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APPLICATION OF NILPOTENT APPROXIMATION AND THE ORBIT METHOD TO THE SEARCH OF THE DIAGONAL ASYMPTOTICS OF SUB-RIEMANNIAN HEAT KERNELS

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Abstract: We propose a general scheme for the search of a fundamental solution to the hypoelliptic diffusion equation in a "sufficiently good" sub-Riemannian manifold and the small-time asymptotics for the solution, which includes the generalized Fourier transform and the orbit method closely related to it, as well as an application of the perturbative method to the nilpotent approximation, and Trotter's formula.

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1. Introduction

The Fourier transform in $\mathbb{R}^n$, one of the most important tools for solving differential equations, admits a natural generalization (but with substantial modifications) to unimodular Lie groups (here we will be interested in exactly this case though an analogous construction can be carried out even on arbitrary locally compact groups).

Definition 1. Let G be a unimodular Lie group endowed with the Haar measure μ and let $\widehat{G}$ be the set of all irreducible unitary representations of G (on, generally speaking, different separable spaces). In each class $\lambda \in \widehat{G}$, choose a representation $\mathfrak{X}_\lambda : G \to \mathrm{U}(H_\lambda)$, where H_λ stands for the Hilbert space of the chosen representation; $\mathrm{U}(H_\lambda)$ stands for the group of all unitary operators on H_λ. The *generalized* (or *noncommutative*) *Fourier transform* of $f \in L^1(G, \mathbb{C})$ is the mapping, denoted by $\mathscr{F}(f)$ or $\widehat{f}$, which assigns to each $\lambda \in \widehat{G}$ the (bounded) operator on H_λ defined by the formula $\widehat{f}(\lambda) = \int_G f(g)\mathfrak{X}_\lambda(g^{-1})\mu(dg)$.

Remark 1. The notation H_λ is correct in the following sense: If we take two equivalent representations R and S from the same class λ then their Hilbert spaces are isometric.

The object $\widehat{G}$ is called the *Pontryagin dual* to G; excluding the case when G is an abelian group, $\widehat{G}$ has no natural group structure. However, some properties of $\widehat{G}$ can be generalized; for example, G can be endowed with a measure P by analogy with the case of abelian groups which is called the *Plancherel measure* and satisfies the *inversion formula* for almost $g \in G$ (provided that $f \in L^1(G, \mathbb{C}) \cap L^2(G, \mathbb{C})$):

$$f(g) = \int\limits_{\widehat{G}} \mathrm{Tr}(\widehat{f}(\lambda) \circ \mathfrak{X}_\lambda(g))P(d\lambda).$$

The trace of a linear operator on H_λ is denoted by Tr in order to avoid confusion with the finite-dimensional (matrix) trace tr. The proof of the existence of the Plancherel measure can be found, for example, in [1, 2].

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The convolution of real- or complex-valued functions with respect to the group operation, defined by the formula

$$(f_1 * f_2)(g) = \int_G f_1(h) f_2(h^{-1}g)\mu(dh),$$

goes to the product (i.e., composition) operators in reverse order. Indeed, if given $\lambda \in \widehat{G}$ we choose $\mathfrak{X}_\lambda \in \lambda$, then

$$\begin{aligned}\widehat{f_1 * f_2}(\lambda) &= \int_{G\times G} f_1(h) f_2(h^{-1}g)\mathfrak{X}_\lambda(g^{-1})\mu(dg)\mu(dh)\\ &= \int_{G\times G} f_1(h') f_2(g')\mathfrak{X}_\lambda((h'g')^{-1})\mu(dg')\mu(dh')\end{aligned}$$

(here the change $g' = h^{-1}g$, $h' = h$ is made in the double integral; the Jacobian of this change is equal to 1 because μ is the Haar measure). On the other hand,

$$\begin{aligned}\widehat{f_2}(\lambda)\widehat{f_1}(\lambda) &= \int_G f_2(g)\mathfrak{X}_\lambda(g^{-1})\mu(dg) \circ \int_G f_1(h)\mathfrak{X}_\lambda(h^{-1})\mu(dh)\\ &= \int_{G\times G} f_1(h) f_2(g)\mathfrak{X}_\lambda(g^{-1}) \circ \mathfrak{X}_\lambda(h^{-1})\mu(dg)\mu(dh),\end{aligned}$$

and since $\mathfrak{X}_\lambda$ is a group homomorphism, we have

$$\mathfrak{X}_\lambda((hg)^{-1}) = \mathfrak{X}_\lambda(g^{-1}h^{-1}) = \mathfrak{X}_\lambda(g^{-1})\mathfrak{X}_\lambda(h^{-1}),$$

whence $\widehat{f_1 * f_2}(\lambda) = \widehat{f_2}(\lambda)\widehat{f_1}(\lambda)$.

The noncommutative Fourier transform can also be extended to generalized functions by analogy with the usual Fourier transform. Of importance is the fact that the Dirac delta-function transforms into the direct integral with respect to the measure P of the identity operators on $(H_\lambda)_{\lambda\in\widehat{G}}$. Indeed, choosing for $\lambda \in \widehat{G}$ a representation $\mathfrak{X}_\lambda \in \lambda$ on H_λ, we obtain the following equalities in the sense of generalized functions

$$\widehat{\delta}(\lambda) = \int_G \delta(g)\mathfrak{X}_\lambda(g^{-1})\mu(dg) = \mathfrak{X}_\lambda(e) = \mathrm{Id}_{H_\lambda},$$

where e is the neutral element of G. The last equality follows from the fact that $\mathfrak{X}_\lambda$ is a group homomorphism. The definitions of direct integral of Hilbert spaces and operations on Hilbert spaces can be found in [3]; the theory of direct integrals is exposed in more detail in [4, 5].

Define the main object of our study—the *sub-Laplacian*. We will first do it in a sufficiently general context and then give some specifications for Lie groups.

Definition 2. (i) Suppose that a smooth distribution H is defined on a smooth manifold M. The sequence of distributions defined recurrently by the equalities $H_1 = H$ and $H_{j+1} = H_j + [H_j, H]$ for positive integers j is called the *Lie flag* of H. It is sometimes assumed that $H_0 = \{0\}$.

(ii) By the *growth vector* for a distribution H we mean the sequence of the dimensions of the spaces in its Lie flag.

(iii) If the growth vector does not depend on the point of the manifold then the distribution (and the manifold itself) are called *equiregular*.

In general, by a flag we mean an inclusion increasing sequence of subspaces in a vector space but we will extend the term "flag" also to increasing sequences of distributions.

Definition 3. Suppose that M is a smooth manifold, H is a distribution on M, and H_j is the jth space of the Lie flag of H. The *degree* $\deg(X)$ of a vector field X on M (more exactly, the *degree of X with respect to H*) is the least number j for which $X \in H_j$.

In what follows, we will deal exactly with the case when the sub-Riemannian manifold M is equiregular. Since, in our context, we assume that the Lie flag stabilizes to the tangent bundle TM (H is totally nonholonomic), we will write down the growth vector in abridged form, cutting the record at j at which $\dim H_j = \dim M$; for example, for the four-dimensional Engel group, we will write the growth vector as $(2, 3, 4)$. Furthermore, we will also have to distinguish between the usual (topological) dimension of M and its Hausdorff dimension with respect to the Carnot–Carathéodory metric. For this reason, we will use the notation $\dim M$ for the first dimension and the notation $\operatorname{hdim} M$ for the second dimension; excluding the case when M is a Riemannian manifold, $\operatorname{hdim} M > \dim M$. This fact together with the definition of Carnot–Carathédory metric and the formula expressing $\operatorname{hdim} M$ in terms of the components of the growth vector, can be found for example in [6]:

$$\operatorname{hdim} M = \sum_{j=1}^{K} j(\dim H_j - \dim H_{j-1}),$$

where K is the minimal natural with $H_K = TM$; it is assumed here that $H_0 = \{0\}$.

Definition 4. Let M be a smooth equiregular sub-Riemannian manifold, for which the horizontal distribution will be denoted by H and the metric on each subspace $H(q)$ for $q \in M$ will be designated by $\langle \cdot, \cdot \rangle_q$. Suppose that the Popp measure is defined on M (by its volume form μ; see [7] for the definitions of μ and Popp measure).

(i) The operator grad_H, assigning to each function ϕ a vector field on M so that $\langle (\operatorname{grad}_H \phi)(q), v \rangle_q = d\phi(q, v)$ for all $q \in M$ and $v \in H(q)$ is called the *horizontal gradient.*

(ii) Refer as the *divergence* div_μ to the operator assigning to each vector field X on M a smooth function by the formula $\operatorname{div}_\mu(X) \cdot \mu = d(i_X(\mu))$, where i_X is the operator of the interior product of differential forms acting by inserting X in the first argument of the form; i.e., the value of the form $i_X(\mu)$ at an arbitrary collection of vector fields $Y_1, \dots, Y_{\dim M-1}$ is equal to $\mu(X, Y_1, \dots, Y_{\dim M-1})$.

(iii) The operator $\Delta_H = \operatorname{div}_\mu \operatorname{grad}_H$ is called the *sub-Laplacian on M with respect to H and μ.*

The equation $\partial_t f(t, x) = \Delta_H f(t, x)$ is called the *heat equation* or *diffusion equation.* Its solution under the generalized initial condition $f(0, x) = \delta_y(x)$ will be referred to as the *heat kernel* and denoted by $\mathrm{HK}(t, x, y)$. Here δ_y is the Dirac generalized function at a point y (the phrase "a measure is concentrated on a set" means that the measure of the complement to the set is zero).

We will also use the operator notation

$$\mathrm{HK}(t, x, y) = (\exp(t\Delta_H)\delta_y)(x).$$

The name "heat kernel" is due to the fact that for each $t > 0$ the function $\mathrm{HK}(t, \cdot, \cdot)$ is the integral kernel of $\exp(t\Delta_H)$.

If the manifold under study has the structure of a Lie group and the horizontal distribution and the metric are left-invariant then μ is the left-invariant Haar measure, and the heat equation is thus invariant. Hence, for Lie groups we will assume the δ-function at the initial condition to be concentrated at the neutral element e; respectively, $\mathrm{HK}(t, x, e)$ will be denoted by $p(t, x)$, or, if t is understood as a parameter, by $p_t(x)$. Since, as this notation, we have $\mathrm{HK}(t, x, y) = p(t, y^{-1}x)$ in the presence of a group structure, we will refer as the *heat kernel* not only to HK but also to the function p from which HK is uniquely recovered.

If the Lie group G under consideration is also unimodular and the distribution H is defined by some orthonormal basis $\{X_j : 1 \le j \le m\}$ then $\Delta_H = \sum_{j=1}^{m} (X_j{}^2)$; a proof can be found in [7]. For each left-invariant field X on G, its Fourier transform $\widehat{X} = \mathscr{F} X \mathscr{F}^{-1}$ decomposes into the direct integral of some operators $\widehat{X}_\lambda : \mathrm{HS}(H_\lambda) \to \mathrm{HS}(H_\lambda)$ (for the definition of $\widehat{X}_\lambda$ and $\widehat{X} = \int_{\widehat{G}^\oplus} \widehat{X}_\lambda P(d\lambda)$, the reader is referred to [7]), and so the Fourier transform of the sub-Laplacian splits into a direct integral: $\widehat{\Delta_H} = \mathscr{F}\Delta_H\mathscr{F}^{-1} = \int_{\widehat{G}}^{\oplus} (\widehat{\Delta_H})_\lambda P(d\lambda)$, where $(\widehat{\Delta_H})_\lambda = \sum_{j=1}^m \big(\widehat{X}_\lambda^2\big)$. Here the symbol $\mathrm{HS}(H_\lambda)$ stands for the class of Hilbert–Schmidt operators on H_λ. If we apply the noncommutative Fourier transform and the inversion formula (for applying this procedure correctly, we will need an approximation of the identity operator; see the proof of Theorem 3) then we will obtain

$$p(t,g) = \exp(t\Delta_H)\delta(g) = \int\limits_{\widehat{G}} \mathrm{Tr}(\exp(t(\widehat{\Delta_H})_\lambda)\mathfrak{X}_\lambda(g))P(d\lambda).$$

Knowing irreducible unitary representations of the group G, we can reduce the initial heat equation to an equation with transformed sub-Laplacian $\widehat{\Delta_H}$, which is usually easier than the initial diffusion equation. For SU(2), SO(3), SL(2), and SE(2), this was done in [8], and for nilpotent groups with growth vectors $(2,3,4)$ and $(2,3,5)$, in [7]. The equivalence classes of irreducible unitary representations can be found with the use of the *orbit method* developed by Kirillov; this method will be briefly exposed in Section 2. For more details on the ideas constituting the orbit method (not always on the level of rigorous theorems), the reader is referred to [9, 10].

Of primarily interest are the nilpotent Lie groups (they are of course unimodular, and so what was exposed above applies to them). The reason behind this is that if an exact solution to the heat equation (over any equiregular sub-Riemannian manifold, even without any group structure) is not required and only its asymptotics for t small are needed then we can pass to the nilpotent approximation at the point and then use Duhamel's formula

$$\exp(t(X+Y)) = \exp(tX) + \int\limits_0^t (\exp((t-s)(X+Y))Y\exp(sX)\,ds).$$

That is now the diagonal asymptotics for the heat kernel was obtained in [11] in the case of a contact three-dimensional manifold in terms of geometric invariants χ and κ defined in [12].

In subsequent arguments, we will also need the fact that the heat kernel $p_t(\cdot)$ in a connected simply-connected Lie group G for each $t>0$ belongs to the Schwartz space $\mathscr{S}(G)$. The proof of this fact and also the definition and some properties of the Schwartz space can be found in [13].

2. The Orbit Method

In formulating the orbit method, we assume that the Lie group is such that the irreducible unitary representations result from one-dimensional representations by the operators of extension from a subgroup, restriction to a subgroup, and induction from a subgroup. Though this assumption is not proved for arbitrary Lie groups, it still holds for nilpotent groups (see [9]). Let us describe the correspondence of orbits and representations in the case when the representation is obtained from a one-dimensional representation in a sole step by induction—this will be enough. Let us give here the definition of induction operator (see also [14]).

Definition 5. Suppose that H is a connected closed subgroup in a Lie group G, $H\diagdown G$ is the set of right cosets of G modulo H, the measure $\mu_{H\diagdown G}$ is the image of the right Haar measure on G under the mapping taking each element $g\in G$ to its right coset Hg, and $T: H \to \mathrm{U}(V)$ is a unitary representation of H in a Hilbert space V with inner product $\langle\cdot,\cdot\rangle_V$ and the corresponding norm $\|\cdot\|_V$.

(i) On the space of cosets (modulo almost everywhere coincidence) of Borel measurable functions $f: G\to V$ such that $f(hg) = T(h)f(g)$ and $\int_{H\diagdown G}\big(\|f(g)\|_V^2\big)\mu_{H\diagdown G}(dg) < \infty$ for all $h\in H$ and $g\in G$, introduce the inner product $\langle f_1, f_2\rangle = \int_{H\diagdown G}\langle f_1(g), f_2(g)\rangle_V \mu_{H\diagdown G}(dg)$. Denote the completion of this space with respect to $\langle\cdot,\cdot\rangle$ by W. The notation $\int_{H\diagdown G}\langle f_1(g), f_2(g)\rangle_V \mu_{H\diagdown G}(dg)$ is correct since $\langle f_1(g), f_2(g)\rangle_V$ is the same for all g in the same right coset.

(ii) Define the representation $\operatorname{Ind}_H^G T : G \to \mathrm{U}(W)$ of G which is induced by a representation T as follows: For each $g \in G$, the operator $\left(\operatorname{Ind}_H^G T\right)_g \in \mathrm{U}(W)$ acts at $f \in W$ by the formula $(\operatorname{Ind}_H^G T)_g(f)(g') = f(g'g)$ for all $g' \in G$.

For describing the structure of $\widehat{G}$, i.e. for classifying irreducible unitary representations of a Lie group G, we will need the *coadjoint action* (or *coadjoint representation*) of G.

DEFINITION 6. Let $\mathfrak{g}$ be the Lie algebra of a Lie group of an algebra G realized by the left-invariant vector fields and let $\mathfrak{g}^*$ be the space of left-invariant differential 1-forms dual to $\mathfrak{g}$. The group G *acts on* $\mathfrak{g}$ *by the adjoint action* Ad defined by the formula $\mathrm{Ad}_g(X) = gXg^{-1}$ for $g \in G$ and $X \in \mathfrak{g}$, and acts on $\mathfrak{g}^*$ by the *coadjoint action* Ad^* defined by the formula $\mathrm{Ad}^*_g(\xi, X) = \xi(g^{-1}Xg)$ for $g \in G$, $X \in \mathfrak{g}$, and $\xi \in \mathfrak{g}^*$.

Abstracting from the variable X, denote by $\mathrm{Ad}^*_g(\xi)$ the differential form $\mathrm{Ad}^*_g(\xi, \cdot)$, to which the form ξ goes for the sake of convenience.

The notation $\mathrm{Ad}_g(X) = gXg^{-1}$ means that the elements of G and $\mathfrak{g}$ are defined by matrices. In coordinate-free form, the definition looks as follows: $\mathrm{Ad}_g(X) = d\Psi_g(e, X)$, where $\Psi_g : G \to G$ is calculated by the formula $\Psi_g(h) = ghg^{-1}$; respectively, $\mathrm{Ad}^*{}_g(\xi) = \xi \circ \mathrm{Ad}_{g^{-1}}$.

DEFINITION 7. $\mathscr{O}_\xi = \{\mathrm{Ad}^*{}_g(\xi) : g \in G\}$ is called the *orbit of the form* ξ in Ad^*.

The set of orbits, which we will denote by $\mathfrak{g}^*/\mathrm{Ad}^*$, is endowed with the quotient topology of the standard topology in $\mathfrak{g}^*$ by the equivalence "membership in the same orbit" and also with the measure that is the decomposition of the Lebesgue measure in $\mathfrak{g}^*$ into the canonical measures on the orbits.

As a "standard" measure on $\widehat{G}$, we take the Plancherel measure, and the topology is introduced as follows: Let T be an irreducible unitary representation of G on some separable Hilbert space, that we will denote by $\mathscr{H}$; the inner product in $\mathscr{H}$ will be denoted by $\langle \cdot, \cdot \rangle_{\mathscr{H}}$. For the point $\lambda \in \widehat{G}$ that is the class of representations equivalent to T, the following neighborhood base of the form $U(K, (v_j)_{j=1,\dots,n})$, where K is a compact subset of G, while $(v_j)_{j=1,\dots,n}$ is a collection of vectors in $\mathscr{H}$: The class of a representation T' defined on a separable Hilbert space $\mathscr{H}'$ with inner product $\langle \cdot, \cdot \rangle_{\mathscr{H}'}$ belongs to $U(K, (v_j)_{j=1,\dots,n})$ if and only if there exists a collection of vectors $(v'_j)_{j=1,\dots,n}$ in $\mathscr{H}'$ such that $|\langle T(g)v_j, v_k\rangle_{\mathscr{H}} - \langle T'(g)v'_j, v'_k\rangle_{\mathscr{H}'}| < 1$ for all $g \in K$ and all indices j, k.

The correspondence between $\widehat{G}$ and $\mathfrak{g}^*/\mathrm{Ad}^*$ must be constructed as an isomorphism between $\widehat{G}$ and $\mathfrak{g}^*/\mathrm{Ad}^*$ as topological and measure spaces. Before constructing it, we give some necessary definitions and facts.

DEFINITION 8. Let G be a Lie group with Lie algebra $\mathfrak{g}$. A Lie subalgebra $\mathfrak{m} \subseteq \mathfrak{g}$ is called *subordinate* to $\xi \in \mathfrak{g}^*$ if $B_\xi(X, Y) = 0$ for all $X, Y \in \mathfrak{m}$, where by definition $B_\xi(X, Y) = \xi([X, Y])$ for all $X, Y \in \mathfrak{g}$.

Denote by $\mathfrak{g}_\xi$ the kernel of the form B_ξ, the set of points $X \in \mathfrak{g}$ such that $B_\xi(X, Y) = 0$ for all $Y \in \mathfrak{g}$.

For each $\xi \in \mathfrak{g}^*$, the Lie subgroup $\{g \in G : \mathrm{Ad}^*{}_g(\xi) = \xi\}$ has the space $\mathfrak{g}_\xi$ as its Lie algebra (see [10]); denote this subgroup by G_ξ.

Each orbit $\mathscr{O}_\xi$ admits a nondegenerate closed G-invariant 2-form turning $\mathscr{O}_\xi$ into a symplectic manifold. All necessary isomorphisms originating from the identification of $\mathscr{O}_\xi$ with the set of right cosets of G modulo the subgroup G_ξ and enabling us to give the term "G-invariance" some exact sense in application to forms on $\mathscr{O}_\xi$ are given in [10]; some method for obtaining a symplectic form on $\mathscr{O}_\xi$ from the form B_ξ is described in [10] too. In particular, $\mathscr{O}_\xi$ has even dimension. On the other hand, if G is connected then every homogeneous symplectic manifold (i.e., a manifold on which G acts and all transformations of G preserve the symplectic form) is locally isomorphic to an orbit in the coadjoint representation either of G itself or of the central extension of G by $\mathbb{R}$.

With an orbit $\mathscr{O}_\xi$, we associate the representation $\operatorname{Ind}_H^G \rho_{\xi,H}$, where H is a subgroup in G with the Lie algebra $\mathfrak{h}$ that is an algebra of maximal dimension subordinate to ξ, equal to $\frac{\dim \mathfrak{g} + \dim \mathfrak{g}_\xi}{2}$, $\rho_{\xi,H}$ is the one-dimensional unitary representation of H defined by the formula $\rho_{\xi,H}(\exp(X)) = \exp(2\pi \mathrm{i} \xi(X))$ for all $X \in \mathfrak{h}$.

As was shown in [9], in our case, this construction gives a full description of $\widehat{G}$:

Theorem 1. *If G is a connected simply-connected nilpotent Lie group with Lie algebra $\mathfrak{g}$ and T is an irreducible unitary representation of G then $T = \operatorname{Ind}_H^G \rho_{\xi,H}$ for some connected subgroup $H \subseteq G$ and some $\xi \in \mathfrak{g}^*$.*

If $H \subseteq G$ is a connected subgroup with Lie algebra $\mathfrak{h}$, $\xi \in \mathfrak{g}^*$ then the representation $T_{\xi,H} = \operatorname{Ind}_H^G \rho_{\xi,H}$ is irreducible if and only if $\mathfrak{h}$ is a subalgebra of maximal dimension subordinate to ξ.

Suppose that $T_{\xi,H}$ and $T_{\xi',H'}$ are irreducible, while λ and λ' are the classes of representations equivalent to $T_{\xi,H}$ and $T_{\xi',H'}$ respectively. Then the conditions $\lambda = \lambda'$ and $\mathscr{O}_\xi = \mathscr{O}_{\xi'}$ are equivalent.

The correspondence of the orbits $\mathscr{O}_\xi$ and the similarity classes of the representations $T_{\xi,H}$ is a homeomorphism in the above-introduced topologies.

In the case of a nilpotent Lie group G, every maximal subalgebra subordinate to an element $\xi \in \mathfrak{g}^*$ includes $\mathfrak{g}_\xi$. This fact, proved by Pukánszky in [15], will be used in considering a concrete example below.

The explicit construction of a subalgebra of maximal dimension which is subordinate to ξ was proposed by Vergne (here we expose her result not in maximal generality; a more complete statement and proof can be found in [16]):

Theorem 2. *Let G be a connected simply-connected Lie group with Lie algebra $\mathfrak{g}$ and $(V_k)_{k=0,\dots,\dim\mathfrak{g}}$ be an inclusion increasing collection of ideals in $\mathfrak{g}$, where $\dim V_k = k$ for all k. Then, for every $\xi \in \mathfrak{g}^*$, $\mathfrak{v}s(\xi) = \sum_{k=0}^{\dim\mathfrak{g}} \ker(B_\xi|_{V_k})$ is a subalgebra of maximal dimension subordinate to ξ.*

In what follows, we use the notations $\exp(\mathfrak{v}s(\xi)) = VS_\xi$ and $T_{\xi,VS_\xi} = R_\xi$, the equivalence class of a representation R_ξ will be denoted by λ_ξ, and the representation space R_ξ, by W_ξ. Sometimes we will write $\mathfrak{v}s(\xi)$ instead of $\mathfrak{v}s_\xi$.

Theorem 2 makes it possible to choose representations in a given class in a canonical way. Moreover, given a collection of ideals $(V_k)_{k=0,\dots,\dim\mathfrak{g}}$, we can naturally construct a Maltsev basis $\mathfrak{g}$ (in the strong sense).

Definition 9. An ordered basis $(Z_k)_{k=1,\dots,\dim\mathfrak{g}}$ of the Lie algebra $\mathfrak{g}$ is called *Maltsev in the weak sense* if all its initial segments $(Z_k)_{k=1,\dots,r}$, $0 \le r \le \dim\mathfrak{g}$, are bases of some subalgebras in $\mathfrak{g}$; if in addition all these subalgebras are ideals in $\mathfrak{g}$ then $(Z_k)_{k=1,\dots,\dim\mathfrak{g}}$ is called *Maltsev in the strong sense.*

For applying the noncommutative Fourier transform (more exactly, of the inversion formula), it remains to calculate its Plancherel measure.

Definition 10. Let A be a real skew-symmetric matrix of order $2n$ whose entries will be denoted by $(a_{i,j})_{i,j=1,\dots,2n}$. The *Pfaffian* $\operatorname{pf}(A)$ is defined by the formula

$$\operatorname{pf}(A) = \frac{1}{2^n n!} \sum_{\sigma\in S_{2n}} \left(\operatorname{sgn}(\sigma) \prod_{i=1}^{n} (a_{\sigma(2i-1),\sigma(2i)}) \right),$$

where S_{2n} is the group of all permutations of a $2n$-element set, while $\operatorname{sgn}(\sigma)$ is the sign of the permutation σ, equal to 1 if σ is even and equal to -1 if σ is odd.

The square of the Pfaffian is equal to the determinant. Below we will see that the sign of the Pfaffian is unimportant in our context; therefore, we can calculate the modulus of the Pfaffian by extracting the square root from the determinant, thus avoiding its direct calculation via permutations.

Let us expose the method of computing the Plancherel measure which is described in [9, 10].

Proposition 1. *If G is a connected simply-connected nilpotent Lie group then*

(i) *for every open dense set $F \subseteq \mathfrak{g}^*/\operatorname{Ad}^*$ consisting of orbits of maximal dimension, the set of elements in $\widehat{G}$ corresponding to the orbits in F has some complement of Plancherel measure 0;*

(ii) *there is a linear subvariety Q in $\mathfrak{g}^*$ so that each orbit in some open dense subset of orbits of maximal dimension intersects with Q at a singleton.*

The Plancherel measure is described in terms of Q as follows: Identify $\mathfrak{g}^{**}$ with $\mathfrak{g}$ by assigning to each $z \in \mathfrak{g}$ some element $\mathfrak{g}^{**}$ that at each $\xi \in \mathfrak{g}^*$ takes the value $\xi(z)$. With this identification in mind, choose *the basis in* $\mathfrak{g}^{**}$

$$\{X_j : 1 \le j \le \dim Q\} \cup \{Y_j : 1 \le j \le \dim \mathfrak{g} - \dim Q\}$$

in which the elements denoted by Y *are constant on* Q*; the coordinates on* Q *are* $(X_j)_{1 \le j \le \dim Q}$*. For each* $\xi \in Q$*, construct the skew-symmetric matrix* $A(\xi)$ *with entries* $a_{j,k} = \xi([Y_j, Y_k])$*. Then the measure on the given open dense set of orbits of maximal dimension taken to the Plancherel measure under the correspondence of* $\widehat{G}$ *and* $\mathfrak{g}^*/\mathrm{Ad}^*$ *is equal to*

$$|\operatorname{pf}(A(\xi))| dX_1 \wedge \dots \wedge dX_{\dim Q}.$$

To formulate the main result, we will need the definition of canonical projection to the subgroup VS_ξ for arbitrary ξ in the above-constructed subspace Q.

Definition 11. Take $\xi \in Q$. Choose a Maltsev basis of $\mathfrak{g}$ in the weak sense, denoted by $(Z_k)_{1 \le k \le \dim \mathfrak{g}}$, for which

$$\mathfrak{v}s(\xi) = \operatorname{span}\left\{Z_k : 1 \le k \le \frac{\dim \mathfrak{g} + \dim \mathfrak{g}_\xi}{2}\right\}.$$

Given $x \in \mathbb{R}^{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}}$, put

$$\gamma_x = \exp(x_1 Z_{\frac{\dim \mathfrak{g} + \dim \mathfrak{g}_\xi}{2}+1}) \cdot \dots \cdot \exp(x_{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}} Z_{\dim \mathfrak{g}}).$$

The canonical projection of $h \in G$ to VS_ξ is defined as $h' \in VS_\xi$ such that $h = h'\gamma_x$ for some $x \in \mathbb{R}^{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}}$. We will denote such h' by $\operatorname{pr}_{VS_\xi}(h)$.

From this decomposition $h = h'\gamma_x$, we can recover $x = \gamma^{-1}((\operatorname{pr}_{VS_\xi}(h))^{-1}h)$.

Remark 2. The notation $(\gamma_x)^{-1}$, which means the element of the group inverse to γ_x, should not be confused with $\gamma^{-1}(\dots)$—the value of the inverse function of γ at some point.

Thus, the formula for $p(t, g)$ is as follows:

Theorem 3. *Let* G *be a connected simply-connected nilpotent Lie group with Haar measure* μ*, left-invariant sub-Riemannian metric, and corresponding sub-Laplacian* Δ_H*. Let the space* Q *and matrix* $A(\xi)$ *for* $\xi \in Q$ *be like those given in Proposition* 1*, and let the mapping* γ *be as in Definition* 11*. Then the heat kernel for* Δ_H *is expressed as*

$$p(t,g) = \int\limits_{Q} \int\limits_{\mathbb{R}^{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}}} \mathrm{e}^{2\pi \mathrm{i}\xi(\log(\operatorname{pr}_{VS_\xi}(\gamma_x g)))} \mathrm{HK}_{\widehat{\Delta_H}(\lambda_\xi)}(t, \gamma^{-1}((\operatorname{pr}_{VS_\xi}(\gamma_x g))^{-1}\gamma_x g), x) |\operatorname{pf}(A(\xi))|\, dx d\xi,$$

where $\mathrm{HK}_{\widehat{\Delta_H}(\lambda_\xi)}(t, \cdot, \cdot)$ *is the integral kernel of the operator* $\exp(t\widehat{\Delta_H}(\lambda_\xi))$ *for all* $t > 0$.

Remark 3. The symbol log in application to an element of a Lie group means the inverse of the exponential mapping. This notation is correct since the exponential mapping of a connected simply-connected Lie group is bijective.

Proof. The main idea is to apply the generalized Fourier transform to the heat equation and then reconstruct the heat kernel from its Fourier transform by the inversion formula. We classify irreducible unitary representations of G by the orbit method; for each such representation, we find an equivalent representation that looks simpler than then initial one.

Choose $\xi \in Q$. The orbit method associates with ξ the representation $R_\xi = \operatorname{Ind}_{VS_\xi}^{G} \rho_{\xi,VS_\xi}$. Here $\rho_{\xi,VS_\xi}(\exp(X)) = \exp(2\pi \mathrm{i}\xi(X))$ for all $X \in \mathfrak{v}s_\xi$ which can be rewritten as $\rho_{\xi,VS_\xi}(h) = \exp(2\pi \mathrm{i}\xi(\log(h)))$ for all $h \in VS_\xi$. Denote the Hilbert space of the representation R_ξ by W_ξ. Its elements are represented by the complex-valued of functions on G defined up to a set of measure zero since ρ_{ξ,VS_ξ} is a one-dimensional representation.

Using the mapping γ and the canonical projection of Definition 11, we construct the transformation $J_\xi : L^2(\mathbb{R}^{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}}) \to W_\xi$ acting on each function $f \in L^2(\mathbb{R}^{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}})$ by the formula

$$J_\xi(f)(g) = \rho_{\xi,VS_\xi}(\mathrm{pr}_{VS_\xi}(g)) f(\gamma^{-1}((\mathrm{pr}_{VS_\xi}(g))^{-1} g))$$

for almost all $g \in G$. The definition of J_ξ is correct because the function $J_\xi(f)$ obtained by this formula possesses the properties of the definition of the Hilbert space on which the induced representation is defined (see Definition 5). Since the modulus of the complex number $\rho_{\xi,VS_\xi}(\mathrm{pr}_{VS_\xi}(g))$ is equal to 1, the so-constructed transformation J_ξ is unitary.

The inverse transformation of J_ξ takes each function $u \in W_\xi$ to the function defined by the formula ${J_\xi}^{-1}(u)(x) = u(\gamma_x)$ for almost all $x \in \mathbb{R}^{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}}$. Indeed, if $f \in L^2(\mathbb{R}^{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}})$ then for all almost all $x \in \mathbb{R}^{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}}$ we have

$${J_\xi}^{-1}(J_\xi(f))(x) = J_\xi(f)(\gamma_x) = \rho_{\xi,VS_\xi}(e) f(\gamma^{-1}(\gamma_x)) = f(x),$$

since $\mathrm{pr}_{VS_\xi}(\gamma_x)$ is equal to the neutral element e. On the other hand, for all $u \in W_\xi$ and almost all $g \in G$, we have

$$\begin{aligned} J_\xi({J_\xi}^{-1}(u))(g) &= \rho_{\xi,VS_\xi}(\mathrm{pr}_{VS_\xi}(g)) \cdot {J_\xi}^{-1}(u)(\gamma^{-1}((\mathrm{pr}_{VS_\xi}(g))^{-1} g)) \\ &= \rho_{\xi,VS_\xi}(\mathrm{pr}_{VS_\xi}(g)) \cdot u((\mathrm{pr}_{VS_\xi}(g))^{-1} g) = u(g). \end{aligned}$$

The last equality follows from the condition $u(hg) = \rho_{\xi,VS_\xi}(h) u(g)$, with $h \in H$ and $g \in G$, which occurs in Definition 5.

Define the representation $R'_\xi : G \to \mathrm{U}(L^2(\mathbb{R}^{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}}))$ equivalent to the representation R_ξ by the formula $R'_\xi(g) = {J_\xi}^{-1} \circ R_\xi(g) \circ J_\xi$ for each $g \in G$, i.e., for each $f \in L^2(\mathbb{R}^{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}})$, the function $R'_\xi(g)(f)$ acts by the formula $R'_\xi(g)(f) = (R_\xi(g)(J_\xi(f))) \circ \gamma$. The last formula takes the following form for almost all $x \in \mathbb{R}^{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}}$:

$$\begin{aligned} R'_\xi(g)(f)(x) &= R_\xi(g)(J_\xi(f))(\gamma_x) = J_\xi(f)(\gamma_x g) \\ &= \rho_{\xi,VS_\xi}(\mathrm{pr}_{VS_\xi}(\gamma_x g)) f(\gamma^{-1}((\mathrm{pr}_{VS_\xi}(\gamma_x g))^{-1} \gamma_x g)) \\ &= \mathrm{e}^{2\pi \mathrm{i} \xi(\log(\mathrm{pr}_{VS_\xi}(\gamma_x g)))} f(\gamma^{-1}((\mathrm{pr}_{VS_\xi}(\gamma_x g))^{-1} \gamma_x g)). \end{aligned}$$

It is with the representation R'_ξ that we will work below. Choosing it as the canonical representative of its equivalence class $\lambda_\xi \in \widehat{G}$, write down the definition of the Fourier transform of $f : G \to \mathbb{C}$:

$$\widehat{f}(\lambda_\xi) = \int_G f(g) R'_\xi(g^{-1}) \mu(dg).$$

Respectively, the inversion formula looks as follows:

$$f(g) = \int_Q \mathrm{Tr}(\widehat{f}(\lambda_\xi) \circ R'_\xi(g)) |\operatorname{pf}(A(\xi))| \, d\xi.$$

Here $\widehat{G}$ is parametrized by orbits in the coadjoint representation (more exactly, by their elements in Q) and the expression is used for the Plancherel measure in terms of this parametrization.

As was shown in [10], the Fourier transform of each $f \in \mathscr{S}(G)$ calculated in λ_ξ has the integral kernel $k_f \in \mathscr{S}(\mathbb{R}^{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}} \times \mathbb{R}^{\frac{\dim \mathfrak{g} - \dim \mathfrak{g}_\xi}{2}})$ such that

$$k_f(x, y) = \int_{VS_\xi} \rho_{\xi,VS_\xi}(h) f((\gamma_x)^{-1} h \gamma_y) dh,$$

where dh stands for the Haar measure on VS_ξ. Since $p_t \in \mathscr{S}(G)$, we can take $f = p_t$; the corresponding function k_{p_t} is equal to $\mathrm{HK}_{\widehat{\Delta_H(\lambda_\xi)}}(t,\cdot,\cdot)$ (see [14]). The fact that $k_{p_t} \in \mathscr{S}(\mathbb{R}^{\frac{\dim\mathfrak{g}-\dim\mathfrak{g}_\xi}{2}} \times \mathbb{R}^{\frac{\dim\mathfrak{g}-\dim\mathfrak{g}_\xi}{2}})$ implies that the operator $\widehat{p_t}(\lambda_\xi)$ has a trace.

As was demonstrated in Section 1, the convolution of two functions $f_1, f_2 : G \to \mathbb{C}$, defined as

$$(f_1 * f_2)(g) = \int_G f_1(h) f_2(h^{-1}g)\mu(dh)$$

for $g \in G$, satisfies $\widehat{f_1 * f_2}(\lambda) = \widehat{f_2}(\lambda) \circ \widehat{f_1}(\lambda)$, $\lambda \in \widehat{G}$. For each $f \in \mathscr{S}(G)$, the solution to the heat equation is written down as $\exp(t\Delta_H)(f) = f * p_t$. Taking the generalized Fourier transform of both sides of this equality, we see that $\mathscr{F}(\exp(t\Delta_H)(f))(\lambda_\xi) = \widehat{p_t}(\lambda_\xi) \circ \widehat{f}(\lambda_\xi)$ for all $\xi \in Q$.

For obtaining $\widehat{p_t}$ from this and then reconstructing p_t by the inversion formula, we must approximate the identity operator $\mathrm{Id}_{L^2(\mathbb{R}^{\frac{\dim\mathfrak{g}-\dim\mathfrak{g}_\xi}{2}})}$ by operators of the form $\widehat{f}(\lambda_\xi)$ for some $f \in \mathscr{S}(G)$. The approximation is necessary because there is no $f \in \mathscr{S}(G)$ such that $\widehat{f}(\lambda_\xi) = \mathrm{Id}_{L^2(\mathbb{R}^{\frac{\dim\mathfrak{g}-\dim\mathfrak{g}_\xi}{2}})}$, since the identity operator is not a Hilbert–Schmidt operator.

Thus, we consecutively take f compactly supported smooth functions ϕ_n converging in the usual sense to the δ-function concentrated at the neutral element such that $\phi_n(g^{-1}) = \phi_n(g)$ and $\phi_n(g) \geq 0$ for all $g \in G$. It is known from [18] that the functions $\phi_n * \psi$ converge in $L^2(G)$ as $n \to \infty$ to ψ for all $\psi \in L^2(G)$ for such a sequence; moreover, the sequence of operators taking each $\psi \in L^2(G)$ to $\phi_n * \psi$ is uniformly bounded in the operator norm. Therefore, $\lim_{n\to\infty} \mathrm{Tr}(\widehat{p_t}(\lambda_\xi) \circ \widehat{\phi_n}(\lambda_\xi)) = \mathrm{Tr}(\widehat{p_t}(\lambda_\xi))$.

If, in the inversion formula, $f(g) = \int_Q \mathrm{Tr}(\widehat{f}(\lambda_\xi) \circ R'_\xi(g))|\,\mathrm{pf}(A(\xi))|\,d\xi$ we put $f = \phi_n * p_t$ and pass to the limit as $n \to \infty$ then we infer

$$\exp(t\Delta_H)\phi_n(g) = \int_Q \mathrm{Tr}(\mathscr{F}(\exp(t\Delta_H)\phi_n)(\lambda_\xi) \circ R'_\xi(g))|\,\mathrm{pf}(A(\xi))|\,d\xi$$

$$= \int_Q \mathrm{Tr}(\widehat{p_t}(\lambda_\xi) \circ \widehat{\phi_n}(\lambda_\xi) \circ R'_\xi(g))|\,\mathrm{pf}(A(\xi))|\,d\xi$$

$$\to \int_Q \mathrm{Tr}(\widehat{p_t}(\lambda_\xi) \circ R'_\xi(g))|\,\mathrm{pf}(A(\xi))|\,d\xi = \int_Q \mathrm{Tr}(R'_\xi(g) \circ \widehat{p_t}(\lambda_\xi))|\,\mathrm{pf}(A(\xi))|\,d\xi$$

(here we have used the circumstance that the composition with the unitary operator $R'_\xi(g)$ does not influence the convergence of the traces) and the formula $\mathrm{Tr}(X \circ Y) = \mathrm{Tr}(Y \circ X)$ either. Thus,

$$p(t,g) = \int_Q \mathrm{Tr}(R'_\xi(g) \circ \widehat{p_t}(\lambda_\xi))|\,\mathrm{pf}(A(\xi))|\,d\xi.$$

For calculating $\mathrm{Tr}(R'_\xi(g) \circ \widehat{p_t}(\lambda_\xi))$, we can use the fact that if U is a unitary operator and K is an operator with trace, whereas the integral kernel of the operator K is a continuous function k; then $U \circ K$ has a trace, its integral kernel k_1 is defined by the formula $k_1(x,y) = (Uk(\cdot,y))(x)$, and $\mathrm{Tr}(U \circ K) = \int Uk(\cdot,x)(x)\,dx$. Taking $U = R'_\xi(g)$ and $K = \widehat{p_t}(\lambda_\xi)$ and inserting the previously found expression for $R'_\xi(g)$, we obtain

$$\mathrm{Tr}(R'_\xi(g) \circ \widehat{p_t}(\lambda_\xi)) = \int_{\mathbb{R}^{\frac{\dim\mathfrak{g}-\dim\mathfrak{g}_\xi}{2}}} (R'_\xi(g)(\mathrm{HK}_{\widehat{\Delta_H(\lambda_\xi)}}(t,\cdot,x)))(x)\,dx$$

$$= \int_{\mathbb{R}^{\frac{\dim\mathfrak{g}-\dim\mathfrak{g}_\xi}{2}}} \mathrm{e}^{2\pi\mathrm{i}\xi(\log(\mathrm{pr}_{VS_\xi}(\gamma_x g)))} \mathrm{HK}_{\widehat{\Delta_H(\lambda_\xi)}}(t, \gamma^{-1}((\mathrm{pr}_{VS_\xi}(\gamma_x g))^{-1}\gamma_x g), x)\,dx.$$

For finishing the proof, it suffices to insert the obtained expression for the trace in the formula

$$p(t,g) = \int\limits_{Q} \operatorname{Tr}(R'_{\xi}(g) \circ \widehat{p_t}(\lambda_{\xi}))|\operatorname{pf}(A(\xi))|\, d\xi. \quad \square$$

Since $\mathrm{HK}_{\widehat{\Delta_H}(\lambda_\xi)}$ usually looks easier than the initial heat kernel, the following terminology is widespread:

Definition 12. The function $\mathrm{HK}_{\widehat{\Delta_H}(\lambda_\xi)}$, introduced in Theorem 3, is called the *reduced kernel* or *transformed kernel.*

3. The Perturbation Method

For applying the perturbation method, we must define the anisotropic dilation.

Definition 13. Suppose that M is an n-dimensional manifold and $F = (H_j)_{j=1,\dots,K}$ is a smooth flag in TM, $H_K = TM$, $d_j = \dim H_j - \dim H_{j-1}$ (here we have put $H_0 = \{0\}$). The coordinates $\vec{x} = (x_k)_{k=1,\dots,n}$ in a neighborhood of $q \in M$ are called *adapted to* F if $\vec{x}(q) = (0,\dots,0)$, and the image of $H_j(q)$ under $d\vec{x}(q)$ is equal to $\bigoplus\limits_{s=1}^{K} \begin{cases} \mathbb{R}^{d_s}, s \le j, \\ \{0\}, s > j, \end{cases}$ for all j.

Definition 14. Let $\vec{x} = (x_k)_{k=1,\dots,n}$ be coordinates on M adapted to the flag $F = (H_j)_{j=1,\dots,K}$. Define the anisotropic ε-dilation with respect to q, where $\varepsilon \ge 0$, by the formula

$$\delta_{\varepsilon,q}(q') = \vec{x}^{-1}((\varepsilon^{\min\{j:\dim H_j \ge k\}} x_k(q'))_{k=1,\dots,n}),$$

where q' is an arbitrary point in the domain of $\vec{x}$.

If M is an equiregular sub-Riemannian manifold then as F we naturally take the Lie flag of the horizontal distribution $H_1 = H$. By K we will denote the *least* j such that $H_j = TM$.

Definition 15. For the differential operators on M representable by monomials in the adapted coordinates, define the homogeneity exponent ν as follows: If α and β are multi-indices then

$$\nu(x^\alpha \partial^\beta) = \sum_{r=1}^{n} ((\alpha_r - \beta_r)\min\{j : \dim H_j \ge r\}).$$

A differential operator with polynomial coefficients is called *homogeneous with exponent* p if all its monomials have the value of ν equal to p.

Definition 16. If $X = \sum_{p=-K}^{\infty}(W_p)$ is the Taylor expansion of a vector field X represented in the adapted coordinates near the point $(0,\dots,0)$, where the vector field W_p is homogeneous with exponent p for all p. We call W_p the *homogeneous part of* X *with exponent* p and denote it by $\mathrm{hg}_p(X)$.

Definition 17. A coordinate system $\vec{x}$ adapted to the Lie flag to an equiregular sub-Riemannian manifold M is called *privileged* if the image of the horizontal bundle under the differential of the coordinate mapping $d\vec{x}$ consists only of homogeneous vector fields with homogeneity exponent at most -1.

In a privileged coordinate system, we can define the nilpotent approximation of M with respect to q whose description is given in the following theorem (see [11, 19–21]):

Theorem 4. *Let* $[X_j, X_k](q') = \sum_{l:\deg X_l \le \deg X_j + \deg X_k} (c_{j,k,l}(q')X_l(q'))$ *be the commutation relation for a smooth basis of an equiregular sub-Riemannian manifold* M*. Then, for every* $q \in M$*, the coefficients*

$$\tilde{c}_{j,k,l} = \begin{cases} c_{j,k,l}(q), & \deg X_l = \deg X_j + \deg X_k, \\ 0, & \deg X_l \ne \deg X_j + \deg X_k, \end{cases}$$

are the structure constants of some nilpotent Lie algebra $\widetilde{\mathfrak{m}}_q$ *and the corresponding Lie group* $\widetilde{M}_q$ *with the natural Carnot–Carathéodory metric* $\lim_{t\to+\infty}(tM)$*, where the limit is understood in the sense* *of Gromov–Hausdorff. Moreover, the vector fields on $\widetilde{M}_q$ defined by the formula $\widetilde{X}_j = \mathrm{hg}_{-\deg X_j} d\vec{x}(X_j)$* (*the basis of the nilpotent approximation*) *are left-invariant.*

Here and below, by deg we mean the degree of a field with respect to the initial horizontal distribution on M. In the sequel, the dimension of the horizontal distribution will be denoted by m; the numbers of the vector fields X_j constituting its basis are as follows: $1 \le j \le m$.

Denote by ${X_j}^*$, $1 \le j \le n$, the 1-forms for which ${X_j}^*(X_j) = 1$ and ${X_j}^*(X_k) = 0$ for $j \ne k$. The basis $\{\widetilde{X}_j : 1 \le j \le n\}$ will be assumed such that the volume form for the Popp measure is the form ${X_1}^* \wedge \cdots \wedge {X_n}^*$; it is known from [7] that this does not diminish generality.

REMARK 4. As the nonhorizontal basis vector fields, we usually choose the vector fields $[[[X_{j_0}, X_{j_1}], X_{j_2}] \dots X_{j_s}]$ with some $s \in \mathbb{N}$, where $1 \le j_l \le m$ for all $l \in \{0, \dots, s\}$. Calculating the coefficient at the volume form for the Popp measure constructed from this basis and dividing one of the basis vector fields with $s = K - 1$, we obtain a new basis in which the Popp measure is defined by a form with coefficient 1.

The nilpotent approximation is itself a sub-Riemannian manifold with horizontal bundle $\mathrm{span}\{\widetilde{X}_j : 1 \le j \le m\}$. If we endow it with a Haar measure and construct the sub-Laplacian, which we will denote by $\widetilde{\Delta}$, then it is expressed as $\widetilde{\Delta} = \sum_{j=1}^{m} (\widetilde{X}_j^2)$.

Now, given the initial sub-Riemannian structure on a manifold M, we define its ε-perturbation. For basis vector fields X_j, $1 \le j \le n$, and $\varepsilon > 0$, we put

$$X_{j,\varepsilon} = \varepsilon^{\deg X_j} \cdot d\delta_{\varepsilon^{-1}} X_j.$$

Similarly, define the 1-forms $X^*_{j,\varepsilon}$, $1 \le j \le n$: namely, $X^*_{j,\varepsilon}(X_{j,\varepsilon}) = 1$ and $X^*_{j,\varepsilon}(X_{k,\varepsilon}) = 0$ for $j \ne k$. We can show (see [11]) that, as $\varepsilon \to 0$, the field $X_{j,\varepsilon}$ converges to $\widetilde{X}_j$ with the first order with respect to ε. As the horizontal distribution of the ε-perturbation, take $\mathrm{span}\{X_{j,\varepsilon} : 1 \le j \le m\}$. The corresponding sub-Laplacian Δ_ε is connected with the initial sub-Laplacian Δ as follows: If $\mathrm{HK}_{\Delta_\varepsilon}$ and HK_Δ are the corresponding heat kernels then

$$\mathrm{HK}_{\Delta_\varepsilon}(t, q', q'') = \varepsilon^{\mathrm{hdim}\, M} \mathrm{HK}_\Delta(\varepsilon^2 t, \delta_{\varepsilon,q}(q'), \delta_{\varepsilon,q}(q'')).$$

The essence of the method is that, alongside this relation, also another one is established between Δ_ε and $\widetilde{\Delta}$. Before describing the latter, we will formulate the new notion of convolution taking into account the variable t, which plays the role of time in the heat equation. This new operation will be denoted by $*$ since we will not need the previous notion of convolution in the present article. Strictly speaking, these are two new notions but there is no conflict between them since one is applied to operator families and the other, to functions of one real variable and two arguments from the manifold. These notions are interrelated as described below.

DEFINITION 18. Let $A = (A(t))_{t \in \mathbb{R}}$ and $B = (B(t))_{t \in \mathbb{R}}$ be two operator families acting at functions on a manifold M with integral kernels $a(t, \cdot, \cdot)$ and $b(t, \cdot, \cdot)$ respectively. Define the convolution of these families by the formula

$$(A * B)(t) = \int_0^t A(t - s) B(s)\, ds.$$

Define the convolution of $a(t, \cdot, \cdot)$ and $b(t, \cdot, \cdot)$ for all $t \in \mathbb{R}$ and $x, y \in M$ by the formula

$$(a * b)(t, x, y) = \int_0^t \left(\int_M a(s, x, z) b(t - s, z, y)\, dz \right) ds.$$

In these terms, $(a * b)(t, \cdot, \cdot)$ is the integral kernel of $(A * B)(t)$. Because of the associativity of $*$, we will omit the parentheses at multiple convolutions.

The relation between Δ_ε and $\widetilde{\Delta}$ can be obtained with the use of Duhamel's formula:

$$\mathrm{e}^{t\Delta_\varepsilon} = \mathrm{e}^{t\widetilde{\Delta}} + \int\limits_0^t (\mathrm{e}^{(t-s)\Delta_\varepsilon}(\Delta_\varepsilon - \widetilde{\Delta})\mathrm{e}^{s\widetilde{\Delta}}\, ds),$$

which is convenient to write as the convolution of the operator family

$$\mathrm{e}^{t\Delta_\varepsilon} = \mathrm{e}^{t\widetilde{\Delta}} + (A * B)\,(t),$$

where $A = (\mathrm{e}^{u\Delta_\varepsilon})_{u\in\mathbb{R}}$ and $B = ((\Delta_\varepsilon - \widetilde{\Delta})\mathrm{e}^{u\widetilde{\Delta}})_{u\in\mathbb{R}}$.

Applying Duhamel's formula for $\exp((t-s)\Delta_\varepsilon)$, we obtain

$$\mathrm{e}^{t\Delta_\varepsilon} = \mathrm{e}^{t\widetilde{\Delta}} + \int\limits_0^t \left(\left(\mathrm{e}^{(t-s)\widetilde{\Delta}} + \int\limits_0^{t-s} (\mathrm{e}^{(t-s-s')\Delta_\varepsilon}(\Delta_\varepsilon - \widetilde{\Delta})\mathrm{e}^{s'\widetilde{\Delta}}\, ds')\right)(\Delta_\varepsilon - \widetilde{\Delta})\mathrm{e}^{s\widetilde{\Delta}}\, ds\right);$$

i.e.,

$$\mathrm{e}^{t\Delta_\varepsilon} = \mathrm{e}^{t\widetilde{\Delta}} + ((\mathrm{e}^{u\widetilde{\Delta}})_{u\in\mathbb{R}} * B)(t) + ((\mathrm{e}^{u\Delta_\varepsilon})_{u\in\mathbb{R}} * B * B)(t).$$

This process can be extended by obtaining thus an expansion of $\exp(t\Delta_\varepsilon)$ in the powers of a small operator (as $\varepsilon \to 0$)

$$\mathrm{e}^{t\Delta_\varepsilon} = \sum_{r=0}^{N-1} ((\mathrm{e}^{u\widetilde{\Delta}})_{u\in\mathbb{R}} \underbrace{*B \cdots * B}_{r \text{ convolutions with } B})(t) + (A \underbrace{*B \cdots * B}_{N \text{ convolutions with } B})(t),$$

which, after passage from operators to their integral kernels, gives the necessary asymptotics of $\mathrm{HK}_{\Delta_\varepsilon}$ (and, hence, HK_Δ) up to any desired order.

Suppose that all horizontal basis vector fields X_j, $1 \le j \le m$, satisfy the condition $\mathrm{hg}_0(X_j) = 0$; in [11], this was achieved by the existence of normal forms for contact distributions on three-dimensional manifolds. Under this assumption, as $\varepsilon \to 0$, we have the asymptotics $X_{j,\varepsilon} = \widetilde{X}_j + \varepsilon^2 \mathrm{hg}_1(X_j) + o(\varepsilon^2)$. Then we obtain the following asymptotics for the operator $\Delta_\varepsilon - \widetilde{\Delta}$:

Theorem 5. *$\Delta_\varepsilon - \widetilde{\Delta} = \varepsilon^2 Y + o(\varepsilon^2)$, where*

$$Y = \sum_{j=1}^m (\widetilde{X}_j \mathrm{hg}_1(X_j) + \mathrm{hg}_1(X_j)\widetilde{X}_j + \Theta_j \widetilde{X}_j), \quad \Theta_j = \sum_{k=1}^n (\widetilde{X}_k(\psi_{j,k}) - \widetilde{X}_j(\psi_{k,k})),$$

the coefficients $\psi_{j,k}$ for $1 \le j \le n$ and $1 \le k \le n$ are smooth functions defined from the asymptotic expansions $X_{j,\varepsilon} = \widetilde{X}_j + \varepsilon^2 \sum_{k=1}^n (\psi_{j,k}\widetilde{X}_k) + o(\varepsilon^2)$, while Y is a second-order differential operator.

Proof. Let us first prove that, for all ordered collections $(j_0, \dots, j_s)$ of naturals from 1 to m, there exists a vector field $R_{j_0,\dots,j_s}$ such that

$$[[[X_{j_0,\varepsilon}, X_{j_1,\varepsilon}], X_{j_2,\varepsilon}] \dots X_{j_s,\varepsilon}] = [[[\widetilde{X}_{j_0}, \widetilde{X}_{j_1}], \widetilde{X}_{j_2}] \dots \widetilde{X}_{j_s}] + \varepsilon^2 R_{j_0,\dots,j_s} + o(\varepsilon^2).$$

Proceed by induction. For $s = 0$, the field $X_{j_0,\varepsilon}$, where $1 \le j_0 \le m$, satisfies this condition with $R_{j_0} = \mathrm{hg}_1(X_{j_0})$ since we have assumed that $\mathrm{hg}_0(X_{j_0}) = 0$.

If the claim holds true for some s then let us prove it for $s+1$:

$$\begin{aligned}
[[[X_{j_0,\varepsilon}, X_{j_1,\varepsilon}], X_{j_2,\varepsilon}] \dots X_{j_{s+1},\varepsilon}] &= [[[[\widetilde{X}_{j_0}, \widetilde{X}_{j_1}], \widetilde{X}_{j_2}] \dots \widetilde{X}_{j_s}] + \varepsilon^2 R_{j_0,\dots,j_s} + o(\varepsilon^2), X_{j_{s+1},\varepsilon}] \\
&= [[[[\widetilde{X}_{j_0}, \widetilde{X}_{j_1}], \widetilde{X}_{j_2}] \dots \widetilde{X}_{j_s}] + \varepsilon^2 R_{j_0,\dots,j_s} + o(\varepsilon^2), \widetilde{X}_{j_{s+1}} + \varepsilon^2 \mathrm{hg}_1(X_{j_{s+1}}) + o(\varepsilon^2)] \\
&= [[[\widetilde{X}_{j_0}, \widetilde{X}_{j_1}], \widetilde{X}_{j_2}] \dots \widetilde{X}_{j_{s+1}}] + \varepsilon^2([R_{j_0,\dots,j_s}, \widetilde{X}_{j_{s+1}}] + [[[[\widetilde{X}_{j_0}, \widetilde{X}_{j_1}], \widetilde{X}_{j_2}] \dots \widetilde{X}_{j_s}], \mathrm{hg}_1(X_{j_{s+1}})]) + o(\varepsilon^2),
\end{aligned}$$

which justifies the induction step with

$$R_{j_0,\dots,j_{s+1}} = [R_{j_0,\dots,j_s}, \widetilde{X}_{j_{s+1}}] + [[[[\widetilde{X}_{j_0}, \widetilde{X}_{j_1}], \widetilde{X}_{j_2}] \dots \widetilde{X}_{j_s}], \mathrm{hg}_1(X_{j_{s+1}})].$$

Since the Lie flag of the distribution $\operatorname{span}\{X_j : 1 \le j \le m\}$ stabilizes to the tangent bundle, each basis vector field X_j for $1 \le j \le n$ can be written down as a linear system of fields of the form $[[[[X_{j_0}, X_{j_1}], X_{j_2}] \dots X_{j_s}]$ with $s \ge 0$ and $1 \le j_l \le m$ for all l such that $0 \le l \le s$; the coefficients of this combination are smooth functions.

Taking $\varepsilon^{\deg X_j} d\delta_{\varepsilon^{-1}}$ of both sides of this expansion and reckoning with the fact $d\delta_{\varepsilon^{-1}}([Z_1, Z_2]) = [d\delta_{\varepsilon^{-1}} Z_1, d\delta_{\varepsilon^{-1}} Z_2]$ for all vector fields Z_1 and Z_2, we conclude that all basis vector fields $X_{j,\varepsilon}$, $1 \le j \le n$, admit the asymptotics $X_{j,\varepsilon} = \widetilde{X}_j + \varepsilon^2 E_j + o(\varepsilon^2)$ with some vector fields E_j, which is convenient to expand in the basis $\{\widetilde{X}_j : 1 \le j \le n\}$ in the form $E_j = \sum_{j'=1}^{n} (\psi_{j,j'} \widetilde{X}_{j'})$, which yields the formula

$$X_{j,\varepsilon} = \widetilde{X}_j + \varepsilon^2 \sum_{j'=1}^{n} (\psi_{j,j'} \widetilde{X}_{j'}) + o(\varepsilon^2).$$

Solve this system of linear equations for $\widetilde{X}_j$ to obtain

$$\widetilde{X}_j = X_{j,\varepsilon} - \varepsilon^2 \sum_{j'=1}^{n} (\psi_{j,j'} X_{j',\varepsilon}) + o(\varepsilon^2).$$

Expressing the sub-Laplacians Δ_ε and $\widetilde{\Delta}$ in the coordinates:

$$\Delta_\varepsilon = \sum_{j=1}^{m} \left(X_{j,\varepsilon}^2 + \sum_{k=1}^{n} X_{k,\varepsilon}^*([X_{k,\varepsilon}, X_{j,\varepsilon}]) X_{j,\varepsilon} \right), \quad \widetilde{\Delta} = \sum_{j=1}^{m} (\widetilde{X}_j^2),$$

we infer

$$\Delta_\varepsilon - \widetilde{\Delta} = \sum_{j=1}^{m} \left((\widetilde{X}_j + \varepsilon^2 \mathrm{hg}_1(X_j) + o(\varepsilon^2))^2 - \widetilde{X}_j^2 + \sum_{k=1}^{n} X_{k,\varepsilon}^*([X_{k,\varepsilon}, X_{j,\varepsilon}]) X_{j,\varepsilon} \right)$$

$$= \sum_{j=1}^{m} \left(\varepsilon^2 \widetilde{X}_j \mathrm{hg}_1(X_j) + \varepsilon^2 \mathrm{hg}_1(X_j) \widetilde{X}_j + \sum_{k=1}^{n} X_{k,\varepsilon}^*([X_{k,\varepsilon}, X_{j,\varepsilon}]) (\widetilde{X}_j + \varepsilon^2 \mathrm{hg}_1(X_j)) \right) + o(\varepsilon^2).$$

For computing ${X_{k,\varepsilon}}^*([X_{k,\varepsilon}, X_{j,\varepsilon}])$, expand $[X_{k,\varepsilon}, X_{j,\varepsilon}]$ in the basis $\{{X_{k,\varepsilon}}^* : 1 \le k \le n\}$ in terms of the structure constants $\tilde{c}_{j,k,l}$, the formula for which is given in Theorem 4, and the coefficient $\psi_{j,j'}$:

$$[X_{k,\varepsilon}, X_{j,\varepsilon}] = \left[\widetilde{X}_k + \varepsilon^2 \sum_{k'=1}^{n} (\psi_{k,k'} \widetilde{X}_{k'}), \widetilde{X}_j + \varepsilon^2 \sum_{j'=1}^{n} (\psi_{j,j'} \widetilde{X}_{j'}) \right] + o(\varepsilon^2)$$

$$= [\widetilde{X}_k, \widetilde{X}_j] + \varepsilon^2 \left(\sum_{k'=1}^{n} ([\psi_{k,k'} \widetilde{X}_{k'}, \widetilde{X}_j]) + \sum_{j'=1}^{n} ([\widetilde{X}_k, \psi_{j,j'} \widetilde{X}_{j'}]) \right) + o(\varepsilon^2)$$

$$= \sum_{l=1}^{n} (\tilde{c}_{k,j,l} \widetilde{X}_l) + \varepsilon^2 \sum_{l=1}^{n} (\psi_{k,l} [\widetilde{X}_l, \widetilde{X}_j] - \psi_{j,l} [\widetilde{X}_l, \widetilde{X}_k] + (\widetilde{X}_k(\psi_{j,l}) - \widetilde{X}_j(\psi_{k,l})) \cdot \widetilde{X}_l)$$

$$+ o(\varepsilon^2) = \sum_{l=1}^{n} \left(\tilde{c}_{k,j,l} \cdot (X_{l,\varepsilon} - \varepsilon^2 \sum_{j'=1}^{n} (\psi_{l,j'} X_{j',\varepsilon})) \right)$$

$$+ \varepsilon^2 \sum_{l=1}^{n} \left(\sum_{j'=1}^{n} ((\psi_{k,l} \tilde{c}_{l,j,j'} - \psi_{j,l} \tilde{c}_{l,k,j'}) X_{j',\varepsilon}) + (\widetilde{X}_k(\psi_{j,l}) - \widetilde{X}_j(\psi_{k,l})) X_{l,\varepsilon} \right) + o(\varepsilon^2).$$

Taking the coefficient at $X_{k,\varepsilon}$, we obtain

$$X^*_{k,\varepsilon}([X_{k,\varepsilon}, X_{j,\varepsilon}]) = \tilde{c}_{k,j,k} - \varepsilon^2 \sum_{l=1}^{n} (\tilde{c}_{k,j,l}\psi_{l,k})$$
$$+\varepsilon^2 \left(\widetilde{X}_k(\psi_{j,k}) - \widetilde{X}_j(\psi_{k,k})\right) + \varepsilon^2 \sum_{l=1}^{n} (\psi_{k,l}\tilde{c}_{l,j,k} - \psi_{j,l}\tilde{c}_{l,k,k}) + o(\varepsilon^2).$$

Sum up these quantities over k. The formula for the structure constants of the nilpotent approximation given in Theorem 4 yields $\tilde{c}_{k,j,k} = \tilde{c}_{j,k,k} = 0$ since no basis vector field X_j satisfies $\deg X_j = 0$. Thus, $\sum_{k=1}^n (\tilde{c}_{k,j,k}) = 0$. With this in mind, we have

$$\sum_{k=1}^{n} (X^*_{k,\varepsilon}([X_{k,\varepsilon}, X_{j,\varepsilon}])) = \varepsilon^2 \Theta_j + o(\varepsilon^2),$$

where

$$\Theta_j = \sum_{k=1}^{n} \left(\widetilde{X}_k(\psi_{j,k}) - \widetilde{X}_j(\psi_{k,k}) + \sum_{l=1}^{n} (\psi_{k,l}\tilde{c}_{l,j,k} - \psi_{j,l}\tilde{c}_{l,k,k} - \tilde{c}_{k,j,l}\psi_{l,k}) \right).$$

For simplifying this expression, utilize alongside the equality $\tilde{c}_{l,k,k} = 0$ the fact that

$$\sum_{k=1}^{n} \sum_{l=1}^{n} (\psi_{k,l}\tilde{c}_{l,j,k} - \tilde{c}_{k,j,l}\psi_{l,k}) = 0$$

because the summands with pairs of numbers (k, l) and (l, k) for $k < l$ are mutually annihilated, and the summands with pairs of numbers (k, k) are equal to 0. Thus,

$$\Theta_j = \sum_{k=1}^{n} (\widetilde{X}_k(\psi_{j,k}) - \widetilde{X}_j(\psi_{k,k})).$$

Inserting the computed expression $\sum_{k=1}^n (X^*_{k,\varepsilon}([X_{k,\varepsilon}, X_{j,\varepsilon}]))$ in the formula for $\Delta_\varepsilon - \widetilde{\Delta}$, we finally get

$$\Delta_\varepsilon - \widetilde{\Delta} = \varepsilon^2 \sum_{j=1}^{m} (\widetilde{X}_j \mathrm{hg}_1(X_j) + \mathrm{hg}_1(X_j)\widetilde{X}_j + \Theta_j \widetilde{X}_j) + o(\varepsilon^2).$$

This is the desired asymptotics. $\square$

Now we have a formula for Y, and so the perturbation method can be applied in the same way as in [11]: taking $N = 2$ in the expansion $\exp(t\Delta_\varepsilon)$ and reckoning with the formula

$$\varepsilon^{\mathrm{hdim}\, M} \mathrm{HK}_\Delta(\varepsilon^2 t, \delta_{\varepsilon,q}(x), \delta_{\varepsilon,q}(y)) = \mathrm{HK}_{\Delta_\varepsilon}(t, x, y),$$

we infer

$$\varepsilon^{\mathrm{hdim}\, M} \mathrm{HK}_\Delta(\varepsilon^2, 0, 0) = \mathrm{HK}_{\Delta_\varepsilon}(1, 0, 0) = \mathrm{HK}_{\widetilde{\Delta}}(1, 0, 0) + \varepsilon^2 (\mathrm{HK}_{\widetilde{\Delta}} * Y(\mathrm{HK}_{\widetilde{\Delta}}))(1, 0, 0) + O(\varepsilon^4),$$

where Y is assumed to act with respect to the first variable from M.

Remark 5. Since $\mathrm{HK}_{\widetilde{\Delta}} * Y(\mathrm{HK}_{\widetilde{\Delta}})(1, 0, 0)$ is equal to

$$\int_0^1 \int_{\widetilde{M}_0} (\mathrm{HK}_{\widetilde{\Delta}}(s, 0, z) Y(\mathrm{HK}_{\widetilde{\Delta}})(1 - s, z, 0))\, dz ds = \int_0^1 \int_{\widetilde{M}_0} (p_{\widetilde{\Delta}}(s, z) Y(p_{\widetilde{\Delta}})(1 - s, z))\, dz ds;$$

to calculate it we must apply Theorem 3 with $G = \widetilde{M}_0$. In the case of three-dimensional contact manifolds, this expression admits further simplification if the integration starts from the coordinates x and y (here $z = (x, y, w)$ has homogeneity exponents $\nu(x) = \nu(y) = 1$, $\nu(w) = 2$). In this case, the calculation amounts to the search for the moments of a two-dimensional normal distribution. In a more general situation (even in the case of Goursat groups, which we examine below), it is not possible to make such a simplification though the qualitative behavior of the kernel $p_{\widetilde{\Delta}}(s, z)$ as $z \to \infty$—exponential decay—still holds (see [22]).

REMARK 6. Without the assumption that $\mathrm{hg}_0(X_j) = 0$, we would obtained the first-order terms with respect to ε in the asymptotic expansion $\varepsilon^{\mathrm{hdim}\, M} \mathrm{HK}_\Delta(\varepsilon^2, 0, 0)$ since $\Delta_\varepsilon - \widetilde{\Delta}$ would be just $O(\varepsilon)$ as $\varepsilon \to 0$, and, after the insertion $t = \varepsilon^2$, there would be no expansion of the form $\mathrm{HK}_\Delta(t, x, x) = t^{-\frac{\mathrm{hdim}\, M}{2}}(a_0 + a_1 t + O(t^2))$.

4. An Example: a Manifold with Growth Vector $(2, 3, \ldots, k, k + 1, \ldots, n)$

In this section, we apply the above methods to a sub-Riemannian manifold whose nilpotent approximation is the n-dimensional Goursat group.

DEFINITION 19. The *Goursat group of dimension* n is the nilpotent Lie group in $\mathbb{R}^n$ with the two-dimensional left-invariant distribution H_1, called the Goursat distribution, which has growth vector $(2, 3 \ldots n - 1, n)$.

The multiplication operation in the Goursat group can be written as

$$\sum_{j=1}^{n} x_j \mathbf{e}_j \star \sum_{k=1}^{n} y_k \mathbf{e}_k = (x_1 + y_1)\mathbf{e}_1 + \sum_{j=2}^{n} \left(x_j + \sum_{k=2}^{j} \left(\frac{{x_1}^{j-k}}{(j-k)!} y_k \right) \right) \mathbf{e}_j,$$

where $\mathbf{0} = \sum_{j=1}^{n} 0\mathbf{e}_j$ is the neutral element.

The distribution H_1 has the left-invariant basis

$$H_1 = \mathrm{span}(\{X_1, X_2\}), \quad X_1 = \partial_1, \quad X_2 = \sum_{k=0}^{n-2} \frac{{x_1}^k}{k!} \partial_{k+2}.$$

Define a sequence of commutators generating the whole tangent bundle with X_1 and X_2 by the formula $X_j = [X_1, X_{j-1}]$ for $j \geq 3$. For $j, j' \geq 2$, we have $[X_j, X_{j'}] = 0$. Introducing the n-dimensional Lebesgue measure on the Goursat group (which is also its Haar measure) and the corresponding volume form, define the sub-Laplacian $\Delta = X_1^2 + X_2^2$.

The elements of the Goursat group are also representable as the square matrices of order n of the form

$$\exp\left(aX_1 + \sum_{j=2}^{n} b_{j-1} X_j \right) = \exp \begin{pmatrix} a \cdot J_{n-1} & \overleftarrow{b}^{\top} \\ \overrightarrow{0}_{n-1} & 0 \end{pmatrix} = \begin{pmatrix} \exp(a \cdot J_{n-1}) & \varphi(a \cdot J_{n-1}) \overleftarrow{b}^{\top} \\ \overrightarrow{0}_{n-1} & 1 \end{pmatrix},$$

where J_{n-1} is the upper triangular matrix of order $n-1$ that is the Jordan cell with eigenvalue 0, $\overrightarrow{0}_{n-1}$ is the zero row vector of length $n-1$, and $\overleftarrow{b}$ is the row vector $(b_{n-1}, \ldots, b_1)$ of length $n-1$ (the left arrow means the reverse order of the components with respect to $\overrightarrow{b} = (b_1, \ldots, b_{n-1})$), while $\top$ stands for transposition,

$$\varphi(z) = \begin{cases} \frac{\exp(z)-1}{z}, & z \neq 0, \\ 1, & z = 0 \end{cases}$$

(the expression $\varphi(a \cdot J_{n-1})$ is understood as a matrix function). As the group operation, we take matrix multiplication, and the matrix exponent serves as the exponential mapping from the Lie algebra into the Lie group. This version of the definition of $\star$, which we will use below, differs insignificantly from the initial one but is equivalent to the latter. This can be checked by associating with each vector $\vec{x} \in \mathbb{R}^n$ the matrix

$$\begin{pmatrix} \exp(x_1 \cdot J_{n-1}) & \overleftarrow{x_{\geq 2}}^\top \\ \overrightarrow{0}_{n-1} & 1 \end{pmatrix} = \exp \begin{pmatrix} x_1 \cdot J_{n-1} & (\varphi(x_1 \cdot J_{n-1}))^{-1} \cdot \overleftarrow{x_{\geq 2}}^\top \\ \overrightarrow{0}_{n-1} & 0 \end{pmatrix},$$

where $\overleftarrow{x_{\geq 2}} = (x_n, \ldots, x_2)$ is the reverse notation of the vector obtained from $\vec{x}$ by removing the first component. The notation $(\varphi(x_1 \cdot J_{n-1}))^{-1}$ is correct since the matrix $\varphi(x_1 \cdot J_{n-1})$ is upper triangular, and all elements on its principal diagonal are equal to 1. This association is a desired automorphism since, for all $\overrightarrow{x}, \overrightarrow{y} \in \mathbb{R}^n$, we have

$$\begin{pmatrix} \exp(x_1 \cdot J_{n-1}) & \overleftarrow{x_{\geq 2}}^\top \\ \overrightarrow{0}_{n-1} & 1 \end{pmatrix} \begin{pmatrix} \exp(y_1 \cdot J_{n-1}) & \overleftarrow{y_{\geq 2}}^\top \\ \overrightarrow{0}_{n-1} & 1 \end{pmatrix} = \begin{pmatrix} \exp(z_1 \cdot J_{n-1}) & \overleftarrow{z_{\geq 2}}^\top \\ \overrightarrow{0}_{n-1} & 1 \end{pmatrix},$$

where $\overrightarrow{z} = \overrightarrow{x} \star \overrightarrow{y}$ by the initial definition of $\star$. In what follows, $\star$ stands for this operation.

We will search for the heat kernel in the Goursat group with the use of Theorem 3. Since its key ingredient is the orbit method, we must perform all calculations that constitute this method. In terms of the new group operation, the adjoint representation looks as

$$\begin{aligned}
&\mathrm{Ad}_{\exp(xX_1 + \sum\limits_{j=2}^{n} y_{j-1}X_j)} \left(aX_1 + \sum_{j=2}^{n} b_{j-1}X_j \right) \\
&= \exp \begin{pmatrix} xJ_{n-1} & \overleftarrow{y}^\top \\ \overrightarrow{0}_{n-1} & 0 \end{pmatrix} \cdot \begin{pmatrix} aJ_{n-1} & \overleftarrow{b}^\top \\ \overrightarrow{0}_{n-1} & 0 \end{pmatrix} \cdot \exp \begin{pmatrix} -xJ_{n-1} & -\overleftarrow{y}^\top \\ \overrightarrow{0}_{n-1} & 0 \end{pmatrix} \\
&= \begin{pmatrix} aJ_{n-1} & \exp(xJ_{n-1})\overleftarrow{b}^\top - aJ_{n-1}\varphi(xJ_{n-1})\overleftarrow{y}^\top \\ \overrightarrow{0}_{n-1} & 0 \end{pmatrix}.
\end{aligned}$$

Defining the functionals X_j^*, where $1 \leq j \leq n$, by the relations $X_j^*(X_j) = 1$ and $X_j^*(X_k) = 0$ for $j \neq k$, we obtain the following formula for the coadjoint representation:

$$\begin{aligned}
&\mathrm{Ad}^*_{\exp\left(xX_1 + \sum\limits_{j=2}^{n} y_{j-1}X_j\right)} \left(\alpha X_1^* + \sum_{j=2}^{n} \beta_{j-1}X_j^* \right) \left(aX_1 + \sum_{j=2}^{n} b_{j-1}X_j \right) \\
&= \left(\alpha X_1^* + \sum_{j=2}^{n} \beta_{j-1}X_j^* \right) \left(\mathrm{Ad}_{\exp\left(-xX_1 - \sum\limits_{j=2}^{n} y_{j-1}X_j\right)} \left(aX_1 + \sum_{j=2}^{n} b_{j-1}X_j \right) \right) \\
&= \alpha a + \overleftarrow{\beta} \cdot (\exp(-xJ_{n-1})\overleftarrow{b}^\top + aJ_{n-1}\varphi(-xJ_{n-1})\overleftarrow{y}^\top),
\end{aligned}$$

which is written down as follows in terms of X_j^*, $1 \leq j \leq n$:

$$\begin{aligned}
&\mathrm{Ad}^*_{\exp\left(xX_1 + \sum\limits_{j=2}^{n} y_{j-1}X_j\right)} \left(\alpha X_1^* + \sum_{j=2}^{n} \beta_{j-1}X_j^* \right) \\
&= (\alpha + \overleftarrow{\beta} J_{n-1}\varphi(-xJ_{n-1})\overleftarrow{y}^\top)X_1^* + \overleftarrow{\beta} \exp(-xJ_{n-1}) \begin{pmatrix} X_n^* \\ \vdots \\ X_2^* \end{pmatrix}.
\end{aligned}$$

The orbits can be found by varying x and $\overrightarrow{y}$, i.e., for every $\xi = \alpha X_1^* + \sum_{j=2}^{n} \beta_{j-1}X_j^*$, by Definition 7, its orbit consists exactly of the elements of the form $\mathrm{Ad}^*_{\exp\left(xX_1 + \sum_{j=2}^{n} y_{j-1}X_j\right)}(\xi)$ for almost all $x \in \mathbb{R}$ and $\overrightarrow{y} \in \mathbb{R}^{n-1}$. Using orbits, we will later classify irreducible unitary representations. To this end, we must find for each $\xi \in \mathfrak{g}^*$ a subalgebra of maximal dimension subordinate to ξ and the corresponding subgroup with which we carry out induction. Use the above-mentioned theorem by Pukánszky [15] stating that if G is a nilpotent Lie group then every maximal subalgebra subordinate to a covector ξ contains $\mathfrak{g}_\xi$; this strongly simplifies the arguments.

For each $\xi = \alpha X_1^* + \sum_{j=2}^n \beta_{j-1} X_j^*$ but for those for which $\overrightarrow{\beta} = \overrightarrow{0}$, denote by $j_{\max}$ the greatest number j such that $\beta_j \neq 0$. The orbit of a covector ξ and the set of maximal subalgebras subordinate to it will depend on what is $j_{\max}$ equal to (and whether it exists at all) for given ξ.

(i) If $j_{\max}$ does not exist (i.e., $\overrightarrow{\beta} = \overrightarrow{0}$) then the orbit consists of the single point αX_1^* for which $\mathfrak{g}_{\alpha X_1^*} = \mathfrak{g}$. In this case, the maximal subordinate subalgebra is unique and equal to $\mathfrak{g}$.

(ii) If $j_{\max} = 1$ then the orbit consists of the single point $\alpha X_1^* + \beta_1 X_2^*$ (the equality $\mathfrak{g}_{\alpha X_1^* + \beta_1 X_2^*} = \mathfrak{g}$ holds). The maximal subordinate subalgebra is also equal to $\mathfrak{g}$.

(iii) The orbit of the covector $\alpha X_1^* + \beta_1 X_2^* + \beta_2 X_3^*$, where $\beta_2 \neq 0$ (i.e., $j_{\max} = 2$), is equal to $\operatorname{span}\{X_1^*, X_2^*\} + \beta_2 X_3^*$ (the sign $+$ designates parallel translation by a given element of $\mathfrak{g}^*$). In this case, $\mathfrak{g}_{\alpha X_1^* + \beta_1 X_2^* + \beta_2 X_3^*} = \operatorname{span}\{X_j : 3 \leq j \leq n\}$. Here a maximal subordinate subalgebra is nonunique; therefore, we apply Vergne's construction (Theorem 2) which for $V_k = \operatorname{span}(\{X_j : n+1-k \leq j \leq n\})$, where $0 \leq k \leq n$, gives the subalgebra span $(\{X_j : 2 \leq j \leq n\})$. Note that, instead of Vergne's subalgebra, we could take the subalgebra $\operatorname{span}(\{X_1\} \cup \{X_j : 3 \leq j \leq n\})$, which leads to another representation of the same equivalence class.

(iv) For $j_{\max} \geq 3$, the orbit is two-dimensional and parametrized by the coefficients at X_1^* and for $X_{j_{\max}}^*$ as follows:

$$\mathscr{O}_{\alpha X_1^* + \sum\limits_{j=2}^{j_{\max}+1} \beta_{j-1} X_j^*} = \left\{ y X_1^* + \sum_{j=1}^{j_{\max}} \left(\sum_{k=j}^{j_{\max}} \left(\frac{(x - \beta_{j_{\max}-1})^{k-j} \beta_k}{\beta_{j_{\max}}{}^{k-j} (k-j)!} \right) \cdot X_{j+1}^* \right) : x, y \in \mathbb{R} \right\}.$$

This parametrization results as follows: Since the $X_{j_{\max}}^*$th component of the covector

$$\operatorname{Ad}^*_{\exp\left(x X_1 + \sum\limits_{j=2}^{n} y_{j-1} X_j\right)} \left(\alpha X_1^* + \sum_{j=2}^{n} \beta_{j-1} X_j^* \right)$$

is equal to x; therefore, it can be defined arbitrarily. Starting from this, the remaining components but the X_1^*th component can be defined uniquely since they do not depend on $\overrightarrow{y}$. The component corresponding to X_1^* has the form $\beta_{j_{\max}} y_{j_{\max}-1} + Z$, where Z does not depend on $y_{j_{\max}-1}$. Since $\beta_{j_{\max}} \neq 0$, the X_1^*th component can be made any a priori given value by choosing $y_{j_{\max}-1}$ suitably. This exhausts all covectors in the orbit of $\alpha X_1^* + \sum_{j=2}^{j_{\max}+1} \beta_{j-1} X_j^*$ with $\beta_{j_{\max}} \neq 0$ for $j_{\max} \geq 3$.

Taking as the representative of the orbit the covector for which the parameters x and y vanish, we obtain $\mathfrak{g}_{\alpha X_1^* + \sum_{j=2}^{j_{\max}+1} \beta_{j-1} X_j^*} = \operatorname{span}(\Phi \cup \Psi)$, where

$$\Phi = \{X_j : j_{\max} + 1 \leq j \leq n\},$$

$$\Psi = \left\{ \left(X_j - \sum_{k=j}^{j_{\max}} \left(\frac{(-\beta_{j_{\max}-1})^{k-j} \beta_k}{\beta_{j_{\max}}{}^{k+1-j} (k-j)!} \right) X_{j_{\max}} \right) : 2 \leq j \leq j_{\max} - 1 \right\}.$$

The maximal subordinate subalgebra is unique and equal to $\operatorname{span}(\{X_j : 2 \leq j \leq n\})$.

Using these data about orbits and maximal subordinate subgroups, we can construct the corresponding representations (in the sense of Kirillov).

In cases (i) and (ii), induction is trivial: the one-dimensional representation corresponding to the covector $\xi = \alpha X_1^* + \beta_1 X_2^*$ (it is unimportant whether β_1 is zero or not), defined by the formula $\rho_{\xi,G}\big(a\mathbf{e}_1 + \sum_{j=2}^n b_{j-1} \mathbf{e}_j\big) = \exp(2\pi \mathrm{i}(\alpha a + \beta_1 b_1)) \cdot \mathrm{Id}$, goes to itself since the subgroup $VS_\xi = \exp(\mathfrak{vs}_\xi)$ is already the whole group G.

Much richer is the structure of representations in cases (iii) and (iv). Since the orbits are two-dimensional in these cases, the Hilbert space of the corresponding representations can be identified with $L^2(\mathbb{R})$ using the equivalent representation R'_ξ instead of R_ξ. This stems from the general fact that the dimension of the space of cosets modulo VS_ξ is equal to one half of the dimension of the orbit $\mathscr{O}_\xi$. The Vergne subalgebra $\mathfrak{vs}_\xi = \operatorname{span}(\{X_j : 2 \le j \le n\})$, common for these cases, will be denoted by $\mathfrak{v}$, since it does not depend on ξ taken from an orbit of type (iii) or (iv); adopt the notation V for the corresponding subgroup $\exp(\mathfrak{v})$.

For finding the induced representation, factorize G into $\mathbb{R}$ and V. The mapping $\gamma : \mathbb{R} \to G$ of Definition 11 is given by the formula $\gamma_x = x\mathbf{e}_1$. Represent $\gamma_x \star g \in G$, where $x \in \mathbb{R}$ and $g \in G$, as $h \star \gamma_w$, where $h \in V$ and $w \in \mathbb{R}$:

$$x\mathbf{e}_1 \star \left(a\mathbf{e}_1 + \sum_{j=2}^{n} b_{j-1}\mathbf{e}_j\right) = \left(\sum_{j=2}^{n}\left(\sum_{k=1}^{j-1}\left(\sum_{l=0}^{k-1}\left(\frac{a^l b_{k-l}}{(l+1)!}\right)\cdot\frac{x^{j-1-k}}{(j-1-k)!}\right)\right)\mathbf{e}_j\right) \star (x+a)\mathbf{e}_1.$$

Consequently, R'_ξ takes the following form: for all $f \in L^2(\mathbb{R})$ and almost all $x \in \mathbb{R}$, we have

$$\begin{aligned}\left(R'_\xi(a\mathbf{e}_1 + \sum_{j=2}^{n} b_{j-1}\mathbf{e}_j)f\right)(x) &= \exp(2\pi\mathrm{i}\xi(\log(h)))f(w)\\ = \exp\Bigg(2\pi\mathrm{i}\xi\Bigg(\sum_{j=2}^{n}&\Bigg(\Bigg(\sum_{k=1}^{j-1}\Bigg(\sum_{l=0}^{k-1}\left(\frac{a^l b_{k-l}}{(l+1)!}\right)\cdot\frac{x^{j-1-k}}{(j-1-k)!}\Bigg)\Bigg)X_j\Bigg)\Bigg)\Bigg)f(x+a)\\ &= \exp\left(2\pi\mathrm{i}\xi\left(\sum_{j=2}^{n}(P_j(a,\overrightarrow{b},x)\cdot X_j)\right)\right)f(x+a)\end{aligned}$$

(the last equality is simply a notation for the coefficients at X_j).

It is at these representations (more exactly, classes of representations) that the Plancherel measure is concentrated. It suffices to consider only $j_{\max} = n-1$ since this condition defines an open dense subset in the set of orbits of maximal dimension. Indeed, the condition $j_{\max} = n-1$ is equivalent to the fact that $\beta_{n-1} \neq 0$, i.e., from the whole of $\mathfrak{g}^*$, we remove an $(n-1)$-dimensional hyperplane. Assigning to each element $\mathfrak{g}^*$ its orbit with account taken of the construction of the topology in $\mathfrak{g}^*/\mathrm{Ad}^*$ takes the complement to the hyperplane to some dense set of orbits.

In each orbit lying in this set, choose a representative of the form $\xi = \sum_{j=2}^{n-2}(\beta_{j-1}X_j^*) + \beta_{n-1}X_n^*$, where $\beta_{n-1} \neq 0$. This can be done for the following reason: As the expression for the orbits shows, we can nullify the coefficients at X_1^* and X_{n-1}^* (there they were denoted by y and x respectively), put β_{n-1} to be an arbitrary nonzero number, and make the remaining coefficients to be equal to any a priori given values by equating the coefficients at X_j^* to these values consecutively (as j decreases) and solving a linear equation with coefficient 1 for each new variable β_j. Thus, we obtain a parametrization of the set of orbits which, under the correspondence between $\mathfrak{g}^*/\mathrm{Ad}^*$ and $\widehat{G}$, goes to some subset in $\widehat{G}$ whose complement has Plancherel measure 0. In terms of the parametrization, the corresponding Plancherel measure has the form $P(d(\beta_j)_{1\le j\le n-1; j\neq n-2}) = |\beta_{n-1}|d(\beta_j)_{1\le j\le n-1; j\neq n-2}$ because, for $\xi = \sum_{j=2}^{n-2}(\beta_{j-1}X_j^*) + \beta_{n-1}X_n^*$, we have $|\operatorname{pf}(\xi)| = |\beta_{n-1}|$. Indeed, using the basis $\{X_1, X_{n-1}\}$ of the space $\mathfrak{g}/\mathfrak{g}_\xi$, find the determinant of the matrix

$$\begin{pmatrix}\xi([X_1,X_1]) & \xi([X_1,X_{n-1}])\\ \xi([X_{n-1},X_1]) & \xi([X_{n-1},X_{n-1}])\end{pmatrix} = \begin{pmatrix}0 & \beta_{n-1}\\ -\beta_{n-1} & 0\end{pmatrix}.$$

It is equal to β_{n-1}^2.

The transformed operator $\widehat{\Delta} = \mathscr{F}\Delta\mathscr{F}^{-1}$ looks as

$$\widehat{\Delta}(\lambda_\xi) = d^2(R'_\xi)(X_1) + d^2(R'_\xi)(X_2),$$

where the differential of R at $X \in \mathfrak{g}$, denoted by $dR(X)$, is the operator on the Hilbert space H_R of the representation R defined at $v \in H_R$ by the formula

$$dR(X)(v) = \left(\frac{d}{dt}(R_{\exp(tX)}(v))\right)\Big|_{t=0}$$

and $d^2R(X) = dR(X) \circ dR(X)$. For expressing $\widehat{\Delta}$ in this form, we used the general formula from [1] which is valid for all unimodular Lie groups.

Straightforward calculation gives $d(R'_\xi)(X_1)(f) = f'$, where the derivative of $f \in L^2(\mathbb{R}, \mathbb{C})$ is understood in the weak sense, and $d(R'_\xi)(X_2)(f) = M_\xi f$ with M_ξ defined as

$$M_\xi(x) = 2\pi \mathrm{i}\left(\sum_{j=1}^{n-3}\left(\beta_j \frac{x^{j-1}}{(j-1)!}\right) + \beta_{n-1}\frac{x^{n-2}}{(n-2)!}\right).$$

Indeed, using the above-derived formula for the representation R'_ξ for $\xi = \sum_{j=2}^{n-2}(\beta_{j-1}X_j^*) + \beta_{n-1}X_n^*$, we obtain $(R'_\xi)_{\exp(tX_1)}(f)(x) = (R'_\xi)_{t\mathbf{e}_1}(f)(x) = f(x+t)$; therefore,

$$d(R'_\xi)(X_1)(f)(x) = \left(\frac{d}{dt}((R'_\xi)_{\exp(tX_1)}(f)(x))\right)\Big|_{t=0} = \left(\frac{d}{dt}(f(x+t))\right)\Big|_{t=0} = f'(x).$$

Similarly,

$$(R'_\xi)_{\exp(tX_2)}(f)(x) = (R'_\xi)_{t\mathbf{e}_2}(f)(x)$$
$$= \exp\left(2\pi \mathrm{i}\xi\left(\sum_{j=2}^{n}(t\frac{x^{j-2}}{(j-2)!}X_j)\right)\right)f(x) = \exp\left(tM_\xi(x)\right)f(x).$$

The last equality follows from the fact that

$$\xi = \sum_{j=2}^{n-2}(\beta_{j-1}X_j^*) + \beta_{n-1}X_n^*.$$

Hence,

$$d(R'_\xi)(X_2)(f)(x) = \left(\frac{d}{dt}((R'_\xi)_{\exp(tX_2)}(f)(x))\right)\Big|_{t=0} = \left(\frac{d}{dt}(\mathrm{e}^{tM_\xi(x)}f(x))\right)\Big|_{t=0} = M_\xi(x)f(x).$$

Consequently, $\widehat{\Delta}(\lambda_\xi)(f) = f'' + M_\xi^2 f$. For the convenience of notations, we will write

$$f'' + (M_{\sum_{j=2}^{n-2}(\beta_{j-1}X_j^*)+\beta_{n-1}X_n^*})^2 f = \widehat{\Delta}_{\overrightarrow{\beta}} f.$$

With the above calculations in mind, Theorem 3, applied to the Goursat group, takes the following form:

Corollary 1. *The heat kernel in the n-dimensional Goursat group corresponding to the sub-Laplacian $\Delta = X_1^2 + X_2^2$, where the horizontal bundle is* $\mathrm{span}(\{X_1, X_2\})$ *with $X_1 = \partial_1$ and $X_2 = \sum_{k=0}^{n-2}\frac{x_1{}^k}{k!}\partial_{k+2}$, is written down as follows:*

$$p\left(t, a\mathbf{e}_1 + \sum_{j=2}^{n} b_{j-1}\mathbf{e}_j\right)$$
$$= \int_{\mathbb{R}^{n-2}}\int_{\mathbb{R}} \mathrm{e}^{2\pi \mathrm{i}\left(\beta_{n-1}P_n(a,\overrightarrow{b},x) + \sum_{j=1}^{n-3}(\beta_j P_{j+1}(a,\overrightarrow{b},x))\right)} \mathrm{HK}_{\widehat{\Delta}_{\overrightarrow{\beta}}}(t, x+a, x)|\beta_{n-1}|\, dx d(\beta_j)_{1\le j\le n-3}\, d\beta_{n-1}.$$

Below this formula will be applied in the perturbation method. For convenience, we will write

$$p\left(t, a\mathbf{e}_1 + \sum_{j=2}^{n} b_{j-1}\mathbf{e}_j\right) = \int\limits_{\mathbb{R}^{n-1}} \mathrm{e}^{Z_{\overrightarrow{\beta},x}(a,\overrightarrow{b})} K_{\overrightarrow{\beta},x,t}(a) d(\overrightarrow{\beta}, x),$$

using the following notations

$$Z_{\overrightarrow{\beta},x}(a, \overrightarrow{b}) = 2\pi\mathrm{i}\left(\beta_{n-1}P_n(a, \overrightarrow{b}, x) + \sum_{j=1}^{n-3} (\beta_j P_{j+1}(a, \overrightarrow{b}, x))\right),$$

$$K_{\overrightarrow{\beta},x,t}(a) = \mathrm{HK}_{\widehat{\Delta}_{\overrightarrow{\beta}}}(t, x+a, x)|\beta_{n-1}|.$$

Whenever dependence on $\overrightarrow{\beta}$ occurs, we imply the omission of the component with index $n-2$. Recall that

$$P_j(a, \overrightarrow{b}, x) = \sum_{k=1}^{j-1}\left(\sum_{l=0}^{k-1}\left(\frac{a^l b_{k-l}}{(l+1)!}\right) \cdot \frac{x^{j-1-k}}{(j-1-k)!}\right).$$

Suppose that the sub-Riemannian manifold has the horizontal distribution $\operatorname{span}\{X_1, X_2\}$ obtained from the Goursat distribution by the perturbation written down in a neighborhood of $(0,\dots,0)$ up to homogeneous vector fields with homogeneity exponent 2 and above as follows. For all $p \le -2$, we have $\mathrm{hg}_p(X_1) = \mathrm{hg}_p(X_2) = 0$; and, moreover,

$$\mathrm{hg}_{-1}(X_1) = \widetilde{X}_1, \quad \mathrm{hg}_0(X_1) = 0, \quad \mathrm{hg}_1(X_1) = \sum_{r=1}^{n}\left(\sum_{\alpha\in\Phi_r} (u_{\alpha,r}x^{\alpha}) \cdot \frac{\partial}{\partial x_r}\right),$$

$$\mathrm{hg}_{-1}(X_2) = \widetilde{X}_2, \quad \mathrm{hg}_0(X_2) = 0, \mathrm{hg}_1(X_2) = \sum_{r=1}^{n}\left(\sum_{\alpha\in\Phi_r} (v_{\alpha,r}x^{\alpha}) \cdot \frac{\partial}{\partial x_r}\right),$$

where Φ_r is the set of all multi-indices $\alpha = (\alpha_1, \dots, \alpha_n)$ for which

$$\alpha_1 + \sum_{j=2}^{n}((j-1)\alpha_j) = \begin{cases} 2, & r = 1, \\ r, & r > 1, \end{cases} \quad \widetilde{X}_1 = \frac{\partial}{\partial x_1}, \quad \widetilde{X}_2 = \sum_{k=0}^{n-2} \frac{{x_1}^k}{k!}\frac{\partial}{\partial x_{k+2}},$$

the homogeneity index 1 is assigned to the variable x_1; the homogeneity exponent $r-1$ is assigned to each variable x_r for $r \ge 2$, and to the operator of derivation with respect to each variable, we assign its homogeneity exponent with the minus sign. The symbols $u_{\alpha,r}$ and $v_{\alpha,r}$ stand for the constants, called *perturbation parameters*, for which for $3 \le j \le n-1$ we have $[X_2, X_j] \in \operatorname{span}(\{X_k : 1 \le k \le j\})$, where $X_j = [X_1, X_{j-1}]$ for $3 \le j \le n$. This condition is imposed because the nilpotent approximation of the manifold is a Goursat group.

The basis vector fields of the nilpotent approximation for $3 \le j \le n$ are $\widetilde{X}_j = [\widetilde{X}_1, \widetilde{X}_{j-1}]$. The volume form for the Popp measure has the form ${X_1}^* \wedge \dots \wedge {X_n}^*$; this can be checked, for example, by a formula from [23].

We will need the fact that the operators $\frac{\partial}{\partial x_j}$, $1 \le j \le n$, are expressible in the basis $\{\widetilde{X}_j : 1 \le j \le n\}$ by coefficients that are polynomials of x_1 because the system of linear equations solved in this case has a unitriangular matrix of polynomials of x_1 whose all elements of the diagonal are equal to 1.

For applying the perturbation method, calculate the operator Y given in Theorem 5:

$$Y = \widetilde{X}_1 \mathrm{hg}_1(X_1) + \mathrm{hg}_1(X_1)\widetilde{X}_1 + \sum_{k=1}^{n}(\widetilde{X}_k(\psi_{1,k}) - \widetilde{X}_1(\psi_{k,k})) \cdot \widetilde{X}_1$$
$$+\widetilde{X}_2 \mathrm{hg}_1(X_2) + \mathrm{hg}_1(X_2)\widetilde{X}_2 + \sum_{k=1}^{n}(\widetilde{X}_k(\psi_{2,k}) - \widetilde{X}_2(\psi_{k,k})) \cdot \widetilde{X}_2,$$

where the coefficients $\psi_{j,j'}$ are the same as in the proof of Theorem 5. They can be calculated explicitly. To this end, in terms of Theorem 5, write down the equality

$$[[[X_{j_0,\varepsilon}, X_{j_1,\varepsilon}], X_{j_2,\varepsilon}] \dots X_{j_s,\varepsilon}] = [[[\widetilde{X}_{j_0}, \widetilde{X}_{j_1}], \widetilde{X}_{j_2}] \dots \widetilde{X}_{j_s}] + \varepsilon^2 R_{j_0,\dots,j_s} + o(\varepsilon^2)$$

with $j_0 = 2$ and $j_k = 1$ for $1 \le k \le s$. For $1 \le s \le n-2$, we obtain

$$(-1)^s X_{s+2,\varepsilon} = (-1)^s \widetilde{X}_{s+2} + \varepsilon^2 R_{2,\underbrace{1,\dots,1}_{s \text{ unities}}} + o(\varepsilon^2).$$

Thus, for all $j \ge 3$, the quantity $\psi_{j,j'}$ is the coefficient at $\widetilde{X}_{j'}$ in the expansion of the operator $E_j = (-1)^j R_{2,\underbrace{1,\dots,1}_{(j-2) \text{ unities}}}$ in the basis $\{\widetilde{X}_{j'} : 1 \le j' \le n\}$. The recurrent formula for $R_{j_0,\dots,j_s}$, deduced at the beginning of the proof of Theorem 5, shows that the coefficients $\psi_{j,j'}$ for $j \ge 3$ and $1 \le j' \le n$ are polynomials of the coordinates and perturbation parameters. For $\psi_{1,j'}$ and $\psi_{2,j'}$, the fact of their polynomial dependence on the coordinates and perturbation parameters is trivial: in the notations given in the proof of Theorem 5, $E_1 = \mathrm{hg}_1(X_1)$ and $E_2 = \mathrm{hg}_1(X_2)$.

Summing up what was said above, we conclude that the coefficients of Y depend polynomially on the coordinates and perturbation parameters.

We observed in Section 3 that, acting by the method given in [11], as $\varepsilon \to 0$, we can obtain the asymptotics

$$\varepsilon^{\mathrm{hdim}\, M} \mathrm{HK}_\Delta(\varepsilon^2, 0, 0) = \mathrm{HK}_{\Delta_\varepsilon}(1,0,0) = \mathrm{HK}_{\widetilde{\Delta}}(1,0,0) + \varepsilon^2 (\mathrm{HK}_{\widetilde{\Delta}} * Y(\mathrm{HK}_{\widetilde{\Delta}}))(1,0,0) + O(\varepsilon^4).$$

We are interested in the coefficient at ε^2 on the right-hand side of the last equality which is equal to $\mathrm{HK}_{\widetilde{\Delta}} * Y(\mathrm{HK}_{\widetilde{\Delta}})(1,0,0)$. Since, for its computation, we must differentiate $p\big(t, a\mathbf{e}_1 + \sum_{j=2}^{n} b_{j-1}\mathbf{e}_j\big)$ twice with respect to the variables a and $\overrightarrow{b}$; this coefficient depends not only on the transformed kernel but also on its derivatives (up to the second order) with respect to a. We will also need to calculate $\mathrm{hdim}\, M$ in the case if the nilpotent approximation of the manifold M is the n-dimensional Goursat group. By the formula given in [6], we obtain $\mathrm{hdim}\, M = \frac{n(n-1)}{2} + 1$.

Further calculations are very cumbersome, and so we give them schematically. If we denote the coefficients of Y by

$$Y = \sum_{j \le k} (F_{j,k}((a, \overrightarrow{b}), \overrightarrow{u}, \overrightarrow{v}) \partial_j \partial_k) + \sum_{j} (G_j((a, \overrightarrow{b}), \overrightarrow{u}, \overrightarrow{v}) \partial_j)$$

(Y contains no summand of zeroth order); then, considering that $\partial_j \partial_k Z_{\overrightarrow{\beta},x}(a, \overrightarrow{b}) = 0$ for all $j, k \ge 2$, we arrive at the expression

$$
\begin{aligned}
Y(p_{\widetilde{\Delta}})(t,a,\overrightarrow{b}) &= \sum_{j\le k}\Bigg(F_{j,k}((a,\overrightarrow{b}),\overrightarrow{u},\overrightarrow{v})\int\limits_{\mathbb{R}^{n-1}} \mathrm{e}^{Z_{\overrightarrow{\beta},x}(a,\overrightarrow{b})}\\
&\quad\times K_{\overrightarrow{\beta},x,t}(a)\partial_j Z_{\overrightarrow{\beta},x}(a,\overrightarrow{b})\partial_k Z_{\overrightarrow{\beta},x}(a,\overrightarrow{b})\,d(\overrightarrow{\beta},x)\Bigg)\\
&+\sum_{k=1}^{n}\Bigg(F_{1,k}((a,\overrightarrow{b}),\overrightarrow{u},\overrightarrow{v})\int\limits_{\mathbb{R}^{n-1}} \mathrm{e}^{Z_{\overrightarrow{\beta},x}(a,\overrightarrow{b})}K_{\overrightarrow{\beta},x,t}(a)\partial_1\partial_k Z_{\overrightarrow{\beta},x}(a,\overrightarrow{b})d(\overrightarrow{\beta},x)\Bigg)\\
&\quad+F_{1,1}((a,\overrightarrow{b}),\overrightarrow{u},\overrightarrow{v})\int\limits_{\mathbb{R}^{n-1}} \mathrm{e}^{Z_{\overrightarrow{\beta},x}(a,\overrightarrow{b})}(\partial_1^2 K_{\overrightarrow{\beta},x,t}(a)\\
&\quad+\partial_1 Z_{\overrightarrow{\beta},x}(a,\overrightarrow{b})\partial_1 K_{\overrightarrow{\beta},x,t}(a))\,d(\overrightarrow{\beta},x)\\
&+\sum_{k=1}^{n}\Bigg(F_{1,k}((a,\overrightarrow{b}),\overrightarrow{u},\overrightarrow{v})\int\limits_{\mathbb{R}^{n-1}} \mathrm{e}^{Z_{\overrightarrow{\beta},x}(a,\overrightarrow{b})}\partial_1 K_{\overrightarrow{\beta},x,t}(a)\partial_k Z_{\overrightarrow{\beta},x}(a,\overrightarrow{b})\,d(\overrightarrow{\beta},x)\Bigg)\\
&+\sum_{j=1}^{n}(G_j((a,\overrightarrow{b}),\overrightarrow{u},\overrightarrow{v})\int\limits_{\mathbb{R}^{n-1}} \mathrm{e}^{Z_{\overrightarrow{\beta},x}(a,\overrightarrow{b})}K_{\overrightarrow{\beta},x,t}(a)\partial_j Z_{\overrightarrow{\beta},x}(a,\overrightarrow{b})\,d(\overrightarrow{\beta},x))\\
&\quad+G_1((a,\overrightarrow{b}),\overrightarrow{u},\overrightarrow{v})\int\limits_{\mathbb{R}^{n-1}} \mathrm{e}^{Z_{\overrightarrow{\beta},x}(a,\overrightarrow{b})}\partial_1 K_{\overrightarrow{\beta},x,t}(a)\,d(\overrightarrow{\beta},x).
\end{aligned}
$$

For making the form of $\mathrm{HK}_{\widetilde{\Delta}} * Y(\mathrm{HK}_{\widetilde{\Delta}})(1,0,0)$ completely explicit, we must have a somewhat constructive method for computing $\mathrm{HK}_{\widehat{\Delta}_{\overrightarrow{\beta}}}$. It is possible to do that by Trotter's formula

$$\mathrm{e}^{A+B} = \lim_{N\to\infty}((\mathrm{e}^{\frac{A}{N}}\mathrm{e}^{\frac{B}{N}})^N).$$

Taking $Bf = tf''$ and $Af = t(M_{n-2 \atop \sum\limits_{j=2}(\beta_{j-1}X_j^*)+\beta_{n-1}X_n^*})^2 f$, we find that

$$(\mathrm{e}^{\frac{B}{N}}f)(x) = \left(\frac{N}{4\pi t}\right)^{\frac{1}{2}}\int\limits_{\mathbb{R}} \mathrm{e}^{-\frac{(x-y)^2N}{4t}}f(y)\,dy,$$

$$(\mathrm{e}^{\frac{A}{N}}f)(x) = \exp\left(-\frac{4\pi^2 t}{N}\left(\sum_{j=1}^{n-3}\left(\beta_j\frac{x^{j-1}}{(j-1)!}\right)+\beta_{n-1}\frac{x^{n-2}}{(n-2)!}\right)^2\right)\cdot f(x),$$

$$\mathrm{HK}_{\widehat{\Delta}_{\overrightarrow{\beta}}}(t,x_1,x_0) = \lim_{N\to\infty}\int\limits_{\mathbb{R}^{N-1}}\prod_{r=0}^{N-1}(L_{t,N}(x_{\frac{r+1}{N}},x_{\frac{r}{N}}))d(x_{\frac{r}{N}})_{1\le r\le N-1},$$

where

$$L_{t,N}(x,y) = \left(\frac{N}{4\pi t}\right)^{\frac{1}{2}}\exp\!\left(-\frac{4\pi^2 t}{n}\left(\sum_{j=1}^{n-3}\left(\beta_j\frac{x^{j-1}}{(j-1)!}\right)+\beta_{n-1}\frac{x^{n-2}}{(n-2)!}\right)^2-\frac{(x-y)^2N}{4t}\right).$$

This formula is applicable under some additional conditions which can be found, for example, in [24]. It is also proved in [24] that they are satisfied for the operators of the form $(\Delta f)(x) = f''(x)-(V(x))^2 f(x)$, where V is a polynomial with real coefficients; the example under study falls under this case.

Inserting the found conditions for $p_{\widetilde{\Delta}}$, $Yp_{\widetilde{\Delta}}$, and $\mathrm{HK}_{\widehat{\Delta}_{\vec{\beta}}}$ into the formula for the desired coefficient

$$\mathrm{HK}_{\widetilde{\Delta}} * Y(\mathrm{HK}_{\widetilde{\Delta}})(1,0,0) = \int\limits_0^1 \int\limits_{\mathbb{R}^n} (p_{\widetilde{\Delta}}(s,(a,\overrightarrow{b}))Y(p_{\widetilde{\Delta}})(1-s,(a,\overrightarrow{b})))d(a,\overrightarrow{b})\,ds,$$

we obtain the following result:

Theorem 6. *For a sub-Riemannian manifold M with nilpotent approximation that is a Goursat group under the assumption that* $\mathrm{hg}_0(X_j) = 0$ *for* $j \in \{1,2\}$, *the coefficient* a_1 *in the asymptotics*

$$\mathrm{HK}_\Delta(t,x,x) = t^{-\frac{n(n-1)+2}{4}}(a_0 + a_1 t + O(t^2))$$

as $t \to 0$ *is a polynomial of the perturbation parameters whose coefficients are expressed in terms of the limits of sequences of some integrals of functions of the form* $P(z_1,\dots,z_k)\exp(Q(z_1,\dots,z_k))$, *where* P *and* Q *are* (*in general, complex*) *polynomials of the real variables* $z_1,\dots,z_k$.

Note that the polynomials under the exponent in these integrals contain information about the representations of the Goursat group and its coadjoint orbits.

Though we have been able to partially complete the calculations only in the case of Goursat groups, we conjecture that, for equiregular sub-Riemannian manifolds with other nilpotent approximations, the coefficient a_1 and also the higher-order coefficients are representable in an analogous form. This mainly depends on how convenient for calculations the formulas for the nilpotent heat kernels will be in the general case. It is not impossible either that there are some nontrivial dependences between the higher-order coefficients.

5. Conclusion

Despite the fact that the existence is known from [25, 26] of asymptotic representation of the form we considered for sub-Riemannian heat kernels, the methods used there (for example, stochastic diffusion) were very unconstructive and related to the geometry of manifolds only indirectly. The approach of the present article gives more explicit formulas for the coefficients though the approach is very cumbersome computationally. It works under not very restrictive assumption that $\mathrm{hg}_0(X_j) = 0$ for the basis horizontal fields X_j which, as we expect, can be removed in many cases.

The novelty of the present article is part concerned with the perturbation method consists in finding very general formulas for the operator Y and the heat kernel in the nilpotent approximation, which is necessary to have at hand in each concrete application of this method.

The special functions that can occur in the expression for $\mathrm{HK}_{\widehat{\Delta_H(R_\xi)}}$ are most likely unsimplifiable. However, $\mathrm{HK}_{\widehat{\Delta_H(R_\xi)}}$ can be expressed with the use of Trotter's formula

$$\exp(A+B) = \lim_{N\to\infty}\left(\left(\exp\left(\frac{A}{N}\right)\exp\left(\frac{B}{N}\right)\right)^N\right)$$

generalized to the case of several summands since the operator $\widehat{\Delta_H}(\lambda)$, where $\lambda \in \widehat{G}$, is expressible in the form of several summands corresponding to the basis horizontal vector fields X_j, $1 \le j \le m$. Each of these summands is the value of $dR(X_j)\circ dR(X_j)$ for some representation $R \in \lambda$ (all definitions involved here are correct for Lie groups).

It is also worth noting that the special functions necessary for solving the sub-Riemannian heat equation are well studied in some cases. For example, for nilpotent Lie groups with growth vectors $(2,3,4)$ and $(2,3,5)$, Heun functions of some special form are enough (see [15]).

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