H}$, satisfies the assumptions (S.1) and (S.2) in Theorem 2.3.

Lemma 2.6: *The operator $\mathcal{H}_{\mathbb{G}}$, as a lifting of $\mathcal{H}$, satisfies assumptions* (S.1)–(S.2) *in Theorem 2.3.*

Proof. (S.1): First of all we observe that, by definition, we have

$$R := \mathcal{H}_{\mathbb{G}} - \mathcal{H} = \mathcal{L}_{\mathbb{G}} - \mathcal{L} \quad \text{on } \mathbb{R}^{1+N};$$

thus, since both $\mathcal{L}_{\mathbb{G}}$ and $\mathcal{L}$ are self-adjoint (as they are sums of squares of homogeneous vector fields) we get $R^* = R$; moreover, as $\mathcal{L}_{\mathbb{G}}$ is a lifting of $\mathcal{L}$, we infer that R annihilates any C^2 function independent of ξ.

(S.2): If N is as in (2.6), we choose a function $\theta \in C_0^\infty(\mathbb{R}^p, [0,1])$ such that

$$\text{supp}(\theta) \subseteq \{\xi \in \mathbb{R}^p : N(\xi) \le 2\}; \quad \theta \equiv 1 \quad \text{on } \{\xi \in \mathbb{R}^p : N(\xi) < 1\}.$$

We define a sequence $\{\theta_j\}_j$ in $C_0^\infty(\mathbb{R}^p)$ by setting, for every $j \in \mathbb{N}$,

$$\theta_j(\xi) := \theta(\delta^*_{2^{-j}}(\xi)), \quad \text{for } \xi \in \mathbb{R}^p.$$

By arguing exactly as in [7, Theorem 4.4], after several technical computations (based on the homogeneity of the Z_j and on the structure of δ^*_λ) one can recognize that $\{\theta_j\}_j$ satisfies the properties in assumption (S.2). ∎

With Lemma 2.6 at hand, the path towards the existence of a global fundamental solution for $\mathcal{H}$ is traced in Theorem 2.3, and it consists of two parts:

(1) firstly, we prove that $\mathcal{H}_{\mathbb{G}}$ admits a fundamental solution $\Gamma_{\mathbb{G}}$;
(2) secondly, we show that such a $\Gamma_{\mathbb{G}}$ satisfies the integrability assumptions (i)–(ii) in Theorem 2.3.

As for (1), it follows from the first statement in the next result; in the sequel, in order to avoid the cumbersome notation $(t,(x,\xi))$ for the points in the product space $\mathbb{R} \times \mathbb{R}^N = \mathbb{R}_t \times (\mathbb{R}^n_x \times \mathbb{R}^p_\xi)$ we often write (t,x,ξ).

THEOREM 2.7 ([13, Theorems 2.1, 2.5]): *There exists a map*

$$\gamma_{\mathbb{G}} : \mathbb{R}^{1+N} \equiv \mathbb{R}^{1+n+p} \to \mathbb{R},$$

smooth away from the origin, such that

$$\Gamma_{\mathbb{G}}(t,x,\xi;s,y,\eta) := \gamma_{\mathbb{G}}(s-t,(x,\xi)^{-1} \star (y,\eta)) \tag{2.11}$$

is a global fundamental solution of the operator $\mathcal{H}_{\mathbb{G}} = \mathcal{L}_{\mathbb{G}} - \partial_t$. *In its turn, there exists a unique symmetric homogeneous norm on* $\mathbb{G}$ *(in the sense of* [15]*)* $d \in C^\infty(\mathbb{R}^N \setminus \{0\})$ *such that*

$$d^{2-Q}((x,\xi)^{-1} \star (y,\eta)), \quad (x,\xi) \ne (y,\eta)$$

is the global fundamental solution of $\mathcal{L}_{\mathbb{G}}$ *(where* Q *is as in* (2.5)*). The following Gaussian estimates for* $\gamma_{\mathbb{G}}$ *hold: there exists a constant* $\mathbf{c} > 0$ *such that, for every* $(x,\xi) \in \mathbb{R}^N$ *and every* $t > 0$, *one has*

$$\mathbf{c}^{-1}\, t^{-Q/2} \exp\Big(-\frac{\mathbf{c}\, d^2(x,\xi)}{t}\Big) \le \gamma_{\mathbb{G}}(t,x,\xi) \le \mathbf{c}\, t^{-Q/2} \exp\Big(-\frac{d^2(x,\xi)}{\mathbf{c}\, t}\Big). \tag{2.12}$$

Via (2.11), *global Gaussian estimates analogous to* (2.12) *hold true for* $\Gamma_{\mathbb{G}}$.

Moreover, $\gamma_{\mathbb{G}}$ satisfies the following additional properties:

(i) $\gamma_{\mathbb{G}} \geq 0$ *and* $\gamma_{\mathbb{G}}(t,x,\xi) = 0$ *if and only if* $t \leq 0$*;*

(ii) $\gamma_{\mathbb{G}}(t,x,\xi) = \gamma_{\mathbb{G}}(t,(x,\xi)^{-1})$ *for every* (t,x,ξ)*;*

(iii) *for every* $\lambda > 0$ *and every* (t,x,ξ)*, we have*

$$\gamma_{\mathbb{G}}(\lambda^2 t, \delta_\lambda x, \delta^*_\lambda \xi) = \lambda^{-Q}\, \gamma_{\mathbb{G}}(t,x,\xi),$$

where $Q = q + q^*$ *is the homogeneous dimension of the group* $\mathbb{G}$*;*

(iv) $\gamma_{\mathbb{G}}$ *vanishes at infinity, that is,* $\gamma_{\mathbb{G}}(t,x,\xi) \to 0$ *as* $\|(t,x,\xi)\| \to \infty$*;*

(v) *for every* $t > 0$*, we have*

$$\int_{\mathbb{R}^n \times \mathbb{R}^p} \gamma_{\mathbb{G}}(t,x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi = 1.$$

Finally, if we consider the function $\Gamma^*_{\mathbb{G}}$ *defined by*

$$\Gamma^*_{\mathbb{G}}(t,x,\xi;s,y,\eta) := \Gamma_{\mathbb{G}}(s,y,\eta;t,x,\xi),$$

then $\Gamma^*_{\mathbb{G}}$ *is a global fundamental solution for the adjoint operator* $\mathcal{H}^*_{\mathbb{G}} = \mathcal{L}_{\mathbb{G}} + \partial_t$*.*

As for (2), the needed integrability properties of $\Gamma_{\mathbb{G}}$ rely on the Gaussian estimates of $\gamma_{\mathbb{G}}$ in (2.12), as we prove in the next result.

Theorem 2.8: *Let the notation of Theorem 2.7 apply. Then the global fundamental solution* $\Gamma_{\mathbb{G}}$ *of* $\mathcal{H}_{\mathbb{G}}$ *satisfies the integrability assumptions* (i) *and* (ii) *in Theorem 2.3.*

Proof. We first prove that $\Gamma_{\mathbb{G}}$ satisfies assumption (i). According to Theorem 2.3, we have to show that, for fixed $(t,x) \neq (s,y) \in \mathbb{R}^{1+n}$, one has

$$\eta \mapsto \Gamma_{\mathbb{G}}(t,x,0;s,y,\eta) \in L^1(\mathbb{R}^p). \tag{2.13}$$

If $s \leq t$, the above (2.13) is an immediate consequence of Theorem 2.7, since

$$\Gamma_{\mathbb{G}}(t,x,0;s,y,\eta) \overset{(2.11)}{=} \gamma_{\mathbb{G}}(s-t,(x,0)^{-1} \star (y,\eta)) = 0, \quad \text{for every } \eta \in \mathbb{R}^p.$$

We can then assume that $s > t$. In this case, by (2.12) and by performing the change of variables $\eta = \Psi^{-1}_{x,y}(u)$ (see (2.9) in Remark 2.5), we obtain the estimate

$$\int_{\mathbb{R}^p} \Gamma_{\mathbb{G}}(t,x,0;s,y,\eta)\,\mathrm{d}\eta \leq \frac{\mathbf{c}}{(s-t)^{Q/2}} \int_{\mathbb{R}^p} \exp\Big(-\frac{d^2((x,0)^{-1} \star (y,\Psi^{-1}_{x,y}(u)))}{\mathbf{c}\,(s-t)}\Big)\mathrm{d}u.$$

On the other hand, since d is a homogeneous norm on $\mathbb{G}$, by (2.7) we know that there exists a constant $\vartheta = \vartheta(\mathbb{G}) \geq 1$ such that, for every $u \in \mathbb{R}^p$ and every $x, y \in \mathbb{R}^n$,

$$d^2((x,0)^{-1} \star (y, \Psi_{x,y}^{-1}(u)) \geq \vartheta^{-2}\, h^2((x,0)^{-1} \star (y, \Psi_{x,y}^{-1}(u))) \overset{(2.10)}{\geq} \vartheta^{-2}\, N^2(u),$$

where h, N are as in (2.6). Hence, (2.13) will follow if we show that

$$u \mapsto \varphi(u) := \exp\Big(-\frac{N^2(u)}{\mathbf{c}\,\vartheta^2\,(s-t)}\Big) \in L^1(\mathbb{R}^p). \tag{2.14}$$

Now, since $\varphi \in C(\mathbb{R}^p)$, we obviously have $\varphi \in L^1_{\text{loc}}(\mathbb{R}^p)$; moreover, since $\exp(-|r|) \leq \beta_Q\,(1+|r|)^{-Q/2}$ (for some constant $\beta_Q > 0$), we get

$$\varphi(u) \leq \frac{\beta_Q\,(\mathbf{c}\,\vartheta^2\,(s-t))^{Q/2}}{(\mathbf{c}\,\vartheta^2\,(s-t) + N^2(u))^{Q/2}} \leq \beta\,(s-t)^{Q/2}\,N^{-Q}(u), \quad \forall\, u \in \mathbb{R}^p \setminus \{0\}.$$

We are then left to prove that N^{-Q} is integrable away from 0, namely on the set $\{N \geq 1\}$. This follows from $Q > q^*$ and by a standard diadic/homogeneous argument using the annuli

$$C_j := \{u \in \mathbb{R}^p : 2^{j-1} \leq N(u) < 2^j\}.$$

To complete the proof, we are left to show that $\Gamma_{\mathbb{G}}$ also satisfies (ii) in Theorem 2.3: for any fixed $(t,x) \in \mathbb{R}^{1+n}$ and any compact set $K \subseteq \mathbb{R}^{1+n}$, we prove

$$((s,y),\eta) \mapsto \Gamma_{\mathbb{G}}(t,x,0;s,y,\eta) \in L^1(K \times \mathbb{R}^p).$$

Let a, b be such that $K \subseteq [a,b] \times \mathbb{R}^n$. We have (see (i)–(v) in Theorem 2.7)

$$\begin{aligned}
&\int_{K\times\mathbb{R}^p} \Gamma_{\mathbb{G}}(t,x,0;s,y,\eta)\,\mathrm{d}s\,\mathrm{d}y\,\mathrm{d}\eta \\
&\qquad \leq \int_a^b \Big(\int_{\mathbb{R}^n\times\mathbb{R}^p} \Gamma_{\mathbb{G}}(t,x,0;s,y,\eta)\,\mathrm{d}y\,\mathrm{d}\eta\Big)\mathrm{d}s \\
&\qquad = \int_a^b \Big(\int_{\mathbb{R}^N} \gamma_{\mathbb{G}}(s-t,(x,0)^{-1}\star(y,\eta))\,\mathrm{d}y\,\mathrm{d}\eta\Big)\mathrm{d}s \\
&\qquad\qquad\qquad \text{(change of variables } (y,\eta) = (x,0)\star(u,v)) \\
&\qquad = \int_a^b \Big(\int_{\mathbb{R}^N} \gamma_{\mathbb{G}}(s-t,u,v)\,\mathrm{d}u\,\mathrm{d}v\Big)\mathrm{d}s \\
&\qquad \leq \int_a^b 1\,\mathrm{d}s = b-a,
\end{aligned}$$

and the proof is complete. ∎

Remark 2.9: The proof of Theorem 2.8 contains the following fact: there exists a constant $\beta > 0$ such that, for every $(t,x),(s,y) \in \mathbb{R}^{1+n}$ with $s > t$ and for every $u \in \mathbb{R}^p \setminus \{0\}$, one has

$$(2.15)\quad \Gamma_{\mathbb{G}}(t,x,0;s,y,\Psi_{x,y}^{-1}(u)) = \gamma_{\mathbb{G}}(s-t,(x,0)^{-1}\star(y,\Psi_{x,y}^{-1}(u))) \le \beta\, N(u)^{-Q}.$$

On the other hand, since $\gamma_{\mathbb{G}}$ identically vanishes on $\{t \le 0\}$, the above estimate holds for every $(t,x) \in \mathbb{R}^{1+n}$ and every $(s,y,u) \in \mathbb{R}^{1+n+p}$.

By gathering together Lemma 2.6, Theorem 2.8 and Theorem 2.3, we are in a position to prove the existence of a global fundamental solution for $\mathcal{H}$.

THEOREM 2.10 (Existence of a fundamental solution for $\mathcal{H}$): *Let $\gamma_{\mathbb{G}}$, $\Gamma_{\mathbb{G}}$ and d be as in Theorem 2.7. Then the following function*

$$(2.16)\quad \Gamma(t,x;s,y) := \int_{\mathbb{R}^p} \Gamma_{\mathbb{G}}(t,x,0;s,y,\eta)\,\mathrm{d}\eta = \int_{\mathbb{R}^p} \gamma_{\mathbb{G}}(s-t,(x,0)^{-1}\star(y,\eta))\,\mathrm{d}\eta$$

is a fundamental solution for $\mathcal{H}$. Moreover, one has the estimates

$$\begin{aligned} &\mathbf{c}^{-1}(s-t)^{-Q/2}\int_{\mathbb{R}^p}\exp\Big(-\frac{\mathbf{c}\,d^2((x,0)^{-1}\star(y,\eta))}{s-t}\Big)\,\mathrm{d}\eta \\ &\qquad \le \Gamma(t,x;s,y) \le \mathbf{c}\,(s-t)^{-Q/2}\int_{\mathbb{R}^p}\exp\Big(-\frac{d^2((x,0)^{-1}\star(y,\eta))}{\mathbf{c}\,(s-t)}\Big)\,\mathrm{d}\eta, \end{aligned}$$

holding true for every $(t,x),(s,y) \in \mathbb{R}^{1+n}$ with $s > t$. Here, $\mathbf{c} > 0$ is a constant only depending on the homogeneous Carnot group $\mathbb{G}$ and on the operator $\mathcal{H}$. Finally, d can be replaced by any homogeneous norm on the homogeneous Carnot group $\mathbb{G} = (\mathbb{R}^N,\star)$.

3. Representation formulas for the derivatives

In this section, in order to prove Theorem 1.6, we use a quite versatile technique, only based on homogeneity arguments. Some of our previous arguments (of dominated-convergence type) may be attacked with this technique also; however, in the previous sections, we preferred to contain the use of homogeneity, in view of future investigations where the latter is not available.

The key ingredients for the proof of Theorem 1.6 are the following technical Lemmas 3.1 and 3.2 (where we use the notations in (2.3) and (2.5)):

Lemma 3.1: *Let* $\Omega := \{(z,\zeta,\eta) \in \mathbb{R}^{1+n} \times \mathbb{R}^{1+n} \times \mathbb{R}^p \,:\, (z,0) \neq (\zeta,\eta)\}$. *Suppose* $g \in C^\infty(\Omega)$ *is homogeneous of degree* $\alpha < -q^*$ *with respect to the family of dilations (with our usual notation)*

$$E_\lambda(z,\zeta,\eta) = E_\lambda((t,x),(s,y),\eta) = (\lambda^2 t, \delta_\lambda(x), \lambda^2 s, \delta_\lambda(y), \delta^*_\lambda(\eta)).$$

Let Z *be any smooth vector field in the* (z,ζ)*-variables, homogeneous of positive degree with respect to the family of dilations*

$$(z,\zeta) = ((t,x),(s,y)) \mapsto (\lambda^2 t, \delta_\lambda(x), \lambda^2 s, \delta_\lambda(y)).$$

Then, the following facts hold:

(1) *for any fixed* $(z,\zeta) \in \mathbb{R}^{1+n} \times \mathbb{R}^{1+n}$ *with* $z \neq \zeta$, *the map* $\eta \mapsto g(z,\zeta,\eta)$ *belongs to* $L^1(\mathbb{R}^p)$;

(2) Z *can pass under the integral sign as follows*

$$Z\left\{(z,\zeta) \mapsto \int_{\mathbb{R}^p} g(z,\zeta,\eta)\,\mathrm{d}\eta\right\} = \int_{\mathbb{R}^p} Z\{(z,\zeta) \mapsto g(z,\zeta,\eta)\}\,\mathrm{d}\eta, \tag{3.1}$$

for every $z,\zeta \in \mathbb{R}^{1+n}$ *with* $z \neq \zeta$.

Proof. (1) Let us fix $z_0,\zeta_0 \in \mathbb{R}^{1+n}$ such that $z_0 \neq \zeta_0$, and let S, N be the homogeneous norms on the spaces $\mathbb{R}^n$ and $\mathbb{R}^p$, respectively, introduced in (2.6). Moreover, we define

$$\widehat{S}(z) = \widehat{S}(t,x) := |t|^{1/2} + S(x) = |t|^{1/2} + \sum_{i=1}^n |x_i|^{1/\sigma_i}.$$

Since, obviously, $\eta \mapsto g(z_0,\zeta_0,\eta)$ belongs to $L^1_{\mathrm{loc}}(\mathbb{R}^p)$, we need to prove that

$$\int_{\{N>1\}} g(z_0,\zeta_0,\eta)\,\mathrm{d}\eta < \infty.$$

To this end, we first choose $\rho > 0$ in such a way that $z_0,\zeta_0 \in \{\widehat{S}(z) \le \rho\}$ and we observe that, since the set

$$K := \{\widehat{S} \le \rho\}^2 \times \{N = 1\}$$

is compact and contained in Ω, there exists $c > 0$ such that

$$|g(z,\zeta,\eta)| \le c \quad \text{for every } z,\zeta \in \{\widehat{S} \le \rho\} \text{ and } \eta \in \{N = 1\}. \tag{3.2}$$

On the other hand, if $\eta\in\mathbb{R}^p$ is such that $N(\eta)>1$ and if we set $\lambda:=1/N(\eta)\in(0,1)$, it is readily seen that $(z_0', \zeta_0', \eta') = E_\lambda(z_0, \zeta_0, \eta) \in K$; thus, by (3.2) and the E_λ-homogeneity of g, we get

$$|g(z_0, \zeta_0, \eta)| \le c\, N(\eta)^\alpha \quad \text{for every } \eta \in \mathbb{R}^p \text{ with } N(\eta) > 1.$$

Since $\alpha < -q^*$, the map

$$\eta \mapsto g(z_0, \zeta_0, \eta)$$

is integrable on $\{N > 1\}$, as desired.

(2) We first prove that, if Z is a smooth vector field as in the statement of the lemma, fixing $z, \zeta \in \mathbb{R}^{1+n}$ with $z \neq \zeta$, the function

$$\Phi(\eta) := Z\{(z, \zeta) \mapsto g(z, \zeta, \eta)\}$$

is η-integrable on the whole of $\mathbb{R}^p$.

To this end we observe that, if we think of Z as a vector field defined on $\mathbb{R}^{1+n}_z \times \mathbb{R}^{1+n}_\zeta \times \mathbb{R}^p_\eta$ but acting only in the (z, ζ) variables (and not on η), then Z is E_λ-homogeneous of degree m; as a consequence, Φ is E_λ-homogeneous of degree $\alpha - m$. Since, by assumption, $m \ge 0$ and $\alpha < -q^*$, we derive from statement (1) that $\Phi(\eta)$ belongs to $L^1(\mathbb{R}^p)$ for every $z, \zeta \in \mathbb{R}^{1+n}$ with $z \neq \zeta$. We now turn to prove identity (3.1). To this aim, we first write

$$\int_{\mathbb{R}^p} \Phi(\eta)\, \mathrm{d}\eta = \int_{\{N(\eta)\le 1\}} \Phi(\eta)\, \mathrm{d}\eta + \int_{\{N(\eta)>1\}} \Phi(\eta)\, \mathrm{d}\eta.$$

We then fix $z_0, \zeta_0 \in \mathbb{R}^{1+n}$ such that $z_0 \neq \zeta_0$ and we show that the function Φ can be dominated, both on $A = \{N \le 1\}$ and on $B = \{N > 1\}$, by an integrable function which does not depend on (z, ζ) (at least for every (z, ζ) in a small neighborhood of (z_0, ζ_0)). As for the first set, we choose two bounded neighborhoods $V_1, V_2 \subseteq \mathbb{R}^{1+n}$ of z_0 and ζ_0, respectively, such that

$$\overline{V}_1 \cap \overline{V}_2 = \varnothing; \tag{3.3}$$

then, we set $K := \overline{V}_1 \times \overline{V}_2 \times \{N \le 1\}$. On account of (3.3), we see that K is a compact subset of Ω; thus, there exists a constant $c > 0$ such that

$$|\Phi(\eta)| = |Z\{(z, \zeta) \mapsto g(z, \zeta, \eta)\}| \le c,$$

for every $z, \zeta \in \overline{V}_1 \times \overline{V}_2$ and every $\eta \in \{N \le 1\}$.

As for the set B, we argue as in the previous statement (1): if $\rho > 0$ is such that $z_0, \zeta_0 \in \{\widehat{S} \le \rho\}$, from the E_λ-homogeneity of Φ we infer the existence of another constant $c' > 0$ such that

$$|\Phi(\eta)| = |Z\{(z,\zeta) \mapsto g(z,\zeta,\eta)\}| \le c' \, N(\eta)^{\alpha - m},$$

for every $z, \zeta \in \{\widehat{S} \le 1\}$ and every $\eta \in \{N > 1\}$; since $\alpha - m \le \alpha < -q^*$, the function $N^{\alpha-m}$ is integrable on B. This ends the proof. ∎

Lemma 3.2: *Let $\rho \in C^\infty(\mathbb{R}^{1+N} \setminus \{0\})$ be homogeneous of degree $d < -q^*$ with respect to the family of dilations (see (2.3))*

$$F_\lambda(t,x,\xi) := (\lambda^2 t, D_\lambda(x,\xi)) = (\lambda^2 t, \delta_\lambda(x), \delta^*_\lambda(\xi)).$$

Then, for every $j = 1, \dots, m$ we have

$$\begin{aligned}\int_{\mathbb{R}^p} X_j^y \{y \mapsto \rho(s-t,(x,0)^{-1} \star (y,\eta))\} \, \mathrm{d}\eta \\ = \int_{\mathbb{R}^p} (Z_j\rho)(s-t,(x,0)^{-1} \star (y,\eta)) \, \mathrm{d}\eta,\end{aligned} \tag{3.4}$$

where Z_j is the lifting vector field of X_j as in Theorem 1.2.

Proof. First of all, by Lemma 3.1-(1), the two integrand functions appearing in (3.4) are η-integrable on $\mathbb{R}^p$; moreover, since Z_j is a lifting of X_j, one has

$$Z_j^{(y,\eta)} = X_j^y + R_j, \quad \text{where } R_j = \sum_{k=1}^p r_{j,k}(y,\eta) \frac{\partial}{\partial \eta_k},$$

where $r_{j,k}$ is smooth and D_λ-homogeneous of degree $\sigma^*_k - 1$ (see (2.4)). In particular, $r_{j,k}$ does not depend on η_k. Now, since Z_j is left-invariant on the group $\mathbb{G} = (\mathbb{R}^N, \star)$, it is not difficult to recognize that[4]

$$Z_j^{(y,\eta)}\{(y,\eta) \mapsto \rho(s-t,(x,0)^{-1} \star (y,\eta))\} = (Z_j\rho)(s-t,(x,0)^{-1} \star (y,\eta)).$$

[4] In fact, Z_j is left-invariant on the product group $(\mathbb{R}^{1+N}, \bullet)$, where

$$(t,x,\xi) \bullet (s,y,\eta) := (t+s,(x,\xi) \star (y,\eta)).$$

As a consequence, we have the following chain of identities

$$\begin{aligned}\int_{\mathbb{R}^p} X_j^y\{y \mapsto \rho(s-t,(x,0)^{-1}\star(y,\eta))\}\,\mathrm{d}\eta \\ &= \int_{\mathbb{R}^p} (Z_j^{(y,\eta)} - R_j)\{(y,\eta)\mapsto \rho(s-t,(x,0)^{-1}\star(y,\eta))\}\,\mathrm{d}\eta \\ &= \int_{\mathbb{R}^p} (Z_j\rho)(s-t,(x,0)^{-1}\star(y,\eta))\,\mathrm{d}\eta \\ &\quad - \int_{\mathbb{R}^p} R_j\{\eta\mapsto \rho(s-t,(x,0)^{-1}\star(y,\eta))\}\,\mathrm{d}\eta.\end{aligned}$$

In view of this computation, the desired Equality (3.4) follows if we show that

$$\int_{\mathbb{R}^p} R_j\{\eta\mapsto \rho(s-t,(x,0)^{-1}\star(y,\eta))\}\,\mathrm{d}\eta = 0. \tag{3.5}$$

In its turn, identity (3.5) can be proved as follows: first of all, since $r_{j,k}$ is independent of η_k, by Fubini's theorem we can write

$$\begin{aligned}\int_{\mathbb{R}^p} R_j\{\eta\mapsto \rho(s-t,(x,0)^{-1}\star(y,\eta))\}\,\mathrm{d}\eta \\ &= \sum_{k=1}^p \int_{\mathbb{R}^p} r_{j,k}(y,\eta)\,\frac{\partial}{\partial\eta_k}\{\eta\mapsto \rho(s-t,(x,0)^{-1}\star(y,\eta))\}\,\mathrm{d}\eta \\ &= \sum_{k=1}^p \int_{\mathbb{R}^p} \frac{\partial}{\partial\eta_k}\{r_{j,k}(y,\eta)\,\rho(s-t,(x,0)^{-1}\star(y,\eta))\}\,\mathrm{d}\eta \\ &= \sum_{k=1}^p \int_{\mathbb{R}^{p-1}} \left(\int_{-\infty}^{\infty} \frac{\partial}{\partial\eta_k}\{r_{j,k}(y,\eta)\,\rho(s-t,(x,0)^{-1}\star(y,\eta))\}\,\mathrm{d}\eta_k\right)\mathrm{d}\widehat{\eta}_k,\end{aligned}$$

where $\widehat{\eta}_k$ denotes the $(p-1)$-tuple of variables obtained by removing η_k from η. On the other hand, since ρ vanishes at infinity (as it is F_λ-homogeneous of negative degree) and since $\|(x,0)^{-1}\star(y,\eta)\|\to\infty$ as $\eta_k\to\pm\infty$, one has

$$\begin{aligned}\lim_{\eta_k\to\pm\infty} r_{j,k}(y,\eta)\,\rho(s-t,(x,0)^{-1}\star(y,\eta)) \\ &= r_{j,k}(y,\eta)\cdot \lim_{\eta_k\to\pm\infty}\rho(s-t,(x,0)^{-1}\star(y,\eta)) \\ &= 0.\end{aligned}$$

This ends the proof. ∎

Thanks to Lemmas 3.1 and 3.2, we can now provide the

Proof of Theorem 1.6. For the sake of readability, we split the proof of formulas (1.10)–(1.12) into three different steps.

Step I: We first prove formula (1.10). To this end we observe that, by repeatedly applying Lemma 3.1, we have the representation

$$\begin{aligned}&\Big(\frac{\partial}{\partial s}\Big)^{\alpha}\Big(\frac{\partial}{\partial t}\Big)^{\beta} X^y_{i_1}\cdots X^y_{i_h}\Gamma(t,x;s,y)\\ &=\int_{\mathbb{R}^p}\Big(\frac{\partial}{\partial s}\Big)^{\alpha}\Big(\frac{\partial}{\partial t}\Big)^{\beta} X^y_{i_1}\cdots X^y_{i_h}\{(t,s,y)\mapsto\gamma_{\mathbb{G}}(s-t,(x,0)^{-1}\star(y,\eta))\}\,\mathrm{d}\eta\\ &=(-1)^{\beta}\int_{\mathbb{R}^p} X^y_{i_1}\cdots X^y_{i_h}\{y\mapsto((\partial_\tau)^{\alpha+\beta}\gamma_{\mathbb{G}})(s-t,(x,0)^{-1}\star(y,\eta))\}\,\mathrm{d}\eta.\end{aligned}\tag{3.6}$$

Formula (1.10) can now be obtained from (3.6) by repeatedly applying Lemma 3.2: in fact, on account of Theorem 2.7-(iii) we know that the functions

$$\begin{aligned}\rho_1 &= (\partial_\tau)^{\alpha+\beta}\gamma_{\mathbb{G}},\\ \rho_2 &= Z_{i_h}(\partial_\tau)^{\alpha+\beta}\gamma_{\mathbb{G}},\\ &\vdots\\ \rho_{h+1} &= Z_{i_2}\cdots Z_{i_h}(\partial_\tau)^{\alpha+\beta}\gamma_{\mathbb{G}}\end{aligned}$$

are smooth on $\mathbb{R}^{1+N}\setminus\{0\}$ and F_λ-homogeneous of degrees

$$\begin{aligned}d_1 &= -Q-2\alpha-2\beta,\\ d_2 &= -Q-2\alpha-2\beta-1,\\ &\vdots\\ d_{h+1} &= -Q-2\alpha-2\beta-h+1,\end{aligned}$$

respectively. Since $Q=q+q^*$, we clearly have $d_1,\dots,d_{h+1}<-q^*$.

Step II: We prove formula (1.11). To this end, in order to apply Lemma 3.2, we first introduce the following map:

$$\phi_{x,y}:\mathbb{R}^p\to\mathbb{R}^p,\quad \phi_{x,y}(u):=\pi_p((x,0)\star(x,u)^{-1}\star(y,0)),$$

where π_p is the projection of $\mathbb{R}^N=\mathbb{R}^n\times\mathbb{R}^p$ onto $\mathbb{R}^p$. By exploiting the D_λ-homogeneity of the component functions of $\star$, it is not difficult to check that $\phi_{x,y}$ is a smooth diffeomorphism of $\mathbb{R}^p$, further satisfying

$$\det|\mathcal{J}_{\phi_{x,y}}(u)|=1,\quad \text{for every } u\in\mathbb{R}^p.$$

Moreover, by using the explicit construction of the group $\mathbb{G}$ in Theorem 2.3 (see [7] for all the details), one can prove that

$$(x,0)^{-1} \star (y, \phi_{x,y}(u)) = (x,u)^{-1} \star (y,0), \quad \forall\, x,y \in \mathbb{R}^n,\, u \in \mathbb{R}^p.$$

Gathering together the above facts, and performing the change of variable $\eta = \phi_{x,y}(u)$, we then obtain the following alternative representation of Γ (also recall the symmetry of $\gamma_{\mathbb{G}}$, see Theorem 2.7-(ii)):

$$\begin{aligned} \Gamma(t,x;s,y) &= \int_{\mathbb{R}^p} \gamma_{\mathbb{G}}(s-t,(x,u)^{-1} \star (y,0))\,\mathrm{d}u \\ &= \int_{\mathbb{R}^p} \gamma_{\mathbb{G}}(s-t,(y,0)^{-1} \star (x,u))\,\mathrm{d}u. \end{aligned} \tag{3.7}$$

Now, starting from (3.7) and repeatedly using Lemma 3.1, we get

$$\begin{aligned} &\Big(\frac{\partial}{\partial s}\Big)^{\alpha}\Big(\frac{\partial}{\partial t}\Big)^{\beta} X^x_{j_1}\cdots X^x_{j_k}\Gamma(t,x;s,y) \\ &\quad = \int_{\mathbb{R}^p} \Big(\frac{\partial}{\partial s}\Big)^{\alpha}\Big(\frac{\partial}{\partial t}\Big)^{\beta} X^x_{j_1}\cdots X^x_{j_k}\{(t,s,x)\mapsto \gamma_{\mathbb{G}}(s-t,(y,0)^{-1}\star(x,u))\}\,\mathrm{d}u \\ &\quad = (-1)^{\beta}\int_{\mathbb{R}^p} X^x_{j_1}\cdots X^x_{j_k}\{x\mapsto ((\partial_\tau)^{\alpha+\beta}\gamma_{\mathbb{G}})(s-t,(y,0)^{-1}\star(x,u))\}\,\mathrm{d}u. \end{aligned}$$

From this, by repeatedly applying Lemma 3.2 (with x in place of y) and by arguing exactly as in the previous step, we obtain the desired (1.11).

Step III: We finally prove formula (1.12). To begin with, we use (1.10) and the change of variable $\eta = \phi_{x,y}(u)$ introduced in Step II to write

$$\begin{aligned} &\Big(\frac{\partial}{\partial s}\Big)^{\alpha}\Big(\frac{\partial}{\partial t}\Big)^{\beta} X^y_{i_1}\cdots X^y_{i_h}\Gamma(t,x;s,y) \\ &\quad = (-1)^{\beta}\int_{\mathbb{R}^p} (Z_{i_1}\cdots Z_{i_h}(\partial_\tau)^{\alpha+\beta}\gamma_{\mathbb{G}})(s-t,(x,u)^{-1}\star(y,0))\,\mathrm{d}u \\ &\qquad\qquad\qquad\qquad \text{(setting } \rho := (Z_{i_1}\cdots Z_{i_h}(\partial_\tau)^{\alpha+\beta}\gamma_{\mathbb{G}})\circ\widetilde{\iota}\,) \\ &\quad = (-1)^{\beta}\int_{\mathbb{R}^p} \rho(s-t,(y,0)^{-1}\star(x,u))\,\mathrm{d}u. \end{aligned}$$

From this, by repeatedly applying Lemma 3.2 and by arguing exactly in Step II (notice that $\rho, Z_{j_k}\rho, \ldots, Z_{j_2}\cdots Z_{j_k}\rho$ are all F_λ-homogeneous of degree less than $-q^*$), we obtain the desired (1.12). This ends the proof. ∎

4. An application to the Cauchy problem for $\mathcal{H}$

In this section we turn our attention to the Cauchy problem for $\mathcal{H}$. In doing this, we shall use many of the properties of Γ in Theorem 1.4, whose proof is postponed to Section 5.

To begin with, let $\varphi \in C(\mathbb{R}^n)$ and $\Omega = (0,\infty)\times\mathbb{R}^n$. We say that a function $u : \Omega \to \mathbb{R}$ is a (classical) solution of the Cauchy problem

$$\begin{cases} \mathcal{H}u = 0 & \text{in } \Omega, \\ u(0,x) = \varphi(x) & \text{for } x \in \mathbb{R}^n, \end{cases} \tag{4.1}$$

if the following conditions are satisfied: $u \in C^2(\Omega)$ and $\mathcal{H}u = 0$ on Ω; u is continuous up to $\overline{\Omega}$ and $u(0,\cdot) = \varphi$ pointwise on $\mathbb{R}^n$. By the C^∞-hypoellipticity of $\mathcal{H}$, any classical solution of (4.1) is smooth on Ω. The following theorem is the main result of this section.

Theorem 4.1: *In the above notations, if φ is continuous and bounded, then*

$$u : \Omega \longrightarrow \mathbb{R} \quad u(t,x) := \int_{\mathbb{R}^n} \Gamma(0,y;t,x)\,\varphi(y)\,\mathrm{d}y \tag{4.2}$$

is the unique bounded classical solution of (4.1)*; furthermore, it satisfies*

$$\sup_{\Omega} |u| \le \sup_{\mathbb{R}^n} |\varphi|. \tag{4.3}$$

Proof. Since the uniqueness problem is of independent interest (and since we prove it with a totally different technique), this is postponed to Proposition 4.2. Then we focus on the rest of the assertion.

First of all, by (ii), (vii) in Theorem 1.4, u is well posed and it satisfies (4.3): indeed, for $t > 0$,

$$|u(t,x)| \le \|\varphi\|_\infty \int_{\mathbb{R}^n} \Gamma(0,y;t,x)\,\mathrm{d}y = \|\varphi\|_\infty \int_{\mathbb{R}^n} \Gamma(0,x;t,y)\,\mathrm{d}y = \|\varphi\|_\infty.$$

The rest of the proof is split in three steps.

Step I: In this step we prove that $u \in C(\Omega)$. To this end, let $z_0 = (t_0, x_0)$ be a fixed point in Ω and let $r > 0$ be such that

$$K := [t_0 - r, t_0 + r] \times \overline{B}(x_0, r) \subseteq \Omega.$$

Moreover, let $z_n \to z_0$; we can assume that $z_n \in K$. By arguing as in the proof of Lemma 5.3-(b), one can easily recognize that

$$(y,\eta) \mapsto \Gamma_{\mathbb{G}}(0,y,0;t,x,\eta) \quad \text{is in } L^1(\mathbb{R}^N), \text{ for every } (t,x) \in \mathbb{R}^{1+n}.$$

Therefore, by Fubini's theorem, for every $n \geq 0$ we can write

$$u(z_n) = u(t_n, x_n) \overset{(2.11)}{=} \int_{\mathbb{R}^n \times \mathbb{R}^p} \gamma_{\mathbb{G}}(t_n, (y,0)^{-1} \star (x_n, \eta))\, \varphi(y)\, \mathrm{d}y\, \mathrm{d}\eta$$
$$= \int_{\mathbb{R}^n \times \mathbb{R}^p} \gamma_{\mathbb{G}}(t_n, u, v)\, \varphi(C_{x_n}^{-1}(u,v))\, \mathrm{d}u\, \mathrm{d}v,$$

where we have used the smooth diffeomorphism $C_x(y,\eta) := (y,0)^{-1} \star (x,\eta)$ (whose Jacobian determinant is 1). A dominated convergence argument is now in order; we skip the details, apart from the non-trivial estimate (based on the Gaussian bound in (2.12))

$$|\gamma_{\mathbb{G}}(t_n, u, v)\, \varphi(C_{x_n}^{-1}(u,v))| \leq \mathbf{c}\, (t_0 - r)^{-Q/2}\, \|\varphi\|_\infty \exp\Big(- \frac{d^2(u,v)}{\mathbf{c}\, (t_0 - r)} \Big) =: f(u,v).$$

In turn, the integrability of f is ensured by the estimate

$$\exp\Big(- \frac{d^2(u,v)}{\mathbf{c}\, (t_0 - r)} \Big) \leq \exp\Big(- \frac{S^2(u)}{\mathbf{c}\, \vartheta^2\, (t_0 - r)} \Big) \exp\Big(- \frac{N^2(v)}{\mathbf{c}\, \vartheta^2\, (t_0 - r)} \Big),$$

where S, N are as in (2.6), and $\vartheta = \vartheta(\mathbb{G}) \geq 1$ is as in (2.7) (by arguing as in the few lines after (2.14), one gets the integrability of the above right-hand side).

Step II: Since u is continuous by Step I, if we show that $\mathcal{H}u = 0$ in $\mathcal{D}'(\Omega)$, the hypoellipticity of $\mathcal{H}$ will imply that $u \in C^\infty(\Omega)$ and $\mathcal{H}u = 0$ on Ω. To this end, let $\psi \in C_0^\infty(\Omega)$. We have

$$\int_{\mathbb{R}^{1+n}} u(t,x)\, \mathcal{H}^* \psi(t,x)\, \mathrm{d}t\, \mathrm{d}x$$
$$= \int_{\mathbb{R}^n} \Big(\int_{\mathbb{R}^{1+n}} \Gamma(0,y;t,x)\, \mathcal{H}^* \psi(t,x)\, \mathrm{d}t\, \mathrm{d}x \Big) \varphi(y)\, \mathrm{d}y$$
$$\overset{(2.1)}{=} - \int_{\mathbb{R}^n} \psi(0,y)\, \varphi(y)\, \mathrm{d}y = 0.$$

Here we applied Fubini's Theorem, whose legitimacy is due to the estimate (see also (vii) in Theorem 1.4)

$$\int_{\mathrm{supp}(\psi)} \Big(\int_{\mathbb{R}^n} \Gamma(0,x;t,y)\, \mathrm{d}y \Big) \mathrm{d}t\, \mathrm{d}x \leq \mathrm{meas}(\mathrm{supp}(\psi)) < \infty.$$

Step III: To end the proof, we must show that u satisfies the needed initial condition. To this end, let $x \in \mathbb{R}^n$ be fixed and let $t_n \in (0,1)$ be vanishing, as $n \to \infty$. Arguing as in Step I (and with the aid of (ii) and (vii) of Theorem 1.4), one gets

$$\begin{aligned}
&|u(t_n, x) - \varphi(x)| \\
&\qquad \le \int_{\mathbb{R}^n \times \mathbb{R}^p} \gamma_{\mathbb{G}}(t_n, u, v)\, |\varphi(C_x^{-1}(u,v)) - \varphi(x)|\, \mathrm{d}u\, \mathrm{d}v \\
&\qquad \overset{(2.12)}{\le} \mathbf{c}\,(t_n)^{-Q/2} \int_{\mathbb{R}^n \times \mathbb{R}^p} \exp\Big(-\frac{d^2(u,v)}{\mathbf{c}\, t_n}\Big) |\varphi(C_x^{-1}(u,v)) - \varphi(x)|\, \mathrm{d}u\, \mathrm{d}v \\
&\qquad = \mathbf{c} \int_{\mathbb{R}^n \times \mathbb{R}^p} \exp\Big(-\frac{d^2(u',v')}{\mathbf{c}}\Big) |\varphi((C_x^{-1} \circ D_{\sqrt{t_n}})(u',v')) - \varphi(x)|\, \mathrm{d}u'\, \mathrm{d}v'.
\end{aligned}$$

In the last equality we used the change of variable $(u,v) = D_{\sqrt{t_n}}(u',v')$, and D_λ-homogeneity of d. Since one clearly has (due to the continuity of φ)

$$\lim_{n \to \infty} \varphi((C_x^{-1} \circ D_{\sqrt{t_n}})(w,z)) = \varphi(C_x^{-1}(0,0)) = \varphi(x),$$

we deduce that $u(t_n, x) \to \varphi(x)$, thanks to a dominated-convergence argument (see Step I) based on

$$\begin{aligned}
\exp\Big(-\frac{d^2(u',v')}{\mathbf{c}}\Big) &|\varphi((C_x^{-1} \circ D_{\sqrt{t_n}})(u',v')) - \varphi(x)| \\
&\le 2\,\|\varphi\|_\infty \exp\Big(-\frac{d^2(u',v')}{\mathbf{c}}\Big).
\end{aligned}$$

This ends the proof. ∎

We now turn to the uniqueness of the solution of the Cauchy problem for $\mathcal{H}$:

Proposition 4.2: *The only bounded classical solution of* (4.1) *when* $\varphi \equiv 0$ *is the null function. As a consequence,* (4.2) *is the unique bounded solution of* (4.1).

Proof. Let u be a bounded classical solution of the homogeneous Cauchy problem for $\mathcal{H}$, and let $v(t,x,\xi) := u(t,x)$ defined on $\mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^p$.

Clearly, $v(0,x,\xi) = u(0,x) = 0$ for every $(x,\xi) \in \mathbb{R}^n \times \mathbb{R}^p$; moreover, since $\mathcal{H}_{\mathbb{G}}$ is a lifting of $\mathcal{H}$ on $\mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^p$, we get $\mathcal{H}_{\mathbb{G}} v = \mathcal{H} u = 0$ point-wise on $(0,\infty) \times \mathbb{R}^n \times \mathbb{R}^p$. Summing up, v is a bounded solution of the homogeneous Cauchy problem for $\mathcal{H}_{\mathbb{G}}$. Since we have transferred our setting to that of Carnot groups $\mathbb{G}$, we are consequently entitled to apply [13, Theorem 2.1], which ensures that $v \equiv 0$, and this ends the proof. ∎

5. Further properties of Γ

This appendix is completely devoted to establishing the properties (i)–(x) of Γ in Theorem 1.4. Throughout the section, Γ is as in (1.9) and all the notations used so far are tacitly understood.

Some of the properties we aim to prove are consequences of Theorem 2.7:

- (i) is a trivial consequence of the integral form of Γ in (1.8) jointly with Theorem 2.7-(i).
- The first part of (ii) comes from (1.8); the symmetry in x, y will be proved later on.
- (iii) follows from (iii) of Theorem 2.7 together with the change of variable $\eta = \delta^*_\lambda(\eta')$ (see also (2.3) and (2.5)).
- (vii) follows from (v) of Theorem 2.7 by making use of the change of variable $(y, \eta) = (x, 0) \star (y', \eta')$.
- (ix) has been proved in Section 4.

Despite the simplicity of its statement, the proof of the following proposition is technical and is a prototype for many of the next proofs.

Proposition 5.1: *The following facts hold true:*

(a) Γ *is continuous out of the diagonal of* $\mathbb{R}^{1+n} \times \mathbb{R}^{1+n}$.

(b) *For every fixed compact set* $K \subseteq \mathbb{R}^{1+n}$, *we have*

$$\sup_{z \in K} \Gamma(z; \zeta) \to 0 \quad \text{as } \|\zeta\| \to \infty.$$

(c) *For every fixed* $\zeta \in \mathbb{R}^{1+n}$, *we have*

$$\Gamma(z; \zeta) \to 0 \quad \text{as } \|z\| \to \infty.$$

Proof. (a) It is a dominated-convergence argument applied to the limit

$$\lim_{n\to\infty} \Gamma(z_n; \zeta_n) = \lim_{n\to\infty} \int_{\mathbb{R}^p} \gamma_{\mathbb{G}}(s_n - t_n, (x_n, 0)^{-1} \star (y_n, \eta))\, \mathrm{d}\eta,$$

where $z_n = (t_n, x_n) \to z_0$, $\zeta_n = (s_n, y_n) \to \zeta_0$ and $z_0 \neq \zeta_0$; this argument is based on the ingredients:

- a proper use of the change of variable $\eta = \Psi^{-1}_{x_n, y_n}(\eta')$ in Remark 2.5;
- the continuity of $\gamma_{\mathbb{G}}$ out of the origin of $\mathbb{R}^{1+N}$;
- the bound (2.15) in Remark 2.15 (together with the integrability of $N^{-Q}(\eta')$ on the set $\{N(\eta') > 1\}$).

(b) It is dominated-convergence, applied to the right-hand limit

$$\lim_{n\to\infty}\sup_{z\in K}\Gamma(z;\zeta_n)\leq \lim_{n\to\infty}\int_{\mathbb{R}^p}\sup_{(t,x)\in K}\gamma_{\mathbb{G}}(s_n-t,(x,0)^{-1}\star(y_n,\eta))\,\mathrm{d}\eta,$$

where $z=(t,x)$, $\zeta_n=(s_n,y_n)\to\infty$ and K is compact in $\mathbb{R}^{1+n}$; we also used:

- another use of the change of variable $\eta=\Psi^{-1}_{x,y_n}(\eta')$;
- the vanishing of $\gamma_{\mathbb{G}}$ at infinity (see (iv) in Theorem 2.7), together with the change of variable $\eta=\Phi_{x,y_n}(\eta')$ and the fact that

$$\lim_{n\to\infty}\|(s_n-t,(x,0)^{-1}\star(y_n,\Psi_{x,y_n}(\eta')))\|=\infty, \tag{5.1}$$

  uniformly for $z\in K$ and $\eta'\in\mathbb{R}^p$;
- the bound (2.15) in Remark 2.15.

(c) This is similar to (b); (5.1) is replaced by the (weaker) information

$$\lim_{n\to\infty}\|(s-t_n,(x_n,0)^{-1}\star(y,\Psi_{x_n,y}(\eta')))\|=\infty\quad\text{uniformly for }\eta'\in\mathbb{R}^p,$$

for any fixed $\zeta=(s,y)$. This ends the proof. ∎

Corollary 5.2: *For every fixed $z\in\mathbb{R}^{1+n}$, the map $\zeta\mapsto\Gamma(z;\zeta)$ is smooth and $\mathcal{H}$-harmonic on $\mathbb{R}^{1+n}\setminus\{z\}$ (i.e., $\mathcal{H}(\Gamma(z;\cdot))=0$ on $\mathbb{R}^{1+n}\setminus\{z\}$).*

Proof. By the C^∞-hypoellipticity of $\mathcal{H}$, we infer that $\Gamma(z;\cdot)$ coincides almost everywhere with a smooth $\mathcal{H}$-harmonic function on $\mathbb{R}^{1+n}\setminus\{z\}$; the 'almost everywhere' can be dropped in view of (a) in Proposition 5.1. ∎

The following results (a) and (c) establish property (vi) of Theorem 1.4, whereas (b) is technical for the study of the Cauchy problem for $\mathcal{H}$.

Lemma 5.3: *The following facts hold true:*

(a) $\Gamma\in L^1_{\mathrm{loc}}(\mathbb{R}^{1+n}\times\mathbb{R}^{1+n})$.

(b) *For every fixed $(s,y)\in\mathbb{R}^{1+n}$, we have*

$$(t,x,\eta)\mapsto\Gamma_{\mathbb{G}}(t,x,0;s,y,\eta)\in L^1_{\mathrm{loc}}(\mathbb{R}^{1+n+p}). \tag{5.2}$$

(c) *For every fixed $\zeta\in\mathbb{R}^{1+n}$, we have $\Gamma(\cdot;\zeta)\in L^1_{\mathrm{loc}}(\mathbb{R}^{1+n})$.*

Proof. (a) Let $K_1,K_2\subseteq\mathbb{R}^{1+n}$ be compact sets and let $T>0$ be so large that $K_2\subseteq[-T,T]\times\mathbb{R}^n$. By Tonelli's Theorem and (vii) in Theorem 1.4, we have

$$\int_{K_1\times K_2}\Gamma(z;\zeta)\,\mathrm{d}z\,\mathrm{d}\zeta\leq 2\,T\,\mathrm{meas}(K_1).$$

(b) Let $\zeta = (s, y) \in \mathbb{R}^{1+n}$, and let $K \subseteq \mathbb{R}^{1+N}$ be compact. It can be proved (see Remark 2.5) that the map

$$H_y : \mathbb{R}^{1+n+p} \longrightarrow \mathbb{R}^{1+n+p}, \quad H_y(t, x, \eta) := (s - t, (x, 0)^{-1} \star (y, \eta))$$

is a smooth diffeomorphism with identically 1 Jacobian determinant. Therefore

$$\begin{aligned}\int_K \Gamma_{\mathbb{G}}(t, x, 0; s, y, \eta)\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}\eta &= \int_K \gamma_{\mathbb{G}}(s - t, (x, 0)^{-1} \star (y, \eta))\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}\eta \\ &= \int_{H_y^{-1}(K)} \gamma_{\mathbb{G}}(\tau, z)\,\mathrm{d}\tau\,\mathrm{d}z < \infty,\end{aligned}$$

since $\gamma_{\mathbb{G}}$ is locally integrable and $H_y^{-1}(K)$ is compact.

(c) Let $K \subseteq \mathbb{R}^{1+n}$ be a compact set. The map $T(t, x, u) := (t, x, \Psi_{x,y}^{-1}(u))$ is a diffeomorphism of $\mathbb{R}^{1+n+p}$ with Jacobian determinant equal to 1. Thus

$$\begin{aligned}\int_K \Gamma(z; \zeta)\,\mathrm{d}z &= \int_{K\times\mathbb{R}^p} \gamma_{\mathbb{G}}(s - t, (x, 0)^{-1} \star (y, \Psi_{x,y}^{-1}(u)))\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}u \\ &= \int_{K\times\{N\le 1\}} \{\cdots\}\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}u + \int_{K\times\{N>1\}} \{\cdots\}\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}u =: \mathrm{I} + \mathrm{II},\end{aligned}$$

where N is as in (2.6). (5.2) implies $\mathrm{I} < \infty$, and (2.15) gives $\mathrm{II} < \infty$. ∎

Thanks to Lemma 5.3, we can prove property (viii) of Theorem 1.4:

Proposition 5.4: *For every fixed $\varphi \in C_0^\infty(\mathbb{R}^{1+n})$, the function*

$$\Lambda_\varphi : \mathbb{R}^{1+n} \longrightarrow \mathbb{R}, \quad \Lambda_\varphi(\zeta) := \int_{\mathbb{R}^{1+n}} \Gamma(z; \zeta)\,\varphi(z)\,\mathrm{d}z$$

is well-defined and it satisfies the following properties:

(a) $\Lambda_\varphi \in C^\infty(\mathbb{R}^{1+n})$ *and* $\mathcal{H}(\Lambda_\varphi) = -\varphi$ *on* $\mathbb{R}^{1+n}$*;*
(b) $\Lambda_\varphi(\zeta) \longrightarrow 0$ *as* $\|\zeta\| \to \infty$*;*
(c) *for every* $\zeta \in \mathbb{R}^{1+n}$*, we have*

$$\Lambda_{\mathcal{H}\varphi}(\zeta) = \int_{\mathbb{R}^{1+n}} \Gamma(z; \zeta)\,\mathcal{H}\varphi(z)\,\mathrm{d}z = -\varphi(\zeta).$$

Proof. By Lemma 5.3-(c), Λ_φ is well-defined. Property (b) is a consequence of Proposition 5.1-(b). By the C^∞-hypoellipticity of $\mathcal{H}$, (a) will follow if we show that Λ_φ is continuous and $\mathcal{H}(\Lambda_\varphi) = -\varphi$ in the sense of distributions. To begin with, let $\zeta_n = (s_n, y_n) \to \zeta_0 = (s_0, y_0)$. Let $T > 0$ be so large that $\mathrm{supp}(\varphi) \subseteq [-T,T] \times \mathbb{R}^n$. We then have

$$\begin{aligned}\Lambda_\varphi(\zeta_n) &= \int_{s_n-T}^{s_n+T} \int_{\mathbb{R}^N} \gamma_{\mathbb{G}}(\tau,u,v)\, \varphi(s_n-\tau, C_{y_n}^{-1}(u,v))\, \mathrm{d}\tau\, \mathrm{d}u\, \mathrm{d}v \\ &= \int_{[-T_0,T_0]\times\mathbb{R}^N} \gamma_{\mathbb{G}}(\tau,u,v)\, \varphi(s_n-\tau, C_{y_n}^{-1}(u,v))\, \mathrm{d}\tau\, \mathrm{d}u\, \mathrm{d}v,\end{aligned}$$

where C_y is as in the proof of Theorem 4.1, and $T_0 \gg 1$ satisfies

$$[s_n - T, s_n + T] \subseteq [-T_0, T_0] \quad \text{for any } n.$$

We can now get $\Lambda_\varphi(\zeta_n) \to \Lambda_\varphi(\zeta_0)$ by a standard dominated convergence argument, based on the integrability of $\gamma_{\mathbb{G}}$ on the strip $[-T_0,T_0]\times\mathbb{R}^N$ (see Theorem 2.7-(v)). Finally, $\mathcal{H}(\Lambda_\varphi) = -\varphi$ in $\mathcal{D}'(\mathbb{R}^{1+n})$ is a consequence of the definition of fundamental solution (and of Lemma 5.3-(a)).

We prove (c). We consider $u := \Lambda_{\mathcal{H}\varphi} + \varphi$. From property (a), we see that u is smooth and $\mathcal{H}$-harmonic on $\mathbb{R}^{1+n}$; moreover, from (b) we get that u vanishes at infinity. Since $\mathcal{H}$ satisfies the Weak Maximum Principle on every bounded open set (and therefore on the whole space $\mathbb{R}^{1+n}$ as well; see [15, Corollary 5.13.7]), we conclude that $u \equiv 0$ throughout $\mathbb{R}^{1+n}$, as desired. ∎

Theorem 5.5 (Fundamental Solution for $\mathcal{H}^*$): *The function*

$$\Gamma^*(z;\zeta) := \Gamma(\zeta;z)$$

is a global fundamental solution for the adjoint operator $\mathcal{H}^* = \mathcal{L} + \partial_t$.

Proof. This follows immediately from (c) of Proposition 5.4. ∎

We can now prove property (iv) of Theorem 1.4.

Theorem 5.6: Γ *is smooth out of the diagonal of* $\mathbb{R}^{1+n}\times\mathbb{R}^{1+n}$.

Proof. We consider the PDO on $\mathbb{R}^{1+n}\times\mathbb{R}^{1+n}$ defined by

$$Q := \sum_{j=1}^m X_j^2(x) + \partial_t + \sum_{j=1}^m X_j^2(y) - \partial_s,$$

where $x,y \in \mathbb{R}^n$ and $t,s \in \mathbb{R}$. Obviously, Q is a Hörmander operator on $\mathbb{R}^{1+n}\times\mathbb{R}^{1+n}$ since this is true of $\sum_{j=1}^m X_j^2$ on $\mathbb{R}^n$. By Theorem 5.6 we deduce that, for any $(t,x) \neq (s,y)$, one has

$$\begin{aligned}Q(\Gamma(t,x;s,y)) &= \mathcal{H}^*((t,x)\mapsto\Gamma(t,x;s,y)) + \mathcal{H}((s,y)\mapsto\Gamma(t,x;s,y)) \\ &= \mathcal{H}^*((t,x)\mapsto\Gamma^*(s,y;t,x)) + \mathcal{H}((s,y)\mapsto\Gamma(t,x;s,y)) = 0.\end{aligned}$$

The C^∞-hypoellipticity of Q and the continuity of Γ out of the diagonal prove the thesis. ∎

The next result establishes the second part of property (ii) of Theorem 1.4.

Theorem 5.7: *For every* $(t,x),(s,y)\in\mathbb{R}^{1+n}$ *we have*

$$\Gamma(t,x;s,y)=\Gamma(t,y;s,x).$$

Proof. To ease the reading, we split the proof into two steps.

Step I: We first prove that the function G defined by

$$G(t,x;s,y):=\Gamma(t,y;s,x)$$

is a global fundamental solution for $\mathcal{H}$, i.e., for every fixed $z=(t,x)\in\mathbb{R}^{1+n}$,

(a) $G(z;\cdot)\in L^1_{\mathrm{loc}}(\mathbb{R}^{1+n})$;
(b) $\mathcal{H}G(z;\cdot)=-\mathrm{Dir}_z$ in $\mathcal{D}'(\mathbb{R}^{1+n})$.

As for assertion (a), let $K\subseteq\mathbb{R}^{1+n}$ be a compact set and let $T>0$ be such that $K\subseteq[-T,T]\times\overline{B(0,T)}=:C(T)$. Since $\Gamma\geq 0$ and $\Gamma(\cdot;\zeta)\in L^1_{\mathrm{loc}}(\mathbb{R}^{1+n})$ for every $\zeta\in\mathbb{R}^{1+n}$, one then has

$$\begin{aligned}\int_K G(t,x;s,y)\,\mathrm{d}s\,\mathrm{d}y&\leq\int_{C(T)}\Gamma(t-s,y;0,x)\,\mathrm{d}s\,\mathrm{d}y\\&=\int_{t-T}^{t+T}\int_{\overline{B(0,T)}}\Gamma(\tau,y;0,x)\,\mathrm{d}\tau\,\mathrm{d}y<\infty.\end{aligned}$$

We now turn to prove assertion (b). To this end, let $\varphi\in C_0^\infty(\mathbb{R}^{1+n})$ and let $\psi(s,y):=\varphi(-s,y)$. Since $\Gamma^*(w;\zeta)=\Gamma(\zeta;w)$ is a global fundamental solution for $\mathcal{H}^*$ (see Theorem 5.5), we have

$$\begin{aligned}-\varphi(t,x)=-\psi(-t,x)&=\int_{\mathbb{R}^{1+n}}\Gamma(s,y;-t,x)\,\mathcal{H}\psi(s,y)\,\mathrm{d}s\,\mathrm{d}y\\&=\int_{\mathbb{R}^{1+n}}\Gamma(0,y;-t-s,x)\,\mathcal{H}\psi(s,y)\,\mathrm{d}s\,\mathrm{d}y\\&=\int_{\mathbb{R}^{1+n}}\Gamma(0,y;-t+\tau,x)\,\mathcal{H}\psi(-\tau,y)\,\mathrm{d}\tau\,\mathrm{d}y\\&\qquad\qquad(\text{since }(\mathcal{H}\psi)(-\tau,y)=\mathcal{H}^*\varphi(\tau,y))\\&=\int_{\mathbb{R}^{1+n}}\Gamma(t,y;\tau,x)\,\mathcal{H}^*\varphi(\tau,y)\,\mathrm{d}\tau\,\mathrm{d}y\\&=\int_{\mathbb{R}^{1+n}}G(t,x;\tau,y)\,\mathcal{H}^*\varphi(\tau,y)\,\mathrm{d}\tau\,\mathrm{d}y,\end{aligned}$$

and this proves that $\mathcal{H}G(z;\cdot)=-\mathrm{Dir}_z$ in $\mathcal{D}'(\mathbb{R}^{1+n})$, as desired.

Step II: In this step we show that, for every $z = (t, x) \in \mathbb{R}^{1+n}$, one has

$$G(z; \cdot) \in C(\mathbb{R}^{1+n} \setminus \{z\}) \quad \text{and} \quad G(z; \zeta) \to 0 \quad \text{as } \|\zeta\| \to \infty.$$

On the one hand, the continuity of $G(z; \cdot)$ out of z is a direct consequence of the continuity of Γ out of the diagonal; on the other hand, since $\Gamma(\cdot; \zeta)$ vanishes at infinity, we have

$$G(t, x; s, y) = \Gamma(t, y; s, x) = \Gamma(t - s, y; 0, x) \longrightarrow 0, \quad \text{as } \|(s, y)\| \to \infty.$$

Due to the uniqueness of Γ, this ends the proof. ∎

The next fact proves what remains to be proved of (v) in Theorem 1.4.

Remark 5.8: (1) In view of $\Gamma(t, x; s, y) = \Gamma(-s, x; -t, y)$ and the symmetry of Γ in $x \leftrightarrow y$, we recognize that, for every compact set $K \subseteq \mathbb{R}^{1+n}$,

$$\lim_{\|\zeta\| \to \infty} \big(\sup_{z \in K} \Gamma(\zeta; z)\big) = \lim_{\|\zeta\| \to \infty} \big(\sup_{z \in K} \Gamma(z; \zeta)\big) = 0.$$

Here we used (b) of Proposition 5.1.

(2) By Theorem 5.7, it is not difficult to prove the following identity:

$$\Gamma^*(t, x; s, y) = \int_{\mathbb{R}^p} \Gamma^*_{\mathbb{G}}(t, x, 0; s, y, \eta)\, \mathrm{d}\eta$$

(where $\Gamma^*_{\mathbb{G}}$ is the fundamental solution of $\mathcal{H}^*_{\mathbb{G}} = \mathcal{L}_{\mathbb{G}} + \partial_t$ on $\mathbb{G}$) which shows that $\Gamma^*_{\mathbb{G}}$ lifts Γ^*.

Furthermore, by the same tricks as above, Γ^* satisfies the dual statement of Proposition 5.4, that is, for every $\varphi \in C_0^\infty(\mathbb{R}^{1+n})$, the function Λ^*_φ defined by

$$\Lambda^*_\varphi(\zeta) := \int_{\mathbb{R}^{1+n}} \Gamma^*(z, \zeta)\, \varphi(z)\, \mathrm{d}z, \quad \zeta \in \mathbb{R}^{1+n},$$

is well-defined and it satisfies the following properties: $\Lambda^*_\varphi \in C^\infty(\mathbb{R}^{1+n})$ and $\mathcal{H}^*(\Lambda^*_\varphi) = -\varphi$ point-wise on $\mathbb{R}^{1+n}$; $\Lambda^*_\varphi(\zeta) \to 0$ as $\|\zeta\| \to \infty$.

Finally, the next proposition proves (x) in Theorem 1.4.

Proposition 5.9: *For every $x, y \in \mathbb{R}^n$ and every $s, t > 0$, we have the following so-called Reproduction Identity:*

$$\Gamma(0, y; t + s, x) = \int_{\mathbb{R}^n} \Gamma(0, w; t, x)\, \Gamma(0, y; s, w)\, \mathrm{d}w. \tag{5.3}$$

Proof. We fix a point $(s,y) \in (0,\infty)\times\mathbb{R}^n$ and we define $\varphi_{s,y}(w) := \Gamma(0,y;s,w)$. Since $\Gamma(0,y;\cdot)$ is smooth out of $(0,y)$ and since $s>0$, it is immediate to check that $\varphi_{s,y} \in C^\infty(\mathbb{R}^N,\mathbb{R})$; moreover, since $\Gamma(0,y;\cdot)$ vanishes at infinity, we see that $\varphi_{s,y}$ is also bounded on $\mathbb{R}^N$. Thus, Theorem 4.1 implies that

$$u(t,x) := \int_{\mathbb{R}^n} \Gamma(0,w;t,x)\,\varphi_{s,y}(w)\,\mathrm{d}w = \int_{\mathbb{R}^n} \Gamma(0,w;t,x)\,\Gamma(0,y;s,w)\,\mathrm{d}w$$

is the unique bounded solution of the Cauchy problem

$$\mathcal{H}u = 0 \quad \text{in } \Omega = (0,\infty)\times\mathbb{R}^n, \quad u(0,x) = \Gamma(0,y;s,x) \quad \text{for } x \in \mathbb{R}^n.$$

We now claim that the function $\overline{\Omega} \ni (t,x) \mapsto v(t,x) := \Gamma(0,y;t+s,x)$ is also a bounded solution of the same Cauchy problem. Indeed, since $s>0$ is fixed, Corollary 5.2 shows that $v \in C^\infty(\Omega,\mathbb{R})$ and that $\mathcal{H}v = 0$ on Ω; moreover, since $\Gamma(0,y;\cdot)$ vanishes at infinity, we deduce that v is bounded on Ω. Since, obviously, $v(0,x) = \Gamma(0,y;s,x)$, we then conclude that $v \equiv u$ on the whole of Ω, and the Reproduction Identity (5.3) follows. ∎

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