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The relative heat content associated with a subset $\Omega \subset M$ of a sub-Riemannian manifold is defined as the total amount of heat contained in Ω at time t, with uniform initial condition on Ω, allowing the heat to flow outside the domain. We obtain a fourth-order asymptotic expansion in the square root of t of the relative heat content associated with relatively compact noncharacteristic domains. Compared to the classical heat content that was studied by Rizzi and Rossi (*J. Math. Pures Appl.* (9) **148** (2021), 267–307), several difficulties emerge due to the absence of Dirichlet conditions at the boundary of the domain. To overcome this lack of information, we combine a rough asymptotics for the temperature function at the boundary, coupled with stochastic completeness of the heat semigroup. Our technique applies to any (possibly rank-varying) sub-Riemannian manifold that is globally doubling and satisfies a global weak Poincaré inequality, including in particular sub-Riemannian structures on compact manifolds and Carnot groups.

1. Introduction

We study the asymptotics of the relative heat content in sub-Riemannian geometry. The latter is a vast generalization of Riemannian geometry; indeed a sub-Riemannian manifold M is a smooth manifold where a metric is defined only on a subset of preferred directions $\mathcal{D}_x \subset T_x M$ at each point $x \in M$ (called horizontal directions). For example, $\mathcal{D}$ can be a sub-bundle of the tangent bundle, but we will consider the most general case of rank-varying distributions. Moreover, we assume that $\mathcal{D}$ satisfies the so-called Hörmander condition, which ensures that M is horizontally path connected, and that the usual length-minimization procedure yields a well-defined metric.

Let M be a sub-Riemannian manifold, equipped with a smooth measure ω, let $\Omega \subset M$ be an open relatively compact subset of M, with smooth boundary, and consider the Cauchy problem for the heat equation in this setting

$$(\partial_t - \Delta)u(t, x) = 0 \quad \text{for all } (t, x) \in (0, \infty) \times M,$$
$$u(0, \cdot) = \mathbb{1}_\Omega \quad \text{in } L^2(M, \omega), \tag{1}$$

where $\mathbb{1}_\Omega$ is the indicator function of the set Ω, and Δ is the sub-Laplacian, defined with respect to ω. By classical spectral theory, there exists a unique solution to (1),

$$u(t, x) = e^{t\Delta}\mathbb{1}_\Omega(x) \quad \text{for all } x \in M, \ t > 0,$$

where $e^{t\Delta}$ denotes the heat semigroup in $L^2(M, \omega)$, associated with Δ. The *relative heat content* is the function

$$H_\Omega(t) = \int_\Omega u(t, x) \, d\omega(x) \quad \text{for all } t > 0.$$

This quantity has been studied in connection with geometric properties of subsets of $\mathbb{R}^n$, starting from the seminal work of De Giorgi [1954], where he introduced the notion of perimeter of a set in $\mathbb{R}^n$ and proved a characterization of sets of finite perimeter in terms of the heat kernel. His result was subsequently refined, using techniques of functions of bounded variation: it was proven in [Ledoux 1994] for balls in $\mathbb{R}^n$, and in [Miranda et al. 2007] for general subsets of $\mathbb{R}^n$, that a borel set $\Omega \subset \mathbb{R}^n$ with finite Lebesgue measure has finite perimeter à la De Giorgi if and only if

$$\text{there exists } \lim_{t \to 0} \frac{\sqrt{\pi}}{\sqrt{t}}(|\Omega| - H_\Omega(t)) = P(\Omega), \tag{2}$$

where $|\cdot|$ is the Lebesgue measure and P is the perimeter measure in $\mathbb{R}^n$. Notice that (2) is equivalent to a first-order[1] asymptotic expansion of $H_\Omega(t)$. A further development in this direction was then obtained in [Angiuli et al. 2013], where the authors extended (2) to an asymptotic expansion of order 3 in $\sqrt{t}$, assuming the boundary of $\Omega \subset \mathbb{R}^n$ to be a $C^{1,1}$ set. For simplicity, we state here the result of [Angiuli et al. 2013, Theorem 1.1] assuming $\partial\Omega$ is smooth:[2]

$$H_\Omega(t) = |\Omega| - \frac{1}{\sqrt{\pi}}P(\Omega)t^{1/2} + \frac{(n-1)^2}{12\sqrt{\pi}}\int_{\partial\Omega}\left(H_{\partial\Omega}^2(x) + \frac{2}{(n-1)^2}c_{\partial\Omega}(x)\right)d\mathcal{H}^{n-1}(x)t^{3/2} + o(t^{3/2}) \tag{3}$$

as $t \to 0$, where $\mathcal{H}^{n-1}$ is the Hausdorff measure and, denoting by $k_i^{\partial\Omega}(x)$ the principal curvatures of $\partial\Omega$ at the point x,

$$H_{\partial\Omega}(x) = \frac{1}{n-1}\sum_{i=1}^{n-1} k_i^{\partial\Omega}(x), \quad c_{\partial\Omega}(x) = \sum_{i=1}^{n-1} k_i^{\partial\Omega}(x)^2.$$

In the Riemannian setting, van den Berg and Gilkey [2015] proved the existence of a complete asymptotic expansion for $H_\Omega(t)$, generalizing (3), when $\partial\Omega$ is smooth. Moreover, they were able to compute explicitly the coefficients of the expansion up to order 4 in $\sqrt{t}$. Their techniques are based

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[1]Here and throughout the paper, the notion of order is computed with respect to $\sqrt{t}$.

[2]The statement of Theorem 1.1 in [Angiuli et al. 2013] differs from (3) by a sign in the third-order coefficient: the correct sign appears a few lines below the statement, in the expansion of the function $K_t(E, E^c)$.

on pseudodifferential calculus and cannot be immediately adapted to the sub-Riemannian setting. In particular, what is missing is a global parametrix estimate for the heat kernel $p_t(x, y)$, see [van den Berg and Gilkey 2015, Section 2.3]: for any $k \in \mathbb{N}$, there exist $J_k, C_k > 0$ such that

$$\left\| p_t(x, y) - \sum_{j=0}^{J_k} p_t^j(x, y) \right\|_{C^k(M \times M)} \leq C_k t^k \quad \text{as } t \to 0, \tag{4}$$

where $p_t^j(x, y)$ are suitable smooth functions, given explicitly in terms of the Euclidean heat kernel and iterated convolutions. The closest estimate analogue to (4) in the sub-Riemannian setting is the one proved recently in [Colin de Verdière et al. 2021, Theorem A] (see Theorem 2.9 for the precise statement), where the authors show an asymptotic expansion of the heat kernel in an *asymptotic neighborhood* of the diagonal, which is not enough to reproduce (4) and thus the argument of van den Berg and Gilkey. Moreover, in this case, $p_t^j(x, y)$ is expressed in terms of the heat kernel of the nilpotent approximation and iterated convolutions, thus posing technical difficulties for the explicit computations of the coefficients (which would be no longer "simple" Gaussian-type integrals).

Under the assumption of not having characteristic points, we prove the existence of the asymptotic expansion of $H_\Omega(t)$, up to order 4 in $\sqrt{t}$, as $t \to 0$. We remark that we include also the rank-varying case. In order to state our main results, let us introduce the following operator, acting on smooth functions compactly supported close to $\partial\Omega$:

$$N\phi = 2g(\nabla\phi, \nabla\delta) + \phi\Delta\delta,$$

where $\delta : M \to \mathbb{R}$ denotes the sub-Riemannian signed distance function from $\partial\Omega$; see Section 4 for precise definitions.

Theorem 1.1. *Let M be a compact sub-Riemannian manifold, equipped with a smooth measure ω, and let $\Omega \subset M$ be an open subset whose boundary is smooth and has no characteristic points. Then, as $t \to 0$,*

$$H_\Omega(t) = \omega(\Omega) - \frac{1}{\sqrt{\pi}}\sigma(\partial\Omega)t^{1/2} - \frac{1}{12\sqrt{\pi}}\int_{\partial\Omega}(N(\Delta\delta) - 2(\Delta\delta)^2)\,d\sigma\,t^{3/2} + o(t^2), \tag{5}$$

where σ denotes the sub-Riemannian perimeter measure.

Remark 1.2. The compactness assumption in Theorem 1.1 is technical and can be relaxed by requiring, instead, global doubling of the measure and a global Poincaré inequality; see Section 7 and in particular Theorem 7.3. Some notable examples satisfying these assumptions are:

• M is a Lie group with polynomial volume growth, the distribution is generated by a family of left-invariant vector fields satisfying the Hörmander condition and ω is the Haar measure. This family includes also Carnot groups.

• $M = \mathbb{R}^n$, equipped with a sub-Riemannian structure induced by a family of vector fields $\{Y_1, \ldots, Y_N\}$ with bounded coefficients together with their derivatives, and satisfying the Hörmander condition.

• M is a complete Riemannian manifold, equipped with the Riemannian measure, and with nonnegative Ricci curvature.

See Section 7.1 for further details. In all these examples, Theorem 1.1 holds.

The strategy of the proof of Theorem 1.1 follows a strategy similar to that of [Rizzi and Rossi 2021], inspired by the method introduced in [Savo 1998], used for the classical heat content (6). However, as we are going to explain in Section 1.1, new technical difficulties arise, the main one being related to the fact that now $u(t, \cdot)|_{\partial\Omega} \neq 0$. At order zero, we obtain the following result; see Section 2 for precise definitions.

Theorem 1.3. *Let M be a sub-Riemannian manifold, equipped with a smooth measure ω and let $\Omega \subset M$ be an open relatively compact subset, whose boundary is smooth and has no characteristic points. Let $x \in \partial\Omega$ and consider a chart of privileged coordinates $\psi : U \to V \subset \mathbb{R}^n$ centered at x such that $\psi(U \cap \Omega) = V \cap \{z_1 > 0\}$. Then,*

$$\lim_{t \to 0} u(t, x) = \int_{\{z_1 > 0\}} \hat{p}_1^x(0, z) \, d\hat{\omega}^x(z) = \frac{1}{2} \quad \text{for all } x \in \partial\Omega,$$

where $\hat{\omega}^x$ denotes the nilpotentization of ω at x and $\hat{p}_t^x$ denotes the heat kernel associated with the nilpotent approximation of M at x and measure $\hat{\omega}^x$.

This result can be seen as a partial generalization of [Capogna et al. 2013, Proposition 3], where the authors proved an asymptotic expansion of $u(t, x)$ up to order 1 in $\sqrt{t}$ for $x \in \partial\Omega$ for a special class of noncharacteristic domains in Carnot groups.

Remark 1.4. Our proof of Theorem 1.3 does not yield an asymptotic series for $u(t, \cdot)|_{\partial\Omega}$ at order higher than 0. Indeed a complete asymptotic series of this quantity seems difficult to achieve; see Section 6.

Remark 1.5. When $\partial\Omega$ has no characteristic points, the conormal bundle

$$\mathcal{A}(\partial\Omega) := \{\lambda \in T^*M : \langle \lambda, T_{\pi(\lambda)}\partial\Omega \rangle = 0\}$$

does not intersect the characteristic set and, as a consequence, the principal symbol of the sub-Laplacian is elliptic near $\mathcal{A}(\partial\Omega)$. Thus, it is likely that microlocal analysis techniques in the spirit of [Colin de Verdière et al. 2018] could yield the existence of a complete asymptotic expansion of the relative heat content (but not an explicit expression and geometric interpretation of the coefficients). We thank Yves Colin de Verdière and the anonymous referee for pointing out this fact.

1.1. *Strategy of the proof of Theorem 1.1.* To better understand the new technical difficulties in the study of the relative heat content $H_\Omega(t)$, let us compare it with the classical heat content $Q_\Omega(t)$ and illustrate the strategy of the proof of Theorem 1.1.

The classical heat content. We highlight the differences between the relative heat content $H_\Omega(t)$ and the classical one $Q_\Omega(t)$: Let $\Omega \subset M$ an open set in M. Then, for all $t > 0$, we have

$$H_\Omega(t) = \int_\Omega u(t, x) \, d\omega(x), \quad Q_\Omega(t) = \int_\Omega u_0(t, x) \, d\omega(x), \tag{6}$$

where $u(t, x)$ is the solution to (1) and $u_0(t, x)$ is the solution to the Dirichlet problem for the heat equation, associated with Ω, i.e.,

$$\begin{aligned} (\partial_t - \Delta)u_0(t, x) &= 0 \quad \text{for all } (t, x) \in (0, \infty) \times \Omega, \\ u_0(t, x) &= 0 \quad \text{for all } (t, x) \in (0, \infty) \times \partial\Omega, \\ u_0(0, x) &= 1 \quad \text{for all } x \in \Omega. \end{aligned} \tag{7}$$

The crucial difference is that $u_0(t, \cdot)|_{\partial\Omega} = 0$ for any $t > 0$, whereas $u(t, \cdot)|_{\partial\Omega} \neq 0$ in general. Thus, there is no a priori relation between $H_\Omega(t)$ and $Q_\Omega(t)$: the only relevant information is given by domain monotonicity, which implies that

$$Q_\Omega(t) \leq H_\Omega(t) \quad \text{for all } t > 0,$$

and clearly this does not give the asymptotics of the latter. See also [van den Berg 2013] for other comparison results in the Euclidean setting.

Failure of Duhamel's principle. In [Rizzi and Rossi 2021], we established a complete asymptotic expansion of $Q_\Omega(t)$, as $t \to 0$, provided that $\partial\Omega$ has no characteristic points. The proof of this result relied on an iterated application of the Duhamel's principle and the fact that $u_0(t, x)|_{\partial\Omega} = 0$. Following the same strategy, we apply Duhamel's principle to a localized version of $H_\Omega(t)$: Fix a function $\phi \in C_c^\infty(M)$, compactly supported in a tubular neighborhood around $\partial\Omega$ and such that $0 \leq \phi \leq 1$ and ϕ is identically 1, close to $\partial\Omega$. Then, using off-diagonal estimates for the heat kernel, one can prove that

$$\omega(\Omega) - H_\Omega(t) = I\phi(t, 0) + O(t^\infty) \quad \text{as } t \to 0, \tag{8}$$

where $I\phi(t, r)$ is defined for $t > 0$ and $r \geq 0$ as

$$I\phi(t, r) = \int_{\Omega_r} (1 - u(t, x))\phi(x)\, d\omega(x), \tag{9}$$

where $\Omega_r = \{x \in \Omega : \delta(x) > r\}$, with $\delta : \Omega \to \mathbb{R}$ denoting the distance function from the boundary. Hence, the small-time behavior of $H_\Omega(t)$ is captured by $I\phi(t, 0)$. By Duhamel's principle and the sub-Riemannian mean value lemma, see Section 4 for details, we obtain

$$I\phi(t, 0) = \frac{1}{\sqrt{\pi}} \int_0^t \int_{\partial\Omega} (1 - u(\tau, y))\phi(y)\, d\sigma(y)\, (t - \tau)^{-1/2}\, d\tau + O(t) \quad \text{as } t \to 0. \tag{10}$$

For the classical heat content, u_0 satisfies Dirichlet boundary condition, see (7); hence (10) would give the first-order asymptotics (and then one could iterate). On the contrary, in this case, we do not have prior knowledge of $u(t, y)$ as $y \in \partial\Omega$ and $t \to 0$. Thus, already for the first-order asymptotics, Duhamel's principle alone is not enough, and we need some information on the asymptotic behavior of $u(t, \cdot)|_{\partial\Omega}$.

First-order asymptotics. We study the asymptotics of $u(t, \cdot)|_{\partial\Omega}$. Using the notion of nilpotent approximation of a sub-Riemannian manifold, see Section 2.3, we deduce the zero-order asymptotic expansion of $u(t, \cdot)|_{\partial\Omega}$ as $t \to 0$, proving Theorem 1.3. This is enough to infer the first-order expansion of $H_\Omega(t)$, by means of (10). At this point, we iterate the Duhamel's principle to obtain the higher-order terms of the expansion of $H_\Omega(t)$. However, already at the first iteration, we obtain the following formula for $I\phi$:

$$I\phi(t, 0) = \frac{1}{\sqrt{\pi}} \int_0^t \int_{\partial\Omega} (1 - u(\tau, \cdot))\phi\, d\sigma\, (t - \tau)^{-1/2}\, d\tau$$

$$+ \frac{1}{2\pi} \int_0^t \int_0^\tau \int_{\partial\Omega} (1 - u(\hat{\tau}, \cdot))N\phi\, d\sigma\, ((\tau - \hat{\tau})(t - \tau))^{-1/2}\, d\hat{\tau}\, d\tau + O(t^{3/2}) \tag{11}$$

as $t \to 0$. Therefore, the zero-order asymptotic expansion of $u(t, \cdot)|_{\partial\Omega}$ no longer suffices for obtaining the second-order asymptotics of $H_\Omega(t)$.

The outside contribution $I^c\phi$. We mentioned that the crucial difference between $H_\Omega(t)$ and $Q_\Omega(t)$, defined in (6), is related to the fact that $u(t, \cdot)|_{\partial\Omega} \neq 0$, whereas $u_0(t, \cdot)|_{\partial\Omega} = 0$ for any $t > 0$. From a physical viewpoint, this distinction comes from the fact that, since the boundary $\partial\Omega$ is no longer insulated, the solution to (1) can flow also outside of Ω, whereas the solution to the Dirichlet problem (7) is confined in Ω, and the external temperature is 0. Hence, we can imagine that the asymptotic expansion of $H_\Omega(t)$ is affected by the boundary, both from the inside and from the outside of Ω.

Interpreting $I\phi$ as the *inside contribution* to the asymptotics of H_Ω, we are going to formalize the physical intuition of having heat flowing outside of Ω, defining an *outside contribution*, $I^c\phi$, to the asymptotics.[3] The starting observation is the following simple relation: Setting

$$K_\Omega(t) = \int_{M\setminus\Omega} u(t, x)\,d\omega(x) \quad \text{for all } t > 0,$$

we have, by the divergence theorem,

$$H_\Omega(t) + K_\Omega(t) = \omega(\Omega) \quad \text{for all } t > 0. \tag{12}$$

Similarly to (9), for a suitable smooth function ϕ, one may define a localized version of $K_\Omega(t)$, which we call $I^c\phi(t, r)$, so that

$$K_\Omega(t) = I^c\phi(t, 0) + O(t^\infty) \quad \text{as } t \to 0; \tag{13}$$

see Section 5.1 for precise definitions. Using (8), (12) and (13), we show the relation

$$I\phi(t, 0) - I^c\phi(t, 0) = O(t^\infty) \quad \text{as } t \to 0,$$

for a suitable smooth function ϕ. On the other hand, for the localized quantity $I\phi(t, 0) - I^c\phi(t, 0)$ we have a Duhamel's principle, thanks to which we are able to study the asymptotic expansion, up to order 3, of the *integral* of $u(t, x)$ over $\partial\Omega$; see Theorem 5.4. The limitation to the order 3 of the asymptotics is technical and seems difficult to overcome; see Remark 5.5. Inserting this asymptotics in (11), we obtain the asymptotics *up to order* 3 of the expansion of $H_\Omega(t)$ as $t \to 0$.

Fourth-order asymptotics. Since we have at disposal only the asymptotics of the integral of $u(t, x)$ over $\partial\Omega$, up to order 3, we need a finer argument to obtain the fourth-order asymptotics of $H_\Omega(t)$. The simple but compelling relation is based once again on (8), (12) and (13), thanks to which we can write

$$\omega(\Omega) - H_\Omega(t) = \tfrac{1}{2}(I\phi(t, 0) + I^c\phi(t, 0)) + O(t^\infty) \quad \text{as } t \to 0.$$

Now for the sum of the contributions $I\phi(t, 0) + I^c\phi(t, 0)$, the Duhamel's principle implies

$$I\phi(t, 0) + I^c\phi(t, 0)$$
$$= \frac{2}{\sqrt{\pi}}\sigma(\partial\Omega)t^{1/2} + \frac{1}{2\pi}\int_0^t\int_0^\tau\int_{\partial\Omega}(1 - 2u(\hat{\tau}, x))N\phi(y)\,d\sigma(y)((\tau - \hat{\tau})(t - \tau))^{-1/2}\,d\hat{\tau}\,d\tau + o(t).$$

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[3]The notation "superscript c" stands for complement. Indeed the outside contribution is the inside contribution of the complement of Ω, see Section 5.1.

This time notice how the integral of $u(t, x)$ over $\partial\Omega$ appears in a first-order term (as opposed to what happened in (10) or (11)); thus its asymptotic expansion up to order 3 implies a fourth-order expansion for $H_\Omega(t)$, concluding the proof of Theorem 1.1.

1.2. *From the heat kernel asymptotics to the relative heat content asymptotics.* In [Colin de Verdière et al. 2021, Theorem A], the authors proved the existence of small-time asymptotics of the hypoelliptic heat kernel, $p_t(x, y)$; see Theorem 2.9 below for the precise statement. In Theorem 1.3 we are able to exploit this result to obtain the zero-order asymptotics of the function

$$u(t, x) = e^{t\Delta}\mathbb{1}_\Omega(x) = \int_\Omega p_t(x, y)\, d\omega(y) \quad \text{for all } t > 0, \; x \in \partial\Omega.$$

However, we are not able to extend Theorem 1.3 to higher-order asymptotics since, roughly speaking, the remainder terms in Theorem 2.9 are not uniform as $t \to 0$. If we had a better control on the remainders, we could indeed integrate (in a suitable way) the small-time heat kernel asymptotics to obtain the corresponding expansion for $u(t, x)$. Finally, from such an expansion, the relative heat content asymptotics would follow from the localization principle (8) and the (iterated) Duhamel's principle (10). This is done in Section 6.

1.3. *Characteristic points.* In order to prove our main results, we need the noncharacteristic assumption on the domain Ω. We recall that for a subset $\Omega \subset M$ with smooth boundary, $x \in \partial\Omega$ is a characteristic point if $\mathcal{D}_x \subset T_x(\partial\Omega)$. As was the case for the classical heat content, see [Rizzi and Rossi 2021], the noncharacteristic assumption is crucial to follow our strategy, since it guarantees the smoothness of the signed distance function close to $\partial\Omega$; see Theorem 4.1. Nevertheless, one might ask whether Theorem 1.1 holds for domains with characteristic points, at least formally.

On the one hand, the coefficients, up to order 2, are well-defined even in presence of characteristic points; see [Balogh 2003]. While, for what concerns the integrand of the third-order coefficient, its integrability, with respect to the sub-Riemannian induced measure σ, is related to integrability of the sub-Riemannian mean curvature $\mathcal{H}$, with respect to the Riemannian induced measure. The latter is a nontrivial property, which has been studied in [Danielli et al. 2012], and holds in the Heisenberg group, for surfaces with mildly degenerate characteristic points in the sense of [Rossi 2023].

On the other hand, differently from what happens in the case of the Dirichlet problem, the heat kernel $p_t(x, y)$ associated with (1) is smooth at the boundary of Ω for positive times, even in presence of characteristic points. Thus, in principle, there is no obstacle in obtaining an asymptotic expansion of $H_\Omega(t)$ also in that case. Moreover, in Carnot groups of step 2, a result similar to (2) holds; see [Bramanti et al. 2012; Garofalo and Tralli 2023]. In particular, the characterization of sets of finite horizontal perimeter in Carnot groups of step 2 is independent of the presence of characteristic points, indicating that an asymptotic expansion such as (5) may still hold, dropping the noncharacteristic assumption.

1.4. *Notation.* Throughout the article, for a set $U \subset M$, we will use the notation $C_c^\infty(U)$, even in the compact case, so that all the statements need not be modified in the noncompact case, when the generalization is possible; see Theorem 7.3. Moreover, in the noncompact and complete case, the set $\Omega \subset M$ is assumed to be open and bounded.

2. Preliminaries

We recall some essential facts in sub-Riemannian geometry, following [Agrachev et al. 2020].

2.1. *Sub-Riemannian geometry.*

Let M be a smooth, connected finite-dimensional manifold. A sub-Riemannian structure on M is defined by a set of N global smooth vector fields $X_1, \ldots, X_N$, called a *generating frame*. The generating frame defines a *distribution* of subspaces of the tangent spaces at each point $x \in M$, given by

$$\mathcal{D}_x = \text{span}\{X_1(x), \ldots, X_N(x)\} \subseteq T_x M. \tag{14}$$

We assume that the distribution satisfies the *Hörmander condition*, i.e., the Lie algebra of smooth vector fields generated by $X_1, \ldots, X_N$, evaluated at the point x, coincides with $T_x M$, for all $x \in M$. The generating frame induces a norm on the distribution at x, namely

$$\|v\|_g = \inf\left\{\sum_{i=1}^N u_i^2 : \sum_{i=1}^N u_i X_i(x) = v\right\} \quad \text{for all } v \in \mathcal{D}_x,$$

which, in turn, defines an inner product on $\mathcal{D}_x$ by polarization, which we denote by $g_x(v, v)$. Let $T > 0$. We say that $\gamma : [0, T] \to M$ is a *horizontal curve* if it is absolutely continuous and

$$\dot{\gamma}(t) \in \mathcal{D}_{\gamma(t)} \quad \text{for a.e. } t \in [0, T].$$

This implies that there exists $u : [0, T] \to \mathbb{R}^N$ such that

$$\dot{\gamma}(t) = \sum_{i=1}^N u_i(t) X_i(\gamma(t)) \quad \text{for a.e. } t \in [0, T].$$

Moreover, we require that $u \in L^2([0, T], \mathbb{R}^N)$. If γ is a horizontal curve, then the map $t \mapsto \|\dot{\gamma}(t)\|_g$ is integrable on $[0, T]$. We define the *length* of a horizontal curve as

$$\ell(\gamma) = \int_0^T \|\dot{\gamma}(t)\|_g \, dt.$$

The *sub-Riemannian distance* is defined, for any $x, y \in M$, by

$$d_{\text{SR}}(x, y) = \inf\{\ell(\gamma) : \gamma \text{ horizontal curve between } x \text{ and } y\}.$$

By the Chow–Rashevsky theorem, the distance $d_{\text{SR}} : M \times M \to \mathbb{R}$ is finite and continuous. Furthermore it induces the same topology as the manifold one.

Remark 2.1. The above definition includes all classical constant-rank sub-Riemannian structures as in [Montgomery 2002; Rifford 2014] (where $\mathcal{D}$ is a vector distribution and g a symmetric and positive tensor on $\mathcal{D}$), but also general rank-varying sub-Riemannian structures. Moreover, the same sub-Riemannian structure can arise from different generating families.

2.2. *The relative heat content.*

Let M be a sub-Riemannian manifold. Let ω be a smooth measure on M, i.e., by a positive tensor density. The *divergence* of a smooth vector field is defined by

$$\text{div}_\omega(X)\omega = \mathcal{L}_X \omega \quad \text{for all } X \in \Gamma(TM),$$

where $\mathcal{L}_X$ denotes the Lie derivative in the direction of X. The *horizontal gradient* of a function $f \in C^\infty(M)$, denoted by ∇f, is defined as the horizontal vector field (i.e., tangent to the distribution at each point) such that

$$g_x(\nabla f(x), v) = v(f)(x) \quad \text{for all } v \in \mathcal{D}_x,$$

where v acts as a derivation on f. In terms of a generating frame as in (14), one has

$$\nabla f = \sum_{i=1}^N X_i(f) X_i \quad \text{for all } f \in C^\infty(M).$$

We recall the divergence theorem (we stress that M is not required to be orientable): Let $\Omega \subset M$ be open with smooth boundary. Then

$$\int_\Omega (f \operatorname{div}_\omega X + g(\nabla f, X)) \, d\omega = - \int_{\partial\Omega} f g(X, v) \, d\sigma \tag{15}$$

for any smooth function f and vector field X such that the vector field fX is compactly supported. In (15), v is the inward-pointing normal vector field to Ω and σ is the induced sub-Riemannian measure on $\partial\Omega$ (i.e., the one whose density is $\sigma = |i_v \omega|_{\partial\Omega}|$).

The *sub-Laplacian* is the operator $\Delta = \operatorname{div}_\omega \circ \nabla$, acting on $C^\infty(M)$. Again, we may write its expression with respect to a generating frame (14), obtaining

$$\Delta f = \sum_{i=1}^N \{X_i^2(f) + X_i(f) \operatorname{div}_\omega(X_i)\} \quad \text{for all } f \in C^\infty(M). \tag{16}$$

We denote by $L^2(M, \omega)$, or simply by L^2, the space of real functions on M which are square-integrable with respect to the measure ω. Let $\Omega \subset M$ be an open relatively compact set with smooth boundary. This means that the closure $\overline{\Omega}$ is a compact manifold with smooth boundary. We consider the *Cauchy problem for the heat equation* on Ω; that is, we look for functions u such that

$$\begin{aligned} (\partial_t - \Delta)u(t, x) &= 0 \quad \text{for all } (t, x) \in (0, \infty) \times M, \\ u(0, \cdot) &= \mathbb{1}_\Omega \quad \text{in } L^2(M, \omega), \end{aligned} \tag{17}$$

where $u(0, \cdot)$ is a shorthand notation for the L^2-limit of $u(t, x)$ as $t \to 0$. Notice that Δ is symmetric with respect to the L^2-scalar product and negative; moreover, if (M, d_{SR}) is complete as a metric space, it is essentially self-adjoint; see [Strichartz 1986]. Thus, there exists a unique solution to (17), and it can be represented as

$$u(t, x) = e^{t\Delta} \mathbb{1}_\Omega(x) \quad \text{for all } x \in M, \ t > 0,$$

where $e^{t\Delta} : L^2 \to L^2$ denotes the heat semigroup, associated with Δ. We remark that, for all $\varphi \in L^2$, the function $e^{t\Delta}\varphi$ is smooth for all $(t, x) \in (0, \infty) \times M$, by the hypoellipticity of the heat operator, and there exists a heat kernel associated with (17), i.e., a positive function $p_t(x, y) \in C^\infty((0, +\infty) \times M \times M)$ such that

$$u(t, x) = \int_M p_t(x, y) \mathbb{1}_\Omega(y) \, d\omega(y) = \int_\Omega p_t(x, y) \, d\omega(y). \tag{18}$$

Definition 2.2 (relative heat content). Let $u(t, x)$ be the solution to (17). We define the *relative heat content*, associated with Ω, as

$$H_\Omega(t) = \int_\Omega u(t, x)\, d\omega(x) \quad \text{for all } t > 0.$$

Remark 2.3. If we consider, instead of Ω, a set which is the closure of an open set, then the Cauchy problem (17) has a unique solution and relative heat content is still well-defined.

We recall here a property of the solution to (17): it satisfies a weak maximum principle, meaning that

$$0 \le u(t, x) \le 1 \quad \text{for all } x \in \Omega, \text{ for all } t > 0. \tag{19}$$

This can be proven following the blueprint of the Riemannian proof (see [Grigoryan 2009, Theorem 5.11]).

Definition 2.4 (characteristic point). We say that $x \in \partial\Omega$ is a *characteristic point*, or tangency point, if the distribution is tangent to $\partial\Omega$ at x, that is,

$$\mathcal{D}_x \subseteq T_x(\partial\Omega).$$

We will assume that $\partial\Omega$ has no characteristic points. We say in this case that Ω is a *noncharacteristic domain*.

2.3. *Nilpotent approximation of M*. We introduce the notion of nilpotent approximation of a sub-Riemannian manifold; see [Jean 2014; Bellaïche 1996] for details. This will be used only in Sections 3 and 6.

Sub-Riemannian flag. Let M be an n-dimensional sub-Riemannian manifold with distribution $\mathcal{D}$. We define the *flag* of $\mathcal{D}$ as the sequence of subsheaves $\mathcal{D}^k \subset TM$ such that

$$\mathcal{D}^1 = \mathcal{D}, \quad \mathcal{D}^{k+1} = \mathcal{D}^k + [\mathcal{D}, \mathcal{D}^k] \quad \text{for all } k \ge 1,$$

with the convention that $\mathcal{D}^0 = \{0\}$. Under the Hörmander condition, the flag of the distribution defines an exhaustion of $T_x M$ for any point $x \in M$; i.e., there exists $r(x) \in \mathbb{N}$ such that

$$\{0\} = \mathcal{D}_x^0 \subset \mathcal{D}_x^1 \subset \cdots \subset \mathcal{D}_x^{r(x)-1} \subsetneq \mathcal{D}_x^{r(x)} = T_x M. \tag{20}$$

The number $r(x)$ is called *degree of nonholonomy* at x. We set $n_k(x) = \dim \mathcal{D}_x^k$ for any $k \ge 0$. Then the collection of $r(x)$ integers

$$(n_1(x), \ldots, n_{r(x)}(x))$$

is called *growth vector* at x, and we have $n_{r(x)}(x) = n = \dim M$. Associated with the growth vector, we can define the *sub-Riemannian weights* $w_i(x)$ at x, setting for any $i \in \{1, \ldots, n\}$,

$$w_i(x) = j \quad \text{if and only if} \quad n_{j-1}(x) + 1 \le i \le n_j(x). \tag{21}$$

A point $x \in M$ is said to be *regular* if the growth vector is constant in a neighborhood of x, and *singular* otherwise. The sub-Riemannian structure on M is said to be *equiregular* if all points of M are regular. In

this case, the weights are constant as well on M. Finally, given any $x \in M$, we define the *homogeneous dimension* of M at x as

$$\mathcal{Q}(x) = \sum_{i=1}^{r(x)} i\,(n_i(x) - n_{i-1}(x)) = \sum_{i=1}^{n} w_i(x).$$

We recall that, if x is regular, then $\mathcal{Q}(x)$ coincides with the Hausdorff dimension of (M, d_{SR}) at x; see [Mitchell 1985]. Moreover, $\mathcal{Q}(x) > n$ for any $x \in M$ such that $\mathcal{D}_x \subsetneq T_x M$.

Privileged coordinates. Let M be a sub-Riemannian manifold with generating frame (14) and f be the germ of a smooth function f at $x \in M$. We call *nonholonomic derivative* of order $k \in \mathbb{N}$ of f the quantity

$$X_{j_1} \cdots X_{j_k} f(x)$$

for any family of indices $\{j_1, \ldots, j_k\} \subset \{1, \ldots, N\}$. Then, the *nonholonomic order* of f at the point x is

$$\mathrm{ord}_x(f) = \min\{k \in \mathbb{N} : \text{there exists } \{j_1, \ldots, j_k\} \subset \{1, \ldots, N\} \text{ such that } X_{j_1} \cdots X_{j_k} f(x) \neq 0\}.$$

Definition 2.5 (privileged coordinates). Let M be a n-dimensional sub-Riemannian manifold and $x \in M$. A system of local coordinates $(z_1, \ldots, z_n)$ centered at x is said to be *privileged* at x if

$$\mathrm{ord}_x(z_j) = w_j(x) \quad \text{for all } j = 1, \ldots, n.$$

Notice that privileged coordinates $(z_1, \ldots, z_n)$ at x satisfy the following property:

$$\partial_{z_i|x} \in \mathcal{D}_x^{w_i}, \quad \partial_{z_i|x} \notin \mathcal{D}_x^{w_i-1} \quad \text{for all } i = 1, \ldots, n. \tag{22}$$

A local frame of TM consisting of n vector fields $\{Z_1, \ldots, Z_n\}$ and satisfying (22) is said to be *adapted* to the flag (20) at x. Thus, privileged coordinates are always adapted to the flag. In addition, given a local frame adapted to the sub-Riemannian flag at x, say $\{Z_1, \ldots, Z_n\}$, we can define a set of privileged coordinates at x, starting from $\{Z_1, \ldots, Z_n\}$, i.e.,

$$\mathbb{R}^n \ni (z_1, \ldots, z_n) \mapsto e^{z_1 Z_1} \circ \cdots \circ e^{z_n Z_n}(x). \tag{23}$$

Moreover, in these coordinates, the vector field Z_1 is exactly ∂_{z_1}.

Nilpotent approximation. Let M be a sub-Riemannian manifold and let $x \in M$ with weights as in (21). Consider $\psi = (z_1, \ldots, z_n) : U \to V$ a chart of privileged coordinates at x, where $U \subset M$ is a relatively compact neighborhood of x and $V \subset \mathbb{R}^n$ is a neighborhood of 0. Then, for any $\varepsilon \in \mathbb{R}$, we can define the *dilation* at x as

$$\delta_\varepsilon : \mathbb{R}^n \to \mathbb{R}^n, \quad \delta_\varepsilon(z) = (\varepsilon^{w_1(x)} z_1, \ldots, \varepsilon^{w_n(x)} z_n). \tag{24}$$

Using such dilations, we obtain the nilpotent (or first-order) approximation of the generating frame (14); indeed setting $Y_i = \psi_* X_i$ for any $i = 1 \ldots, N$, define

$$\widehat{X}_i^x = \lim_{\varepsilon \to 0} \varepsilon \delta_{(1/\varepsilon)*}(Y_i) \quad \text{for all } i = 1 \ldots, N, \tag{25}$$

where the limit is taken in the C^∞-topology of $\mathbb{R}^n$. Notice that the vector field $\widehat{X}_i^x$ is defined on the whole $\mathbb{R}^n$, even though Y_i was defined only on $V \subset \mathbb{R}^n$.

Theorem 2.6. *Let M be a n-dimensional sub-Riemannian manifold with generating frame $\{X_1, \ldots, X_N\}$ and consider its first-order approximation at x as in* (25). *Then, the frame $\{\widehat{X}_1^x, \ldots, \widehat{X}_N^x\}$ of vector fields on $\mathbb{R}^n$ generates a nilpotent Lie algebra of step $r(x) = w_n(x)$ and satisfies the Hörmander condition.*

The proof of this theorem can be found in [Jean 2014]. Recall that a Lie algebra is said to be nilpotent of step s if s is the smallest integer such that all the brackets of length greater than s are zero.

Definition 2.7 (nilpotent approximation). Let M be a sub-Riemannian manifold and let $x \in M$. Then, Theorem 2.6 implies that the frame $\{\widehat{X}_1^x, \ldots, \widehat{X}_N^x\}$ is a generating frame for a sub-Riemannian structure on $\mathbb{R}^n$: we denote the resulting sub-Riemannian manifold by $\widehat{M}^x$. This is the so-called *nilpotent approximation* of M at the point x.

Notice that the sub-Riemannian distance of $\widehat{M}^x$, denoted by $\hat{d}^x$, is 1-homogeneous with respect to the dilations (24).

Remark 2.8. Up to isometries, the nilpotent approximation of M at x coincides with the Gromov–Hausdorff metric tangent space of (M, d_{SR}) at x. Moreover, $\widehat{M}^x$ is isometric to a quotient of a Carnot group. See [Gromov 1996; Bellaïche 1996; Montgomery 2002] for further details.

Nilpotentized sub-Laplacian. Let M be a sub-Riemannian manifold, equipped with a smooth measure ω, and let $(z_1, \ldots, z_n)$ be a set of privileged coordinates at $x \in M$. We will use the same symbol ω to denote measure in coordinates. The *nilpotentization* $\hat{\omega}^x$ of ω at x is defined as

$$\langle \hat{\omega}^x, f \rangle = \lim_{\varepsilon \to 0} \frac{1}{|\varepsilon|^{\mathcal{Q}(x)}} \langle \delta_\varepsilon^* \omega, f \rangle \quad \text{for all } f \in C_c^\infty(\mathbb{R}^n). \tag{26}$$

Notice that, denoting by $dz = dz_1 \cdots dz_n$ the Lebesgue measure on $\mathbb{R}^n$, we have

$$\delta_\varepsilon^*(dz) = |\varepsilon|^{\mathcal{Q}(x)} dz \quad \text{for all } \varepsilon \neq 0.$$

Thus, the limit in (26) exists. Finally, we can define the *nilpotentized sub-Laplacian* according to (16), acting on $C^\infty(\mathbb{R}^n)$, i.e.,

$$\hat{\Delta}^x = \mathrm{div}_{\hat{\omega}^x}(\hat{\nabla}^x) = \sum_{i=1}^N (\widehat{X}_i^x)^2. \tag{27}$$

We remark that in (27) there is no divergence term, since

$$\mathrm{div}_{\hat{\omega}^x}(\widehat{X}_i^x) = 0 \quad \text{for all } i \in \{1, \ldots, N\}.$$

As in the general sub-Riemannian context, in the nilpotent approximation $\widehat{M}^x$, we may consider the Cauchy heat problem (17) in $L^2(\mathbb{R}^n, \hat{\omega}^x)$. We will the denote the associated heat kernel as

$$\hat{p}_t^x(z, z') \in C^\infty((0, +\infty) \times \mathbb{R}^n \times \mathbb{R}^n).$$

Heat kernel asymptotics. Let M be a sub-Riemannian manifold, equipped with a smooth measure ω and denote by $p_t(x, y)$ the heat kernel (18). We have the following result.

Theorem 2.9 [Colin de Verdière et al. 2021, Theorem A]. *Let M be a sub-Riemannian manifold and let $\psi : U \to V$ be a chart of privileged coordinates at $x \in M$. Then, for any $m \in \mathbb{N}$,*

$$|\varepsilon|^{\mathcal{Q}(x)} p_{\varepsilon^2 \tau}(\delta_\varepsilon(z), \delta_\varepsilon(z')) = \hat{p}_\tau^x(z, z') + \sum_{i=1}^m \varepsilon^i f_i^x(\tau, z, z') + o(|\varepsilon|^m) \quad as \ \varepsilon \to 0, \tag{28}$$

in the C^∞-topology of $(0, \infty) \times V \times V$, where the f_i^x are smooth functions satisfying the following homogeneity property: for $i = 0, \ldots, m$,

$$|\varepsilon|^{\mathcal{Q}(x)} \varepsilon^{-i} f_i^x(\varepsilon^2 \tau, \delta_\varepsilon(z), \delta_\varepsilon(z')) = f_i^x(\tau, z, z') \quad for \ all \ (\tau, z, z') \in (0, \infty) \times \mathbb{R}^n \times \mathbb{R}^n, \tag{29}$$

where, for $i = 0$, we set $f_0^x(\tau, z, z') = \hat{p}_\tau^x(z, z')$. In (28), we are considering the heat kernel p_t in coordinates, with a little abuse of notation.

Remark 2.10. We will drop the dependence on the center of the privileged coordinates if there is no confusion.

3. Small-time asymptotics of $u(t, x)$ at the boundary

We prove here Theorem 1.3, regarding the zero-order asymptotics of $u(t, \cdot)|_{\partial \Omega}$ as $t \to 0$.

Theorem 3.1. *Let M be a compact sub-Riemannian manifold, equipped with a smooth measure ω and let $\Omega \subset M$ be an open subset, whose boundary is smooth and has no characteristic points. Let $x \in \partial \Omega$ and consider a chart of privileged coordinates $\psi : U \to V \subset \mathbb{R}^n$ centered at x such that $\psi(U \cap \Omega) = V \cap \{z_1 > 0\}$. Then,*

$$\lim_{t \to 0} u(t, x) = \int_{\{z_1 > 0\}} \hat{p}_1^x(0, z) \, d\hat{\omega}^x(z) = \frac{1}{2} \quad for \ all \ x \in \partial \Omega,$$

where $\hat{\omega}^x$ denotes the nilpotentization of ω at x and $\hat{p}_t^x$ denotes the heat kernel associated with the nilpotent approximation of M at x and measure $\hat{\omega}^x$.

Remark 3.2. A chart of privileged coordinates such that $\psi(U \cap \Omega) = V \cap \{z_1 > 0\}$ always exists, provided that $\partial \Omega$ has no characteristic points. Indeed, in this case, there exists a tubular neighborhood of the boundary, see Theorem 4.1, which is built through the flow of $\nabla \delta$, namely

$$G : (-r_0, r_0) \times \partial \Omega \to \Omega_{-r_0}^{r_0}, \quad G(t, q) = e^{t \nabla \delta}(q),$$

is a diffeomorphism such that $G_* \partial_t = \nabla \delta$ and $\delta(G(t, q)) = t$. Here $\delta : M \to \mathbb{R}$ is the signed distance function[4] from $\partial \Omega$ and $\Omega_{-r_0}^{r_0} = \{-r_0 < \delta < r_0\}$; see Section 4.1 for precise definitions. Therefore, choosing

---

[4]We warn the reader that δ without a subscript always denotes the signed distance function and should not be confused with dilations δ_ε.

an adapted frame for the distribution at x, say $\{Z_1, \ldots, Z_n\}$, where $Z_1 = \nabla \delta$, we can define a set of privileged coordinates as in (23):

$$\mathbb{R}^n \ni (z_1, \ldots, z_n) \mapsto e^{z_1 Z_1} \circ \underbrace{e^{z_2 Z_2} \circ \cdots \circ e^{z_n Z_n}(x)}_{\varphi(z_2, \ldots, z_n)} = G(z_1, \varphi(z_2, \ldots, z_n)). \tag{30}$$

The resulting set of coordinates ψ satisfies $\psi_*(\nabla \delta) = \partial_{z_1}$ and, denoting by V the neighborhood of 0 in $\mathbb{R}^n$ where ψ is invertible, $\psi(U \cap \Omega) = \{z_1 > 0\} \cap V$. Here, $e^{sX}(q)$ denotes the flow of the vector field X, starting at q, evaluated at time s.

Proof of Theorem 3.1. Let $p_t(x, y)$ be the heat kernel of M. Then we may write

$$u(t, x) = \int_\Omega p_t(x, y)\, d\omega(y) \quad \text{for all } x \in M.$$

For a fixed $x \in M$, denoting by U any relatively compact neighborhood of x, we have

$$\begin{aligned}
u(t, x) &= \int_{U \cap \Omega} p_t(x, y)\, d\omega(y) + \int_{\Omega \setminus U} p_t(x, y)\, d\omega(y) \\
&= \int_{U \cap \Omega} p_t(x, y)\, d\omega(y) + O(t^\infty)
\end{aligned}$$

as $t \to 0$. Indeed, since the heat kernel is exponentially decaying outside the diagonal, see [Jerison and Sánchez-Calle 1986, Proposition 3],

$$\int_{\Omega \setminus U} p_t(x, y)\, d\omega(y) \le \omega(\Omega \setminus U) C_U e^{-c_U/t} = O(t^\infty) \quad \text{as } t \to 0. \tag{31}$$

Now, for $x \in \partial\Omega$, fix the set of privileged coordinates $\psi : U \to V \subset \mathbb{R}^n$, defined as in the statement, and assume without loss of generality that $\delta_\varepsilon(V) \subset V$ for any $|\varepsilon| \le 1$, where δ_ε is the dilation (24) of the nilpotent approximation of M. Also set

$$V_\varepsilon = \delta_\varepsilon(V \cap \{z_1 > 0\}) \quad \text{for all } |\varepsilon| \le 1.$$

When the limits exist, we have

$$\lim_{t \to 0} u(t, x) = \lim_{t \to 0} \int_{U \cap \Omega} p_t(x, y)\, d\omega(y) = \lim_{t \to 0} \int_{V_1} p_t(0, z)\, d\omega(z), \tag{32}$$

where, in the last equation, we are considering the expression of the heat kernel and the measure in coordinates. We want to apply (28) at order 1 in ε, so let us rephrase the statement as follows: for any compact set $K \subset V$,

$$|\varepsilon|^Q p_{\varepsilon^2 \tau}(0, \delta_\varepsilon(z)) = \hat{p}_\tau(0, z) + \varepsilon R(\varepsilon, \tau, z) \quad \text{as } \varepsilon \to 0, \tag{33}$$

where R is a smooth function such that

$$\sup_{\varepsilon \in [-1,1],\ z \in K} |R(\varepsilon, \tau, z)| \le C(\tau, K), \tag{34}$$

with $C(\tau, K) > 0$. Notice that (34) is not uniform in τ, in the sense that $\tau \mapsto C(\tau, K)$ can explode as $\tau \to 0$, in general. Moreover, without loss of generality and, up to restrictions of U, we can assume that

(34) holds globally on $\overline{V}_1$. For a fixed parameter $L > 1$, we set $\tau = 1/L$ and $\varepsilon^2 = tL$ in (33), obtaining

$$|tL|^{\mathcal{Q}/2} p_t(0, \delta_{\sqrt{tL}}(z)) = \hat{p}_{1/L}(0, z) + \sqrt{tL} R(\sqrt{tL}, 1/L, z) \quad \text{as } t \to 0,$$

where the remainder R is bounded as $t \to 0$ on the compact sets of V, but with a constant depending on L. Inserting the above expansion in (32), and writing the measure in coordinates $d\omega(z) = \omega(z) \, dz$, with $\omega(\cdot) \in C^\infty(V_1)$, we have

$$
\begin{aligned}
u(t, x) &= \int_{V_1} p_t(0, z) \omega(z) \, dz + O(t^\infty) \\
&= \int_{V_{\sqrt{tL}}} p_t(0, z) \omega(z) \, dz + \int_{V_1 \setminus V_{\sqrt{tL}}} p_t(0, z) \, d\omega(z) + O(t^\infty) \\
&= \int_{V_1} |tL|^{\mathcal{Q}/2} p_t(0, \delta_{\sqrt{tL}}(z)) \omega(\delta_{\sqrt{tL}}(z)) \, dz + \int_{V_1 \setminus V_{\sqrt{tL}}} p_t(0, z) \, d\omega(z) + O(t^\infty) \\
&= \int_{V_1} \left(\hat{p}_{1/L}(0, z) + \sqrt{tL} R(\sqrt{tL}, 1/L, z) \right) \omega(\delta_{\sqrt{tL}}(z)) \, dz \quad\quad\quad\quad (35) \\
&\qquad\qquad\qquad\qquad\qquad + \int_{V_1 \setminus V_{\sqrt{tL}}} p_t(0, z) \, d\omega(z) + O(t^\infty), \quad\quad (36)
\end{aligned}
$$

where in the third equality we performed the change of variable $z \mapsto \delta_{1/\sqrt{tL}}(z)$ in the first integral. Let us discuss the terms appearing in (35) and (36). First of all, for any $L > 1$, by definition of the nilpotentization of ω given in (26), we get

$$\lim_{t \to 0} \int_{V_1} \hat{p}_{1/L}(0, z) \omega(\delta_{\sqrt{tL}}(z)) \, dz = \int_{V_1} \hat{p}_{1/L}(0, z) \, d\hat{\omega}(z).$$

Moreover, for a fixed $L > 1$, the integral of R is bounded as $t \to 0$; Therefore, using (34), we have

$$\left| \sqrt{tL} \int_{V_1} R(\sqrt{tL}, 1/L, z) \, d\omega(z) \right| \le C_L \sqrt{t} \quad \text{for all } t \le 1,$$

where $C_L > 0$ is a constant depending on the fixed L. Secondly, by an upper Gaussian bound for the heat kernel in compact sub-Riemannian manifold [Jerison and Sánchez-Calle 1986, Theorem 2], we obtain the following estimate for (36):

$$\int_{V_1 \setminus V_{\sqrt{tL}}} p_t(0, z) \, d\omega(z) \le \int_{V_1 \setminus V_{\sqrt{tL}}} \frac{C_1 e^{-\beta \, d_{\mathrm{SR}}^2(0, z)/t}}{t^{\mathcal{Q}/2}} \, d\omega(z), \quad\quad (37)$$

where $C_1, \beta > 0$ are positive constants. Now, by the ball-box theorem [Jean 2014, Theorem 2.1], the sub-Riemannian distance function at the origin is comparable with the sub-Riemannian distance of $\widehat{M}^x$, denoted by $\hat{d}$. In particular, there exists a constant $c > 0$ such that

$$d_{\mathrm{SR}}^2(0, z) \ge c \, \hat{d}^2(0, z) \quad \text{for all } z \in V. \quad\quad (38)$$

Since in (37) we are integrating over the set $V_1 \setminus V_{\sqrt{tL}}$ and $\hat{d}$ is 1-homogeneous with respect to δ_ε, we conclude that

$$d_{\mathrm{SR}}^2(0, z) \ge c \, tL \quad \text{for all } z \in V_1 \setminus V_{\sqrt{tL}}.$$

Therefore, using also (38), the term (37) can be estimated as follows:

$$
\int_{V_1 \setminus V_{\sqrt{tL}}} p_t(0, z) \, d\omega(z) \leq C_1 e^{-c\beta L/2} \int_{V_1} \frac{e^{-\beta d_{\mathrm{SR}}^2(0,z)/(2t)}}{t^{Q/2}} \, d\omega(z)
$$
$$
\leq C_1 e^{-c\beta L/2} \int_{V_1} \frac{e^{-\beta c \, \hat{d}^2(0,z)/(2t)}}{t^{Q/2}} \omega(z) \, dz \leq \widetilde{C} e^{-c\beta L/2},
\tag{39}
$$

where $\widetilde{C} > 0$ is independent of t and L. The last inequality in (39) follows from the fact that, after a change of variable $z \mapsto \delta_{1/\sqrt{t}}(z)$, the integral

$$
\int_{V_1} \frac{e^{-\beta c \hat{d}^2(0,z)/(2t)}}{t^{Q/2}} \omega(z) \, dz < +\infty
$$

is uniformly bounded with respect to $t \in [0, \infty)$.

Therefore, for any $L > 1$, we obtain the following estimates for the limit of u:

$$
\limsup_{t \to 0} u(t, x) \leq \int_{V_1} \hat{p}_{1/L}(0, z) \, d\hat{\omega}(z) + \widetilde{C} e^{-c\beta L/2},
$$
$$
\liminf_{t \to 0} u(t, x) \geq \int_{V_1} \hat{p}_{1/L}(0, z) \, d\hat{\omega}(z) - \widetilde{C} e^{-c\beta L/2}.
\tag{40}
$$

In order to evaluate the limits in (40), let us firstly notice that, since $\hat{p}$ enjoys upper and lower Gaussian bounds (see for example [Colin de Verdière et al. 2021, Appendix C]), reasoning as we did for (39), we can prove

$$
\int_{V_1} \hat{p}_{1/L}(0, z) \, d\hat{\omega}(z) = \int_{\{z_1 > 0\}} \hat{p}_{1/L}(0, z) \, d\hat{\omega}(z) + O(e^{-\beta' L}).
\tag{41}
$$

Secondly, thanks to (29) for $\hat{p}$, we have the parity property

$$
\hat{p}_t(0, z) = \hat{p}_t(0, \delta_{-1}(z)) \quad \text{for all } t > 0, \ z \in \mathbb{R}^n,
$$

and, by the choice of privileged coordinates, $\delta_{-1}(\{z_1 > 0\}) = \{z_1 < 0\}$. Thus, using also the stochastic completeness of the nilpotent approximation, we obtain, for any $t \geq 0$,

$$
1 = \int_{\mathbb{R}^n} \hat{p}_t(0, z) \, d\hat{\omega}(z) = \int_{\{z_1 > 0\}} \hat{p}_t(0, z) \, d\hat{\omega}(z) + \int_{\{z_1 < 0\}} \hat{p}_t(0, z) \, d\hat{\omega}(z) = 2 \int_{\{z_1 > 0\}} \hat{p}_t(0, z) \, d\hat{\omega}(z),
$$

having performed the change of variables $z \mapsto \delta_{-1}(z)$ in the last equality. Hence, the integral in (41) is

$$
\int_{V_1} \hat{p}_{1/L}(0, z) \, d\hat{\omega}(z) = \frac{1}{2} + O(e^{-\beta' L}).
$$

Finally, we optimize the inequalities (40) with respect to L, taking $L \to \infty$ and concluding the proof. $\square$

Remark 3.3. In the noncompact case, if M is globally doubling and supports a global Poincaré inequality, the proof above is still valid; see Theorem 7.3. Otherwise, a different proof is needed; see [Rossi 2021, Appendix D] for details.

4. First-order asymptotic expansion of $H_\Omega(t)$

In this section, we introduce the technical tools that allow us to prove the first-order asymptotic expansion of the relative heat content starting from Theorem 3.1. The new ingredient is a definition of an operator I_Ω, which depends on the base set Ω.

4.1. *A mean value lemma.* Define $\delta : M \to \mathbb{R}$ to be the signed distance function from $\partial\Omega$, i.e.,

$$\delta(x) = \begin{cases} d_{\mathrm{SR}}(x, \partial\Omega), & x \in \Omega, \\ -d_{\mathrm{SR}}(x, \partial\Omega), & x \in M \setminus \Omega, \end{cases}$$

where $d_{\mathrm{SR}}(\cdot, \partial\Omega) : M \to [0, +\infty)$ denotes the usual distance function from $\partial\Omega$. Let us introduce the following notation: for any $a, b \in \mathbb{R}$, with $a < b$, we set

$$\Omega_a^b = \{x \in M : a < \delta(x) < b\},$$

with the understanding that if b (or a) is omitted, it is assumed to be $+\infty$ (or $-\infty$), for example[5]

$$\Omega_r = \Omega_r^{+\infty} = \{x \in M : r < \delta(x)\}.$$

In the noncharacteristic case, [Franceschi et al. 2020, Proposition 3.1] can be extended without difficulties to the signed distance function.

Theorem 4.1 (double-sided tubular neighborhood). *Let M be a sub-Riemannian manifold and let $\Omega \subset M$ be an open relatively compact subset of M whose boundary is smooth and has no characteristic points. Let $\delta : M \to \mathbb{R}$ be the signed distance function from $\partial\Omega$. Then, we have*:

(i) *δ is Lipschitz with respect to the sub-Riemannian distance and $\|\nabla\delta\|_g \le 1$ a.e.*

(ii) *There exists $r_0 > 0$ such that $\delta : \Omega_{-r_0}^{r_0} \to \mathbb{R}$ is smooth.*

(iii) *There exists a smooth diffeomorphism $G : (-r_0, r_0) \times \partial\Omega \to \Omega_{-r_0}^{r_0}$ such that*

$$\delta(G(t, y)) = t \quad and \quad G_*\partial_t = \nabla\delta \quad for\ all\ (t, y) \in (-r_0, r_0) \times \partial\Omega.$$

Moreover, $\|\nabla\delta\|_g \equiv 1$ on $\Omega_{-r_0}^{r_0}$.

In particular, the following coarea formula for the signed distance function holds:

$$\int_{\Omega_0^r} v(x)\, d\omega(x) = \int_0^r \int_{\partial\Omega_s} v(s, y)\, d\sigma(y)\, ds \quad \text{for all } r \ge 0, \tag{42}$$

where σ is the induced measure on $\partial\Omega_s$, namely the positive measure with density $|i_{\nabla\delta}\omega|_{|\partial\Omega_s}$. From (42), we deduce the sub-Riemannian mean value lemma; see [Rizzi and Rossi 2021, Theorem 4.1] for a proof.

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[5]Notice that the set $\Omega_{-\infty}^{+\infty}$ is equal to M; thus omitting both indices can create confusion. We will never do that and Ω will always denote the starting subset of M.

Proposition 4.2. *Let M be a compact sub-Riemannian manifold, equipped with a smooth measure ω, let $\Omega \subset M$ be an open subset of M with smooth boundary and no characteristic points and let $\delta : M \to \mathbb{R}$ be the signed distance function from $\partial\Omega$. Fix a smooth function $v \in C^\infty(M)$ and define*

$$F(r) = \int_{\Omega_r} v(x) d\omega(x) \quad \text{for all } r \geq 0. \tag{43}$$

Then there exists $r_0 > 0$ such that the function F is smooth on $[0, r_0)$ and, for $0 \leq r < r_0$,

$$F''(r) = \int_{\Omega_r} \Delta v(x) \, d\omega(x) - \int_{\partial\Omega_r} v(y) \operatorname{div}_\omega(\nu(y)) \, d\sigma(y),$$

where ν is the inward-pointing unit normal to Ω_r, and σ is the induced measure on $\partial\Omega_r$.

Remark 4.3. If $v \in C_c^\infty(M)$, then neither M nor Ω is required to be compact for [Proposition 4.2](#) to be true; indeed its proof relies on [(42)](#), which continues to hold, and the divergence theorem [(15)](#), which applies if $\operatorname{supp}(v)$ is compact. Moreover, we remark that ν_r is equal to $\nabla\delta$ up to sign. We prefer to keep ν_r in [(43)](#), since we are going to apply it when the integral is performed over Ω_r or its complement.

If we choose the function v in the definition of F to be $1 - u(t, x)$, where $u(t, \cdot) = e^{t\Delta}\mathbb{1}_\Omega$, then F satisfies a nonhomogeneous one-dimensional heat equation.

Corollary 4.4. *Under the hypotheses of [Proposition 4.2](#), the function*

$$F(t, r) = \int_{\Omega_r} (1 - u(t, x)) \, d\omega(x) \quad \text{for all } t > 0, \ r \geq 0, \tag{44}$$

where $u(t, x) = e^{t\Delta}\mathbb{1}_\Omega(x)$, satisfies the following nonhomogeneous one-dimensional heat equation:

$$(\partial_t - \partial_r^2)F(t, r) = \int_{\partial\Omega_r} (1 - u(t, \cdot)) \operatorname{div}_\omega(\nu) \, d\sigma, \quad t > 0, \ r \in [0, r_0). \tag{45}$$

Here ν is the inward-pointing unit normal to Ω_r, and σ is the induced measure on $\partial\Omega_r$.

[Corollary 4.4](#) holds only for $r \leq r_0$; however, we would like to extend it to the *whole* positive half-line, in order to apply a Duhamel's principle. This can be done up to an error which is exponentially small.

4.2. *Localization principle.*

Proposition 4.5. *Let M be a compact sub-Riemannian manifold, equipped with a smooth measure ω, and let $\Omega \subset M$ be an open subset of M, with smooth boundary. Moreover, let $K \subset M$ be a closed set such that $K \cap \partial\Omega = \varnothing$. Then*

$$\mathbb{1}_\Omega(x) - u(t, x) = O(t^\infty) \quad \text{uniformly for } x \in K,$$

where $u(t, x) = e^{t\Delta}\mathbb{1}_\Omega(x)$.

Proof. The statement is a direct consequence of the off-diagonal estimate for the heat kernel in compact sub-Riemannian manifold (see [Jerison and Sánchez-Calle 1986, Proposition 3]):

$$p_t(x, y) \leq C_a e^{-c_a/t} \quad \text{for all } x, y \text{ with } d(x, y) \geq a, \ t < 1, \tag{46}$$

for suitable constants $C_a, c_a > 0$, depending only on a. Now, since $K \cap \partial\Omega = \varnothing$, we can write K as a disjoint union

$$K = K_1 \sqcup K_2, \quad \text{with } K_1 \subset \Omega, \ K_2 \subset M \setminus \Omega.$$

At this point, for $i = 1, 2$, set $a_i = d_{SR}(K_i, \partial\Omega) > 0$ by hypothesis, and let $x \in K_1$. Then, using the stochastic completeness of M, we have

$$|\mathbb{1}_\Omega(x) - u(t, x)| = 1 - u(t, x) = \int_{M \setminus \Omega} p_t(x, y) \, d\omega(y) \le C_1 e^{-c_1/t} \omega(M \setminus \Omega), \tag{47}$$

which is exponentially decaying, uniformly in K_1. Analogously, if $x \in K_2$, we have

$$|\mathbb{1}_\Omega(x) - u(t, x)| = u(t, x) = \int_M p_t(x, y) \mathbb{1}_\Omega(y) \, d\omega(y) = \int_\Omega p_t(x, y) \, d\omega(y) \le C_2 e^{-c_2/t} \omega(\Omega),$$

uniformly in K_2. $\square$

Remark 4.6. In the noncompact case, Proposition 4.5 may fail. Indeed, on the one hand the off-diagonal estimate (46) is not always available; on the other hand the measure of $M \setminus \Omega$ appearing in (47) is infinite. Under additional assumption on M, we are able to recover a localization principle; see Section 7.

Let M be compact. Thanks to Proposition 4.5, we can extend the function F defined in (44) to a solution to a nonhomogeneous heat equation such as (45) on the whole half-line. More precisely, let $\phi, \eta \in C_c^\infty(M)$ such that

$$\phi + \eta \equiv 1, \quad \text{supp}(\phi) \subset \Omega_{-r_0}^{r_0}, \quad \text{supp}(\eta) \subset \Omega^{-r_0/2} \cup \Omega_{r_0/2}, \tag{48}$$

where r_0 is defined in Proposition 4.2. We have then, for $r \in [0, r_0)$,

$$\begin{aligned}
F(t, r) &= \int_{\Omega_r} (1 - u(t, x))\phi(x) \, d\omega(x) + \int_{\Omega_r} (1 - u(t, x))\eta(x) \, d\omega(x) \\
&= \int_{\Omega_r} (1 - u(t, x))\phi(x) \, d\omega(x) + \int_{\text{supp}(\eta) \cap \Omega_r} (1 - u(t, x))\eta(x) \, d\omega(x) \\
&= \int_{\Omega_r} (1 - u(t, x))\phi(x) \, d\omega(x) + O(t^\infty), \tag{49}
\end{aligned}$$

where we used Proposition 4.5 to deal with the second term, having set $K = \text{supp}(\eta) \cap \Omega_r$. For this reason, we may focus on the first term in (49).

Definition 4.7. For all $t > 0$ and $r \ge 0$, we define the operators $I_\Omega, \Lambda_\Omega : C_c^\infty(\Omega_{-r_0}^{r_0}) \to C^\infty((0, \infty) \times [0, \infty))$, associated with Ω, by

$$I_\Omega \phi(t, r) = \int_{\Omega_r} (1 - u(t, x))\phi(x) \, d\omega(x),$$

$$\Lambda_\Omega \phi(t, r) = -\partial_r I_\Omega \phi(t, r) = -\int_{\partial\Omega_r} (1 - u(t, y))\phi(y) \, d\sigma(y)$$

for any $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$, and where σ denotes the induced measure on $\partial\Omega_r$ and $u(t, \cdot) = e^{t\Delta}\mathbb{1}_\Omega(\cdot)$.

Remark 4.8. We stress that, for every $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$, $I_\Omega \phi$, $\Lambda_\Omega \phi$ are indeed smooth in both variables thanks to the choice of the parameter $r_0 > 0$ as in Proposition 4.2, together with the smoothness of the solution to the heat equation. Moreover, $\Lambda_\Omega \phi$ is compactly supported in the r-variable.

Thanks to the localization principle, we can improve Corollary 4.4, obtaining a better result for $I_\Omega \phi(t, r)$.

Lemma 4.9. *Let $L = \partial_t - \partial_r^2$ be the one-dimensional heat operator. Then, for any $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$,*

$$L(I_\Omega \phi(t, r)) = I_\Omega \Delta \phi(t, r) + \Lambda_\Omega N_\Omega \phi(t, r) \quad \text{for all } t > 0, \ r \geq 0,$$

where N_Ω is the operator defined by

$$N_\Omega \phi = 2g(\nabla \phi, \nu) + \phi \ \mathrm{div}_\omega(\nu) \quad \text{for all } \phi \in C_c^\infty(\Omega_{-r_0}^{r_0}), \tag{50}$$

and ν is the inward-pointing unit normal to Ω.

4.3. *Duhamel's principle for $I_\Omega \phi$.* We recall for the convenience of the reader a one-dimensional version of the Duhamel's principle; see [Rizzi and Rossi 2021, Lemma 5.4].

Lemma 4.10 (Duhamel's principle). *Let $f \in C((0, \infty) \times [0, \infty))$, $v_0, v_1 \in C([0, \infty))$, such that $f(t, \cdot)$ and v_0 are compactly supported and assume that*

$$\text{there exists } \lim_{t \to 0} f(t, r) \quad \text{for all } r \geq 0.$$

Consider the nonhomogeneous heat equation on the half-line:

$$\begin{aligned}
Lv(t, r) &= f(t, r) \quad \text{for } t > 0, \ r > 0, \\
v(0, r) &= v_0(r) \quad \text{for } r > 0, \\
\partial_r v(t, 0) &= v_1(t) \quad \text{for } t > 0,
\end{aligned} \tag{51}$$

where $L = \partial_t - \partial_r^2$. Then, for $t > 0$ and $r \geq 0$, the solution to (51) is given by

$$v(t, r) = \int_0^\infty e(t, r, s) v_0(s) \, ds + \int_0^t \int_0^\infty e(t - \tau, r, s) f(\tau, s) \, ds \, d\tau - \int_0^t e(t - \tau, r, 0) v_1(\tau) \, d\tau, \tag{52}$$

where $e(t, r, s)$ is the Neumann heat kernel on the half-line, that is,

$$e(t, r, s) = \frac{1}{\sqrt{4\pi t}} (e^{-(r-s)^2/(4t)} + e^{-(r+s)^2/(4t)}). \tag{53}$$

Finally, we apply Lemma 4.10 to obtain an asymptotic equality for $I_\Omega \phi$. The main difference with the result of [Rizzi and Rossi 2021, Theorem 5.6] is that the former will not be a true first-order asymptotic expansion.

Corollary 4.11. *Let M be a compact sub-Riemannian manifold, equipped with a smooth measure ω, and let $\Omega \subset M$ be an open subset whose boundary is smooth and has no characteristic points. Then, for any*

function $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$,

$$I_\Omega \phi(t, 0) = \frac{1}{\sqrt{\pi}} \int_0^t \int_{\partial \Omega} (1 - u(\tau, y)) \phi(y) \, d\sigma(y) (t - \tau)^{-1/2} \, d\tau + O(t)$$

as $t \to 0$, *where* $u(t, \cdot) = e^{t\Delta} \mathbb{1}_\Omega(\cdot)$.

Proof. By Lemma 4.9, the function $I_\Omega \phi(t, r)$ satisfies the following Neumann problem on the half-line:

$$LI_\Omega \phi(t, r) = f(t, r) \qquad \text{for } t > 0, \ r > 0,$$
$$I_\Omega \phi(0, r) = 0 \qquad \text{for } r > 0,$$
$$\partial_r I_\Omega \phi(t, 0) = -\Lambda_\Omega \phi(t, 0) \quad \text{for } t > 0,$$

where the source is given by $f(t, r) = I_\Omega \Delta \phi(t, r) + \Lambda_\Omega N_\Omega \phi(t, r)$. Thus, applying Duhamel's formula (52), we have

$$I_\Omega \phi(t, 0) = \int_0^t \int_0^{+\infty} e(t - \tau, 0, s) f(\tau, s) \, ds \, d\tau + \frac{1}{\sqrt{\pi}} \int_0^t \frac{1}{\sqrt{t - \tau}} \Lambda_\Omega \phi(t, 0) \, d\tau.$$

Since the source is uniformly bounded by the weak maximum principle (19), the first integral is a remainder of order t as $t \to 0$, concluding the proof. $\qquad \square$

Remark 4.12. We mention that a relevant role in the sequel will be played by the operators I_Ω, see Definition 4.7, associated with either Ω or its complement Ω^c.

4.4. *First-order asymptotics.* In this section we prove the first-order asymptotic expansion of $H_\Omega(t)$; see Theorem 1.1 at order 1. We will use Corollary 4.11 for the *inside contribution*:

$$I\phi(t, r) = \int_{\Omega_r} (1 - u(t, x)) \phi(x) \, d\omega(x) \quad \text{for all } t > 0, \ r \geq 0, \tag{54}$$

for any $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$, and where σ denotes the induced measure on $\partial \Omega_r$ and $u(t, \cdot) = e^{t\Delta} \mathbb{1}_\Omega(\cdot)$ is the solution to (17). The quantity (54) is just Definition 4.7, applied with base set $\Omega \subset M$.

Theorem 4.13. *Let M be a compact sub-Riemannian manifold, equipped with a smooth measure ω, and let $\Omega \subset M$ be an open subset whose boundary is smooth and has no characteristic points. Then,*

$$H_\Omega(t) = \omega(\Omega) - \frac{1}{\sqrt{\pi}} \sigma(\partial \Omega) t^{1/2} + o(t^{1/2}) \quad \text{as } t \to 0.$$

Proof. Let $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$ be as in (48); namely

$$0 \leq \phi \leq 1 \qquad \text{and} \qquad \phi \equiv 1 \quad \text{in } \Omega_{-r_0/2}^{r_0/2}.$$

Then, by the localization principle, see (49), we have that

$$\omega(\Omega) - H_\Omega(t) = I\phi(t, 0) + O(t^\infty) \quad \text{as } t \to 0. \tag{55}$$

Applying Corollary 4.11, we have

$$I\phi(t, 0) = \frac{1}{\sqrt{\pi}} \int_0^t \int_{\partial \Omega} (1 - u(\tau, y)) \phi(y) \, d\sigma(y) (t - \tau)^{-1/2} \, d\tau + O(t) \quad \text{as } t \to 0. \tag{56}$$

Thus, to infer the first-order term of the asymptotic expansion we have to compute the following limit:

$$\lim_{t \to 0} \frac{I\phi(t, 0)}{t^{1/2}} = \lim_{t \to 0} \frac{1}{t^{1/2}\sqrt{\pi}} \int_0^t \int_{\partial\Omega} (1 - u(\tau, y))\phi(y)\, d\sigma(y)(t - \tau)^{-1/2}\, d\tau. \tag{57}$$

Firstly, by the change of variable in the integral $\tau \mapsto t\tau$, we rewrite the argument of the limit (57) as

$$\frac{1}{\sqrt{\pi}} \int_0^1 \int_{\partial\Omega} (1 - u(t\tau, y))\phi(y)\, d\sigma(y)(1 - \tau)^{-1/2}\, d\tau.$$

Secondly, we apply the dominated convergence theorem. Indeed, on the one hand, by Theorem 3.1 we have pointwise convergence

$$(1 - u(t\tau, y))\phi(y) \xrightarrow{t \to 0} \tfrac{1}{2}\phi(y) \quad \text{for all } y \in \partial\Omega,\ \tau \in (0, 1),$$

and on the other hand, by the maximum principle

$$\left| \int_{\partial\Omega} (1 - u(t\tau, y))\phi(y)\, d\sigma(y)(1 - \tau)^{-1/2} \right| \le \int_{\partial\Omega} |\phi|\, d\sigma (1 - \tau)^{-1/2} \in L^1(0, 1)$$

for any $t > 0$. Therefore, we finally obtain that

$$I\phi(t, 0) = \sqrt{\frac{t}{\pi}} \int_{\partial\Omega} \phi(y)\, d\sigma(y) + o(t^{1/2}) \quad \text{as } t \to 0.$$

Recalling that $\phi_{|\partial\Omega} \equiv 1$, we conclude the proof. $\qquad\square$

Remark 4.14. The above technique used to evaluate the first-order coefficient causes a loss of precision in the remainder, with respect to the expression (56), where the remainder is $O(t)$. This loss comes from the application of Theorem 3.1, which does not contain any remainder estimate.

5. Higher-order asymptotic expansion of $H_\Omega(t)$

We iterate Duhamel's formula (52) for the inside contribution to study the higher-order asymptotics of $H_\Omega(t)$. We obtain the following expression for $I\phi$ at order 3:

$$I\phi(t, 0) = \frac{1}{\sqrt{\pi}} \int_0^t \int_{\partial\Omega} (1 - u(\tau, \cdot))\phi\, d\sigma (t - \tau)^{-1/2}\, d\tau$$
$$+ \frac{1}{2\pi} \int_0^t \int_0^\tau \int_{\partial\Omega} (1 - u(\hat\tau, \cdot))N\phi\, d\sigma ((\tau - \hat\tau)(t - \tau))^{-1/2}\, d\hat\tau\, d\tau + O(t^{3/2}), \tag{58}$$

where $u(t, \cdot) = e^{t\Delta}\mathbb{1}_\Omega(\cdot)$ denotes the solution to (17) and N is the operator defined by

$$N\phi = 2g(\nabla\phi, \nabla\delta) + \phi\Delta\delta \quad \text{for all } \phi \in C_c^\infty(\Omega_{-r_0}^{r_0}), \tag{59}$$

with $\delta : M \to \mathbb{R}$ the signed distance function from $\partial\Omega$. The computations for deriving (58) are technical. We refer to the Appendix for further details, and in particular to Lemma A.6. Motivated by (58), we introduce the following functional.

Definition 5.1. Let M be a sub-Riemannian manifold, equipped with a smooth measure ω, let $\Omega \subset M$ be a relatively compact subset with smooth boundary and let $v \in C^\infty((0, +\infty) \times M)$. Define the functional $\mathcal{G}_v$, for any $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$ as

$$\mathcal{G}_v[\phi](t) = \frac{1}{2\sqrt{\pi}} \int_0^t \int_{\partial\Omega} v(\tau, \cdot)\phi \, d\sigma (t - \tau)^{-1/2} \, d\tau \quad \text{for all } t \geq 0, \tag{60}$$

where σ is the sub-Riemannian induced measure on $\partial\Omega$.

Notice that the functional $\mathcal{G}_v$ is linear with respect to the subscript function v, by linearity of the integral. Moreover, when the function v is chosen to be the solution to (17), we easily obtain the following corollary of Theorem 3.1, which is just a rewording of (57).

Corollary 5.2. *Let M be a compact sub-Riemannian manifold, equipped with a smooth measure ω, and let $\Omega \subset M$ be an open subset whose boundary is smooth and has no characteristic points. Let $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$. Then,*

$$\mathcal{G}_u[\phi](t) = \frac{1}{2\sqrt{\pi}} \int_{\partial\Omega} \phi(y) \, d\sigma(y) t^{1/2} + o(t^{1/2}) \quad \text{as } t \to 0.$$

Then, we can rewrite (58) in a compact notation:

$$I\phi(t, 0) = 2\mathcal{G}_{1-u}[\phi](t) + \frac{1}{\sqrt{\pi}} \int_0^t \mathcal{G}_{1-u}[N\phi](t) \, d\sigma (t - \tau)^{-1/2} \, d\tau + O(t^{3/2}). \tag{61}$$

However, on the one hand, the application of Corollary 5.2 to (58) does not give any new information on the asymptotics of $H_\Omega(t)$, as the first term produces an error of $o(t^{1/2})$. On the other hand, it is clear that an asymptotic series of $\mathcal{G}_u$ is enough to deduce the small-time expansion of $H_\Omega(t)$.

5.1. *The outside contribution and an asymptotic series for $\mathcal{G}_u[\phi]$.* In this section, we deduce an asymptotic series, at order 3, of $\mathcal{G}_u[\phi](t)$ as $t \to 0$. This is done by exploiting the fact that the diffusion of heat is not confined in Ω, and as a result we can define an *outside contribution*, namely the quantity obtained from Definition 4.7, applied with base set $\Omega^c \subset M$:

$$I^c\phi(t, r) = \int_{(\Omega^c)_r} (1 - u^c(t, x))\phi(x) \, d\omega(x) \quad \text{for all } t > 0, \ r \geq 0, \tag{62}$$

for any $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$, and where σ denotes the induced measure on the boundary of $(\Omega^c)_r$ and $u^c(t, x) = e^{t\Delta}\mathbb{1}_{\Omega^c}(x)$. We remark that, since Ω and its complement share the boundary, then $(\Omega^c)_{-r_0}^{r_0} = \Omega_{-r_0}^{r_0}$. It is convenient to introduce (62), because it turns out that the quantity $I\phi - I^c\phi$, where $I\phi$ is the inside contribution (54), has an explicit asymptotic series in integer powers of t.

Proposition 5.3. *Let M be a compact sub-Riemannian manifold, equipped with a smooth measure ω, and let $\Omega \subset M$ be an open subset with smooth boundary. Let $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$. Then, for any $k \in \mathbb{N}$,*

$$I\phi(t, 0) - I^c\phi(t, 0) = \sum_{i=1}^k a_i(\phi)t^i + O(t^{k+1}) \quad \text{as } t \to 0, \tag{63}$$

where

$$a_i(\phi) = \int_{\partial\Omega} g(\nabla(\Delta^{i-1}\phi), \nabla\delta) \, d\sigma \quad \text{for } i \geq 1.$$

Proof. Recall that in the definition of the outside contribution (62), the integrand function involves $u^c(t, x) = e^{t\Delta}\mathbb{1}_{\Omega^c}(x)$. Since M is compact, and hence stochastically complete, we have

$$1 - u^c(t, x) = e^{t\Delta}1(x) - e^{t\Delta}\mathbb{1}_{\Omega^c}(x) = u(t, x) \quad \text{for all } t > 0, \ x \in M,$$

having used the pointwise equality $1 - \mathbb{1}_{\Omega^c} = \mathbb{1}_\Omega$ in $M \setminus \partial\Omega$. Therefore, we can write the difference $I\phi(t, 0) - I^c\phi(t, 0)$ as follows:

$$\begin{aligned}
I\phi(t, 0) - I^c\phi(t, 0) &= \int_\Omega (1 - u(t, \cdot))\phi \, d\omega - \int_{\Omega^c} (1 - u^c(t, \cdot))\phi \, d\omega \\
&= \int_\Omega (1 - u(t, \cdot))\phi \, d\omega - \int_{\Omega^c} u(t, \cdot)\phi \, d\omega \\
&= \int_\Omega \phi(x) \, d\omega(x) - \int_M u(t, x)\phi(x) \, d\omega(x).
\end{aligned} \tag{64}$$

Since $u(t, x)$ is the solution to (17), the function (64) is smooth as $t \in [0, \infty)$. Indeed, the smoothness in the open interval is guaranteed by hypoellipticity of the sub-Laplacian. At $t = 0$, the divergence theorem, together with the fact that ϕ has compact support in M, implies that

$$\begin{aligned}
\partial_t^i \left(\int_M u(t, x)\phi(x) \, d\omega(x) \right) &= \int_M \partial_t^i(u(t, x)\phi(x)) \, d\omega(x) = \int_M \Delta^i u(t, x)\phi(x) \, d\omega(x) \\
&= \int_M u(t, x)\Delta^i\phi(x) \, d\omega(x) \xrightarrow{t \to 0} \int_\Omega \Delta^i\phi(x) \, d\omega(x).
\end{aligned}$$

The previous limit shows that (64) is smooth at $t = 0$, and also that its asymptotic expansion at order k, as $t \to 0$, coincides with its k-th Taylor polynomial at $t = 0$. Finally, we recover (63), applying once again the divergence theorem:

$$\int_\Omega \Delta^i\phi \, d\omega = -\int_{\partial\Omega} g(\nabla(\Delta^{i-1}\phi), \nu) \, d\sigma = -\int_{\partial\Omega} g(\nabla(\Delta^{i-1}\phi), \nabla\delta) \, d\sigma,$$

recalling that $\nu = \nabla\delta$ is the inward-pointing normal vector to Ω at its boundary. $\qquad\square$

Applying the (iterated) Duhamel's principle (52) to the difference $I\phi - I^c\phi$, we are able to obtain relevant information on the functional $\mathcal{G}_u$.

Theorem 5.4. *Let M be a compact sub-Riemannian manifold, equipped with a smooth measure ω, and let $\Omega \subset M$ be an open subset whose boundary is smooth and has no characteristic points. Then, for any $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$,*

$$\mathcal{G}_u[\phi](t) = \frac{1}{2\sqrt{\pi}} \int_{\partial\Omega} \phi \, d\sigma \, t^{1/2} + \frac{1}{8} \int_{\partial\Omega} \phi\Delta\delta \, d\sigma \, t + o(t^{3/2}) \quad \text{as } t \to 0. \tag{65}$$

Proof. Let us study the difference of the inside and outside contributions $I\phi(t, 0) - I^c\phi(t, 0)$. On the one hand, we have an iterated Duhamel's principle, see Lemma A.7, which we report here:

$$(I\phi - I^c\phi)(t, 0) = 2\mathcal{G}_{1-2u}[\phi](t) + \frac{1}{2} \int_{\partial\Omega} N\phi \, d\sigma \, t + \frac{1}{2\pi} \int_0^t \int_0^\tau \mathcal{G}_{1-2u}[N^2\phi](\hat{\tau})((\tau - \hat{\tau})(t - \tau))^{-1/2} \, d\hat{\tau} \, d\tau$$

$$+ \frac{1}{4\sqrt{\pi}} \int_0^t \int_{\partial\Omega} (1 - 2u(\tau, \cdot))(4\Delta - N^2)\phi \, d\sigma \, (t - \tau)^{1/2} \, d\tau + O(t^2), \tag{66}$$

where we recall that N is the operator acting on smooth functions compactly supported close to $\partial\Omega$ defined by

$$N\phi = 2g(\nabla\phi, \nabla\delta) + \phi\Delta\delta \quad \text{for all } \phi \in C_c^\infty(\Omega_{-r_0}^{r_0}).$$

Using Corollary 5.2 and the linearity of $\mathcal{G}_v$ with respect to v, we know that

$$\mathcal{G}_{1-2u}[\phi](t) = o(t^{1/2}) \quad \text{as } t \to 0, \text{ for all } \phi \in C_c^\infty(\Omega_{-r_0}^{r_0}). \tag{67}$$

Therefore, applying (67) to the function $N^2\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$, we obtain

$$\frac{1}{2\pi} \int_0^t \int_0^\tau \mathcal{G}_{1-2u}[N^2\phi](\hat{\tau})((\tau - \hat{\tau})(t - \tau))^{-1/2} \, d\hat{\tau} \, d\tau = o(t^{3/2}) \quad \text{as } t \to 0. \tag{68}$$

In addition, an application of Theorem 3.1 and the dominated convergence theorem implies that

$$\int_0^t \int_{\partial\Omega} (1 - 2u(\tau, \cdot))(4\Delta - N^2)\phi \, d\sigma (t - \tau)^{1/2} \, d\tau = o(t^{3/2}) \quad \text{as } t \to 0. \tag{69}$$

Thus, using (68) and (69), we can improve (66), obtaining

$$I\phi(t, 0) - I^c\phi(t, 0) = 2\mathcal{G}_{1-2u}[\phi](t) + \frac{1}{2} \int_{\partial\Omega} N\phi \, d\sigma \, t + o(t^{3/2}). \tag{70}$$

On the other hand, the quantity $I\phi(t, 0) - I^c\phi(t, 0)$ has a complete asymptotic series by Proposition 5.3, which at order 3 becomes

$$I\phi(t, 0) - I^c\phi(t, 0) = \int_{\partial\Omega} g(\nabla\phi, \nabla\delta) \, d\sigma \, t + o(t^{3/2}) \quad \text{as } t \to 0. \tag{71}$$

Comparing (70) and (71), we deduce that, as $t \to 0$,

$$\begin{aligned}
2\mathcal{G}_{1-2u}[\phi](t) &= -\frac{1}{2} \int_{\partial\Omega} N\phi \, d\sigma \, t + o(t^{3/2}) + \int_{\partial\Omega} g(\nabla\phi, \nabla\delta) \, d\sigma \, t + o(t^{3/2}) \\
&= -\frac{1}{2} \int_{\partial\Omega} \phi\Delta\delta \, d\sigma \, t + o(t^{3/2}).
\end{aligned}$$

Finally, using the linearity of the functional $\mathcal{G}_v[\phi]$ with respect to v, we conclude the proof. $\qquad\square$

Remark 5.5. The asymptotics (65) for the functional $\mathcal{G}_u[\phi](t)$ is the best result that we are able to achieve. In the expression (66), the problematic term is given by (69), i.e.,

$$\int_0^t \int_{\partial\Omega} (1 - 2u(\tau, \cdot))(4\Delta - N^2)\phi \, d\sigma (t - \tau)^{1/2} \, d\tau,$$

which cannot be expressed in terms of $\mathcal{G}_u$; hence the only relevant information is given by Theorem 3.1. In conclusion, we cannot repeat the strategy of the proof of Theorem 5.4, replacing the series of $\mathcal{G}_u$ at order 3 in (66) to deduce the higher-order terms.

5.2. Fourth-order asymptotics. In this section we prove Theorem 1.1. We recall here the statement.

Theorem 5.6. *Let M be a compact sub-Riemannian manifold, equipped with a smooth measure ω, and let $\Omega \subset M$ be an open subset whose boundary is smooth and has no characteristic points. Then, as $t \to 0$,*

$$H_\Omega(t) = \omega(\Omega) - \frac{1}{\sqrt{\pi}}\sigma(\partial\Omega)t^{1/2} - \frac{1}{12\sqrt{\pi}}\int_{\partial\Omega}(2g(\nabla\delta, \nabla(\Delta\delta)) - (\Delta\delta)^2)\,d\sigma\, t^{3/2} + o(t^2).$$

Before giving the proof of the theorem, let us comment on its strategy. Recall that, on the one hand, for a cutoff function $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$ which is identically 1 close to $\partial\Omega$, see (48), the localization principle (55) holds, namely

$$\omega(\Omega) - H_\Omega(t) = I\phi(t, 0) + O(t^\infty) \quad \text{as } t \to 0. \tag{72}$$

Moreover, by the iterated Duhamel's principle for $I\phi(t, 0)$, see Lemma A.6, we can deduce expression (61), namely

$$I\phi(t, 0) = 2\mathcal{G}_{1-u}[\phi](t) + \frac{1}{\sqrt{\pi}}\int_0^t \mathcal{G}_{1-u}[N\phi](t)\,d\sigma\,(t - \tau)^{-1/2}\,d\tau + O(t^{3/2}). \tag{73}$$

On the other hand, we have an asymptotic series of the functional $\mathcal{G}_u$ at order 3; see Theorem 3.1. Therefore, if we naively insert this series in (73), we can obtain, at most, a third-order asymptotic expansion of the relative heat content $H_\Omega(t)$, whereas we are interested in the fourth-order expansion.

Using the outside contribution, we are able to overcome this difficulty. In particular, applying Proposition 5.3, for a function $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$ which is identically 1 close to $\partial\Omega$, we have the following asymptotic relation:

$$I\phi(t, 0) = I^c\phi(t, 0) + O(t^\infty) \quad \text{as } t \to 0. \tag{74}$$

Notice that (74) is a direct consequence of Proposition 5.3 since all the coefficients of the expansion vanish. Therefore, thanks to (74), we can rephrase (72) as

$$\omega(\Omega) - H_\Omega(t) = \tfrac{1}{2}(I\phi(t, 0) + I^c\phi(t, 0)) + O(t^\infty) \quad \text{as } t \to 0. \tag{75}$$

The advantage of (75) is that we can now apply the iterated Dirichlet principle for the sum $I\phi + I^c\phi$; see Lemma A.8. Already at order 3, we obtain

$$(I\phi + I^c\phi)(t, 0) = \frac{2}{\sqrt{\pi}}\int_{\partial\Omega}\phi\,d\sigma\,t^{1/2} + \frac{1}{\sqrt{\pi}}\int_0^t \mathcal{G}_{1-2u}[N\phi](\tau)(t - \tau)^{-1/2}\,d\tau + O(t^{3/2}), \tag{76}$$

where N is the operator defined in (59). As we can see, in (76), the functional $\mathcal{G}_u$ occurs for the first time in the second iteration of the Duhamel's principle, as opposed to the expansion for $I\phi$, where it appeared already in the first application; see (73). Hence we gain an order with respect to the asymptotic series of $\mathcal{G}_u$. More generally, if we were able to develop the k-th order asymptotics for $\mathcal{G}_u$, this would imply the $(k+1)$-th order expansion for $H_\Omega(t)$.

Proof of Theorem 5.6. Following the discussion above, it is enough to expand the sum $I\phi + I^c\phi$, with $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$. For this quantity, Lemma A.8 holds, namely we have the following iterated version of

Duhamel's principle:

$$
\begin{aligned}
(I\phi + I^c\phi)(t,0) = {} & \frac{2}{\sqrt{\pi}} \int_{\partial\Omega} \phi \, d\sigma \, t^{1/2} + \frac{1}{\sqrt{\pi}} \int_0^t \mathcal{G}_{1-2u}[N\phi](\tau)(t-\tau)^{-1/2} \, d\tau \\
& + \frac{1}{6\sqrt{\pi}} \int_{\partial\Omega} (4\Delta + N^2)\phi \, d\sigma \, t^{3/2} \\
& + \frac{1}{4\pi^{3/2}} \int_0^t \int_0^\tau \int_0^{\hat{\tau}} \mathcal{G}_{1-2u}[N^3\phi](s)((\hat{\tau}-s)(\tau-\hat{\tau})(t-\tau))^{-1/2} \, ds \, d\hat{\tau} \, d\tau \\
& + \frac{1}{4\sqrt{\pi}} \int_0^t \mathcal{G}_{1-2u}[(6N\Delta - N^3 - 2\Delta N)\phi](\tau)(t-\tau)^{1/2} \, d\tau + O(t^{5/2}), \quad (77)
\end{aligned}
$$

where N is defined in (59). Moreover, recall that by Theorem 5.4, the functional $\mathcal{G}_{1-2u}[\phi]$ has the following expansion for any $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$:

$$
\mathcal{G}_{1-2u}[\phi](t) = -\frac{1}{4} \int_{\partial\Omega} \phi \Delta\delta \, d\sigma \, t + o(t^{3/2}) \quad \text{as } t \to 0. \tag{78}
$$

Thus, replacing the term $\mathcal{G}_{1-2u}[N\phi]$ in (77) with the expansion (78) for $N\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$, we obtain the following asymptotic as $t \to 0$:

$$
\begin{aligned}
I\phi(t,0) + I^c\phi(t,0) = {} & \frac{2}{\sqrt{\pi}} \int_{\partial\Omega} \phi \, d\sigma \, t^{1/2} - \frac{1}{3\sqrt{\pi}} \left(\int_{\partial\Omega} N\phi \Delta\delta \, d\sigma \right) t^{3/2} \\
& + \frac{1}{6\sqrt{\pi}} \int_{\partial\Omega} (4\Delta + N^2)\phi \, d\sigma \, t^{3/2} + o(t^2) \quad (79)
\end{aligned}
$$

for any $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$. In particular, if we choose $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$ such that $\phi \equiv 1$ close to $\partial\Omega$, then on the one hand, from (79), we obtain, as $t \to 0$,

$$
I\phi(t,0) + I^c\phi(t,0) = \frac{2}{\sqrt{\pi}} \sigma(\partial\Omega) t^{1/2} + \frac{1}{6\sqrt{\pi}} \int_{\partial\Omega} (2g(\nabla\delta, \nabla(\Delta\delta)) - (\Delta\delta)^2) \, d\sigma \, t^{3/2} + o(t^2).
$$

On the other hand, the asymptotic relation (75) holds. □

Third-order vs. fourth-order asymptotics. We stress that we could have obtained the third-order asymptotic expansion of $H_\Omega(t)$ *without* introducing the sum of the inside and outside contributions $I\phi + I^c\phi$, and only using the Duhamel's principle for $I\phi$, see Lemma A.6, and the asymptotic series for $\mathcal{G}_u$, see Theorem 5.4. However, for the improvement to the fourth-order asymptotics, the argument of the sum of contributions seems necessary.

5.3. *The weighted relative heat content.* Adapting the proof of Theorem 5.6, one can prove a slightly more general result which we state here for completeness.

Proposition 5.7. *Let M be a compact sub-Riemannian manifold, equipped with a smooth measure ω, and let $\Omega \subset M$ be an open subset whose boundary is smooth and has no characteristic points. Let $\chi \in C_c^\infty(M)$ and define the **weighted relative heat content***

$$
H_\Omega^\chi(t) = \int_\Omega u(t,x)\chi(x) \, d\omega(x) \quad \text{for all } t > 0.
$$

Then, as $t \to 0$,

$$H_\Omega^\chi(t) = \int_\Omega \chi \, d\omega - \frac{1}{\sqrt{\pi}} \int_{\partial\Omega} \chi \, d\sigma \, t^{1/2} - \frac{1}{2} \int_{\partial\Omega} g(\nabla\chi, \nabla\delta) \, d\sigma \, t$$
$$- \left(\frac{1}{12\sqrt{\pi}} \int_{\partial\Omega} (4\Delta + N^2)\chi \, d\sigma - \frac{1}{6\sqrt{\pi}} \int_{\partial\Omega} (N\chi)\Delta\delta \, d\sigma \right) t^{3/2}$$
$$- \frac{1}{2} \int_{\partial\Omega} g(\nabla(\Delta\chi), \nabla\delta) \, d\sigma \, t^2 + o(t^2).$$

Proof. Let us consider a cutoff function ϕ as in (48). Then, applying the usual localization argument, see (49), we have

$$\int_\Omega \chi(x) \, d\omega(x) - H_\Omega^\chi(t) = I[\phi\chi](t, 0) + O(t^\infty) \quad \text{as } t \to 0,$$

where now the function $\phi\chi \in C_c^\infty(\Omega_{-r_0}^{r_0})$ and $\phi\chi = \chi$ close to $\partial\Omega$.

As we did in the proof of Theorem 5.6, we relate $H_\Omega^\chi(t)$ with the sum of contributions. Applying Proposition 5.3, we have the following asymptotic relation at order 4:

$$I[\phi\chi](t, 0) - I^c[\phi\chi](t, 0) = \int_{\partial\Omega} g(\nabla\chi, \nabla\delta) \, d\sigma \, t + \int_{\partial\Omega} g(\nabla(\Delta\chi), \nabla\delta) \, d\sigma \, t^2 + o(t^2),$$

as $t \to 0$, having used the fact that $\phi\chi \equiv \chi$ close to $\partial\Omega$. Notice that this relation coincides with (74) when $\chi \equiv 1$ close to $\partial\Omega$. Thus, we obtain

$$\int_\Omega \chi(x) \, d\omega(x) - H_\Omega^\chi(t) = \frac{1}{2}(I[\phi\chi](t, 0) + I^c[\phi\chi](t, 0))$$
$$+ \int_{\partial\Omega} g(\nabla\chi, \nabla\delta) \, d\sigma \, t + \int_{\partial\Omega} g(\nabla(\Delta\chi), \nabla\delta) \, d\sigma \, t^2 + o(t^2) \quad \text{as } t \to 0.$$

Finally, applying (79) for $I[\phi\chi](t, 0) + I^c[\phi\chi](t, 0)$, we conclude. $\square$

Remark 5.8. We compare the coefficients of the expansions of $H_\Omega(t)$ and $Q_\Omega(t)$, defined in (6), respectively. On the one hand, by [Rizzi and Rossi 2021, Theorem 5.8], the k-th coefficient of the expansion of $Q_\Omega(t)$ is of the form

$$- \int_{\partial\Omega} D_k(\chi) \, d\sigma \quad \text{for all } \chi \in C_c^\infty(M),$$

where D_k is a differential operator acting on $C_c^\infty(M)$ and belonging to $\text{span}_\mathbb{R}\{\Delta, N\}$ as algebra of operators. On the other hand, Proposition 5.7 shows that this is no longer true for the third coefficient of the expansion of $H_\Omega(t)$, as we need to add the operator multiplication by $\Delta\delta$.

6. An alternative approach using the heat kernel asymptotics

As we can see by a first application of Duhamel's principle, see (10), and its iterations, the small-time asymptotics of $u(t, \cdot)|_{\partial\Omega}$, together with uniform estimates on the remainder with respect to $x \in \partial\Omega$, would be enough to determine the asymptotic expansion of the relative heat content, at any order.

In Theorem 3.1, we studied the zero-order asymptotics of $u(t, \cdot)|_{\partial\Omega}$. The technique used for its proof does not work at higher-order, since the exponential remainder term in (40) would be unbounded as $t \to 0$.

In this section, we comment how such a higher-order asymptotics of $u(t, \cdot)|_{\partial\Omega}$ can be obtained exploiting the asymptotic formula for the heat kernel proved in [Colin de Verdière et al. 2021, Theorem A].

Let M be a compact sub-Riemannian manifold and $\Omega \subset M$ an open subset with smooth boundary. For $x \in \partial\Omega$, let us consider $\psi = (z_1, \ldots, z_n) : U \to V$ a chart of privileged coordinates centered at x, with U a relatively compact set. Since the heat kernel is exponentially decaying outside the diagonal, see (31),

$$
\begin{aligned}
u(t, x) &= \int_\Omega p_t(x, y)\, d\omega(y) = \int_{\Omega \cap U} p_t(x, y)\, d\omega(y) + O(t^\infty) \\
&= \int_{V_1} p_t(0, z)\, d\omega(z) + O(t^\infty),
\end{aligned}
\tag{80}
$$

where $V_1 = \psi(U \cap \Omega)$, and we denote with the same symbols ω and $p_t(0, z)$ the coordinate expression of the measure and heat kernel, respectively. For example, if $x \in \partial\Omega$ is noncharacteristic, we may choose ψ as in (30), and then $V_1 = V \cap \{z_1 > 0\}$. Recall the asymptotic expansion of the heat kernel of Theorem 2.9, evaluated in $(0, z)$: for any $m \in \mathbb{N}$ and compact set $K \subset (0, \infty) \times V$,

$$
|\varepsilon|^{\mathcal{Q}} p_{\varepsilon^2 \tau}(0, \delta_\varepsilon(z)) = \hat{p}_\tau(0, z) + \sum_{i=0}^m \varepsilon^i f_i(\tau, 0, z) + o(|\varepsilon|^m) \quad \text{as } \varepsilon \to 0,
\tag{81}
$$

uniformly as $(\tau, z) \in K$, where $\mathcal{Q}$, $\hat{p}$ and the f_i are defined in Section 2. We will omit the dependence on the center of the privileged coordinates, x, it being fixed for the moment. At this point, we would like to integrate (81) to get information of $u(t, x)$ as $t \to 0$. Proceeding formally, let us choose the parameters ε, τ in (81) such that

$$
\varepsilon^2 \tau = t, \quad \varepsilon = t^{\alpha/(2\alpha+1)}, \quad \tau = t^{1/(2\alpha+1)},
\tag{82}
$$

for some $\alpha > 0$ to be fixed. For convenience of notation, set

$$
V_s = \delta_s(V_1) \quad \text{for all } s \in [-1, 1].
$$

Then, split the integral over V_1 in (80) in two, so that the first one is computed on V_ε and the second one is computed on its complement in V_1, i.e., $V_1 \setminus V_\varepsilon$. Notice that, by usual off-diagonal estimates, see [Jerison and Sánchez-Calle 1986, Proposition 3] and our choice of the parameter ε as in (82), the following is a remainder term, independent of the value of α:

$$
\int_{V_1 \setminus V_\varepsilon} p_t(0, z)\, d\omega(z) = O(e^{-\beta \varepsilon^2/t}) = O(t^\infty) \quad \text{as } t \to 0.
$$

Thus, writing the measure in coordinates $d\omega(z) = \omega(z)\, dz$ with $\omega(\cdot) \in C^\infty(V_1)$, we have, as $t \to 0$,

$$
\begin{aligned}
u(t, x) &= \int_{V_\varepsilon} p_t(0, z)\omega(z)\, dz + O(t^\infty) = \int_{V_1} \varepsilon^{\mathcal{Q}} p_{\varepsilon^2 \tau}(0, \delta_\varepsilon(z))\omega(\delta_\varepsilon(z))\, dz + O(t^\infty) \\
&= \int_{V_1} \left(\hat{p}_\tau(0, z) + \sum_{i=0}^{m-1} \varepsilon^i f_i(\tau, 0, z) + \varepsilon^m R_m(\varepsilon, \tau, z) \right) \omega(\delta_\varepsilon(z))\, dz + O(t^\infty),
\end{aligned}
\tag{83}
$$

where R_m is a smooth function on $[-1, 1] \times (0, \infty) \times \mathbb{R}^n$ such that

$$\sup_{\varepsilon \in [-1,1], \; z \in K} |R_m(\varepsilon, \tau, z)| \leq C_m(\tau, K) \tag{84}$$

for any compact set $K \subset \mathbb{R}^n$, according to (81). Up to restricting the domain of privileged coordinates U, we can assume that (84) holds on $\overline{V}$. By our choices (82), we would like the term

$$t^{m\alpha/(2\alpha+1)} \int_{V_1} |R_m(t^{\alpha/(2\alpha+1)}, t^{1/(2\alpha+1)}, z)| \omega(\delta_{t^{\alpha/(2\alpha+1)}}(z)) \, dz \tag{85}$$

to be an error term of order greater than $(m-1)/2$ as $t \to 0$. Thus, assume for the moment that for all $K \subset V$ compact and, for all $m \in \mathbb{N}$, there exist $\ell = \ell(m, K) \in \mathbb{N}$ and $C_m(K) > 0$ such that

$$\sup_{\substack{\varepsilon \in [-1,1] \\ z \in K}} |R_m(\varepsilon, \tau, z)| \leq \frac{C_m(K)}{\tau^\ell} \quad \text{for all } \tau \in (0, 1). \tag{H}$$

Thanks to assumption (H), choosing α large enough, we see that (85) is a $o(t^{(m-1)/2})$. Performing the change of variable $z \mapsto \delta_{1/\sqrt{\tau}}(z)$ in (83), and exploiting the homogeneity properties of $\hat{p}$ and f_i, namely (29), we finally obtain the following expression for u as $t \to 0$:

$$u(t, x) = \int_{V_{t^{-1/(2(2\alpha+1))}}} \left(\hat{p}_1(0, z) + \sum_{i=0}^{m-1} t^{i/2} a_i(z) \right) \omega(\delta_{\sqrt{t}}(z)) \, dz + o(t^{(m-1)/2}), \tag{86}$$

having set $a_i(z) = f_i(1, 0, z)$, for all $i \in \mathbb{N}$. Therefore, we find an asymptotic expansion of $u(t, x)$ under assumption (H), which is crucial to overcome the fact that (81) is formulated on an asymptotic neighborhood of the diagonal, and not uniformly as $\tau \to 0$. It is likely[6] that (H) can be proven in the nilpotent case, and more generally when the ambient manifold is $M = \mathbb{R}^n$ and the generating family of the sub-Riemannian structure, $\{X_1, \ldots, X_N\}$ satisfies the uniform Hörmander polynomial condition; see [Colin de Verdière et al. 2021, Appendix B] for details. Although this strategy could be used to prove the existence of an asymptotic expansion of $H_\Omega(t)$, we refrain to go in this direction since two technical difficulties would arise nonetheless:

• *Uniformity of the expansion of $u(t, x)$ with respect to $x \in \partial\Omega$.* In the nonequiregular case, see Section 2.3 for details, the expansion (81) is not uniform as x varies in compact subsets of M; hence the same would be true for the expansion (86).

• *Computations of the coefficients.* The coefficients appearing in (86) depend on the nilpotent approximation at $x \in \partial\Omega$ and are not clearly related to the invariants of $\partial\Omega$.

Our strategy avoids almost completely the knowledge of the small-time asymptotics of $u(t, \cdot)_{\partial\Omega}$, it being based on an asymptotic series of the auxiliary functional $\mathcal{G}_u$. Moreover, we stress that our method to prove the asymptotics of $H_\Omega(t)$ up to order 4, see Theorem 1.1, holds for any sub-Riemannian manifold, including also the nonequiregular ones.

---

[6]Personal communication by Yves Colin de Verdière, Luc Hillairet and Emmanuel Trélat.

Remark 6.1. In order to pass from (86) to the asymptotic expansion of $H_\Omega(t)$, we would use Duhamel's formula, which holds under the noncharacteristic assumption. This means that, even though (81) of course is true even in presence of characteristic points, we can't say much about the asymptotics of $H_\Omega(t)$ in the general case.

7. The noncompact case

In the noncompact case, we have the following difficulties:

- The localization principle, see Proposition 4.5, may fail.

- Set $u(t, x) = e^{t\Delta}\mathbb{1}_\Omega(x)$ and $u^c(t, x) = e^{t\Delta}\mathbb{1}_{\Omega^c}(x)$. If the manifold is not stochastically complete, the relation $u(t, x) + u^c(t, x) = 1$ does not hold.

- The Gaussian bounds for the heat kernel and its time-derivatives, à la [Jerison and Sánchez-Calle 1986, Theorem 3], may not hold; thus Lemma A.3 may not be true.

Definition 7.1. Let M be a sub-Riemannian manifold, equipped with a smooth measure ω. We say that (M, ω) is (*globally*) *doubling* if there exist constants $C_D > 0$ such that

$$V(x, 2\rho) \leq C_D V(x, \rho) \quad \text{for all } \rho > 0, \ x \in M,$$

where $V(x, \rho) = \omega(B_\rho(x))$. We say that (M, ω) satisfies a (*global*) *weak Poincaré inequality*, if there exist constants $C_P > 0$ such that

$$\int_{B_\rho(x)} |f - f_{x,\rho}|^2 \, d\omega \leq C_P \rho^2 \int_{B_{2\rho}(x)} \|\nabla f\|^2 \, d\omega, \quad \rho > 0, \ x \in M,$$

for any smooth function $f \in C^\infty(M)$. Here

$$f_{x,\rho} = \frac{1}{V(x, \rho)} \int_{B_\rho(x)} f \, d\omega.$$

We refer to these properties as local whenever they hold for any $\rho < \rho_0$.

Remark 7.2. If M is a sub-Riemannian manifold, equipped with a smooth globally doubling measure ω, then it is stochastically complete, namely

$$\int_M p_t(x, y) \, d\omega(y) = 1 \quad \text{for all } t > 0, \ x \in M.$$

This is a straightforward consequence of the characterization given by [Sturm 1994, Theorem 4] on the volume growth of balls.

Theorem 7.3. *Let M be a complete sub-Riemannian manifold, equipped with a smooth measure ω. Assume that (M, ω) is globally doubling and satisfies a global weak Poincaré inequality. Then, there exist constants $C_k, c_k > 0$ for any integer $k \geq 0$, depending only on C_D, C_P, such that, for any $x, y \in M$ and $t > 0$,*

$$|\partial_t^k p_t(x, y)| \leq \frac{C_k t^{-k}}{V(x, \sqrt{t})} \exp\left(-\frac{d_{SR}^2(x, y)}{c_k t}\right), \tag{87}$$

where we recall $V(x, \sqrt{t}) = \omega(B_{\sqrt{t}}(x))$.

In addition, there exist constants $C_\ell, c_\ell > 0$, depending only on C_D, C_P, such that, for any $x, y \in M$ and $t > 0$,

$$p_t(x, y) \geq \frac{C_\ell}{V(x, \sqrt{t})} \exp\left(-\frac{d_{SR}^2(x, y)}{c_\ell t}\right). \tag{88}$$

Proof. Define the sub-Riemannian Hamiltonian as the smooth function $H : T^*M \to \mathbb{R}$,

$$H(\lambda) = \frac{1}{2} \sum_{i=1}^{N} \langle \lambda, X_i \rangle^2, \quad \lambda \in T^*M,$$

where $\{X_1, \ldots, X_N\}$ is a generating family for the sub-Riemannian structure. Then, following the notation of [Sturm 1996], one can easily verify that

$$\mathcal{E}(u, v) = \int_M 2H(du, dv) \, d\omega \quad \text{for all } u, v \in C_c^\infty(M),$$

where H is the sub-Riemannian Hamiltonian viewed as a bilinear form on fibers, defines a strongly local Dirichlet form with domain $\mathrm{dom}(\mathcal{E}) = C_c^\infty(M)$. Notice that the Friedrichs extension of $\mathcal{E}$ is exactly the sub-Laplacian. Moreover, the intrinsic metric

$$d_I(x, y) = \sup\{|u(x) - u(y)| : u \in C_c^\infty(M), |2H(du, du)| \leq 1\} \quad \text{for all } x, y \in M$$

coincides with the usual sub-Riemannian distance, as $|2H(du, du)| = \|\nabla u\|^2$; see [Barilari et al. 2016, Chapter 2, Proposition 12.4]. Thus, $\mathcal{E}$ is also strongly regular and, by our assumptions on (M, ω), [Saloff-Coste 1992, Theorem 4.3] holds true, proving (87). For the Gaussian lower bound (88), it is enough to apply [Sturm 1996, Corollary 4.10]; see also [Saloff-Coste 1992, Theorem 4.2]. □

Remark 7.4. Theorem 7.3 ensures that the time-derivatives of the heat kernel satisfy Gaussian bounds, which are sufficient to prove Lemma A.3 in the noncompact case. This lemma is crucial to obtain the asymptotics expansion of $H_\Omega(t)$ at order *strictly greater* than 1.

We prove now the noncompact analogue of Proposition 4.5.

Corollary 7.5. *Under the assumptions of Theorem 7.3, let $\Omega \subset M$ be an open subset with smooth boundary. Then, for any $K \subset M$ closed subset of M such that $K \cap \partial\Omega = \varnothing$, we have*

$$\mathbb{1}_\Omega(x) - u(t, x) = O(t^\infty) \quad \text{as } t \to 0, \text{ uniformly for } x \in K,$$

where $u(t, x) = e^{t\Delta}\mathbb{1}_\Omega(x)$ is the solution to (17).

Proof. Let us assume that $K \subset \Omega$ such that $K \cap \partial\Omega = \varnothing$. The other part of the statement can be done similarly.

Since M is stochastically complete, see Remark 7.2, for any $x \in K$, we can write

$$\mathbb{1}_\Omega(x) - u(t, x) = 1 - e^{t\Delta}\mathbb{1}_\Omega(x) = e^{t\Delta}1(x) - e^{t\Delta}\mathbb{1}_\Omega(x) = \int_{M\setminus\Omega} p_t(x, y) \, d\omega(y).$$

Thanks to Theorem 7.3, we can apply (87) for $k = 0$, obtaining

$$\int_{M \setminus \Omega} p_t(x, y) \, d\omega(y) \leq \int_{M \setminus \Omega} \frac{C_0}{V(x, \sqrt{t})} \exp\left(-\frac{d_{\mathrm{SR}}^2(x, y)}{c_0 t}\right) d\omega(y)$$

for suitable constants $C_0, c_0 > 0$ not depending on $x, y \in M$, $t > 0$. Now, fix $L > 1$; since $K \subset \Omega$ is closed with empty intersection with $\partial \Omega$, and thus well-separated from $\partial \Omega$, we deduce there exists $a = a(K) > 0$ such that $d_{\mathrm{SR}}(x, y) > a$ for any $x \in K$, $y \in M \setminus \Omega$, and so

$$\int_{M \setminus \Omega} p_t(x, y) \, d\omega(y) \leq \int_{M \setminus \Omega} \frac{C_0}{V(x, \sqrt{t})} \exp\left(-\frac{d_{\mathrm{SR}}^2(x, y)}{c_0 t}\right) d\omega(y)$$

$$\leq \exp\left(-\frac{C(a, L)}{c_0 t}\right) \int_{M \setminus \Omega} \frac{C_0}{V(x, \sqrt{t})} \exp\left(-\frac{d_{\mathrm{SR}}^2(x, y)}{2^L c_0 t}\right) d\omega(y), \qquad (89)$$

where $C(a, L) = a^2(2^L - 1)/2^L > 0$. Thus, if we prove that the integral in (89) is finite, we conclude. Firstly, recall the Gaussian lower bound (88), which holds thanks to Theorem 7.3:

$$p_t(x, y) \geq \frac{C_\ell}{V(x, \sqrt{t})} \exp\left(-\frac{d_{\mathrm{SR}}^2(x, y)}{c_\ell t}\right) \qquad (90)$$

for suitable constants $C_\ell, c_\ell > 0$, not depending on $x, y \in M$, $t > 0$. Secondly, by the doubling property of ω, it is well known that there exists C_D', $s > 0$ depending only on C_D such that

$$V(x, R) \leq C_D'\left(\frac{R}{\rho}\right)^s V(x, \rho) \quad \text{for all } \rho \leq R. \qquad (91)$$

Therefore, choosing $L > 1$ so big that $\tilde{c}^2 = (2^L c_0)/c_\ell > 1$ and applying (91) for $\rho = \sqrt{t}$ and $R = \tilde{c}\sqrt{t}$, we have $R > \rho$ and

$$V(x, \tilde{c}\sqrt{t}) \leq \tilde{C} V(x, \sqrt{t}) \quad \text{for all } t > 0, \qquad (92)$$

having let $\tilde{C} = C_D'\tilde{c}^s > 0$. Finally, using (92) and the Gaussian lower bound (90), we can estimate the integral in (89) as follows:

$$\int_{M \setminus \Omega} \frac{1}{V(x, \sqrt{t})} \exp\left(-\frac{d_{\mathrm{SR}}^2(x, y)}{2^L c_0 t}\right) d\omega(y) \leq \int_M \frac{\tilde{C}}{V(x, \tilde{c}\sqrt{t})} \exp\left(-\frac{d_{\mathrm{SR}}^2(x, y)}{c_\ell \tilde{c} t}\right) d\omega(y)$$

$$\leq \frac{\tilde{C}}{C_\ell} \int_M p_{\tilde{t}}(x, y) \, d\omega(y) \leq \frac{\tilde{C}}{C_\ell},$$

where $\tilde{t} = \tilde{c}t$. Since the resulting constant does not depend on $x \in K$, we conclude the proof. $\qquad \square$

Using Corollary 7.5 and adopting the same strategy of the compact case, one can finally prove the following result.

Theorem 7.6. *Let M be a complete sub-Riemannian manifold, equipped with a smooth measure ω. Assume that (M, ω) is globally doubling and satisfies a global weak Poincaré inequality. Let $\Omega \subset M$ be*

an open and bounded subset whose boundary is smooth and has no characteristic points. Then, as $t \to 0$,

$$H_\Omega(t) = \omega(\Omega) - \frac{1}{\sqrt{\pi}}\sigma(\partial\Omega)t^{1/2} - \frac{1}{12\sqrt{\pi}}\int_{\partial\Omega}\left(2g(\nabla\delta, \nabla(\Delta\delta)) - (\Delta\delta)^2\right)d\sigma\, t^{3/2} + o(t^2).$$

Remark 7.7. Theorem 7.6 holds true also for the weighted relative heat content; see Section 5.3. In both cases, we do not know whether its assumptions are sharp in the noncompact case.

7.1. *Notable examples.* We list here some notable examples of sub-Riemannian manifolds satisfying the assumptions of Theorem 7.3. For these examples Theorem 7.6 is valid.

- *M* is a Lie group with polynomial volume growth, the distribution is generated by a family of left-invariant vector fields satisfying the Hörmander condition and ω is the Haar measure. This family includes also Carnot groups. See for example [Varopoulos 1996; Saloff-Coste 1992; Gallagher and Sire 2012].

- $M = \mathbb{R}^n$, equipped with a sub-Riemannian structure induced by a family of vector fields $\{Y_1, \dots, Y_N\}$ with bounded coefficients together with their derivatives, and satisfying the Hörmander condition. Under these assumptions, the Lebesgue measure is doubling, see [Nagel et al. 1985, Theorem 1], and the Poincaré inequality is verified in [Jerison 1986]. We remark that these works provide the local properties of Definition 7.1, with constants depending only on the C^k-norms of the vector fields Y_i for $i = 1, \dots, N$. Thus, if the C_k-norms are globally bounded, we obtain the corresponding global properties.

- *M* is a complete Riemannian manifold with metric *g*, equipped with the Riemannian measure, and with nonnegative Ricci curvature.

We mention that a Riemannian manifold *M* with Ricci curvature bounded below by a negative constant satisfies only locally Definition 7.1, i.e., for some $\rho_0 < \infty$, depending on the Ricci bound. Nevertheless, we can prove Corollary 7.5 in this case, as [Li and Yau 1986, Corollary 3.1] provides an upper Gaussian bound, and a lower bound as (88) holds; see [Bakry and Qian 1999, Corollary 2]. Thus, the first-order asymptotic expansion of $H_\Omega(t)$, see Theorem 4.13, is valid in this setting.

Appendix: Iterated Duhamel's principle for $I_\Omega\phi(t, 0)$

In this section, we study the iterated Duhamel's principle for the $I_\Omega\phi$; see Definition 4.7. The main result is Lemma A.6, which will imply formulas (58), (66) and (77).

The next proposition is a version of the iterated Duhamel's principle taken from [Rizzi and Rossi 2021, Proposition A.1], which we recall here.

Proposition A.1. *Let $F \in C^\infty((0, \infty) \times [0, +\infty))$ be a smooth function compactly supported in the second variable and let $L = \partial_t - \partial_r^2$. Assume that the following conditions hold:*

(i) *$L^k F(0, r) = \lim_{t\to 0} L^k F(t, r)$ exists in the sense of distributions[7] for any $k \geq 0$.*

(ii) *$L^k F(t, 0)$ and $\partial_r L^k F(t, 0)$ converge to a finite limit as $t \to 0$ for any $k \geq 0$.*

---

[7] Namely, for any $\psi \in C^\infty([0, \infty))$, there exists finite $\lim_{t\to 0}\int_0^\infty f(t, r)\psi(r)\,dr$. With a slight abuse of notation, we define $\int_0^\infty f(0, r)\psi(r)\,dr = \lim_{t\to 0}\int_0^\infty f(t, r)\psi(r)\,dr$.

Then, for all $m \in \mathbb{N}$ and $t > 0$, we have

$$F(t, 0) = \sum_{k=0}^{m} \left(\frac{t^k}{k!} \int_0^\infty e(t, r, 0) L^k F(0, r) \, dr - \frac{1}{\sqrt{\pi} k!} \int_0^t \partial_r L^k F(\tau, 0)(t - \tau)^{k-1/2} \, d\tau \right)$$

$$+ \frac{1}{m!} \int_0^t \int_0^\infty e(t - \tau, r, 0) L^{m+1} F(\tau, r)(t - \tau)^m \, dr \, d\tau, \quad (93)$$

where $e(t, r, s)$ is the Neumann heat kernel on the half-line; see (53).

We want to apply Proposition A.1 to the function $I_\Omega \phi(t, 0)$; thus, we study in detail the operators $L^k I_\Omega$ for any $k \geq 1$. Define iteratively the family of matrices of operators, acting on smooth functions,

$$M_{kj} = \begin{pmatrix} Q_{kj} & S_{kj} \\ P_{kj} & R_{kj} \end{pmatrix},$$

as follows. Set

$$M_{10} = \begin{pmatrix} \Delta & -\Delta N_\Omega \\ N_\Omega & -N_\Omega^2 + \Delta \end{pmatrix} \quad \text{and} \quad M_{11} = \begin{pmatrix} 0 & N_\Omega \\ 0 & 0 \end{pmatrix},$$

and, for all $k \geq 1$ and $0 \leq j \leq k$, set

$$M_{kj} = M_{10} M_{k-1, j} + M_{11} M_{k-1, j-1}, \quad (94)$$

while $M_{kj} = 0$ for all other values of the indices, i.e., $k < 0$, $j < 0$ or $k < j$. Here N_Ω is the operator defined in (50), namely

$$N_\Omega \phi = 2g(\nabla \phi, \nu) + \phi \, \text{div}_\omega(\nu) \quad \text{for all } \phi \in C_c^\infty(\Omega_{-r_0}^{r_0}), \quad (95)$$

where ν is the inward-pointing normal from Ω.

Recall the definition of I_Ω and Λ_Ω: for any $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$ and for all $t > 0$, $r \geq 0$,

$$I_\Omega \phi(t, r) = \int_{\Omega_r} (1 - u(t, x))\phi(x) \, d\omega(x),$$

$$\Lambda_\Omega \phi(t, r) = -\partial_r I_\Omega \phi(t, r) = - \int_{\partial \Omega_r} (1 - u(t, y))\phi(y) \, d\sigma(y),$$

where $u(t, \cdot) = e^{t\Delta} \mathbb{1}_\Omega(\cdot)$. Iterations of $L^k I_\Omega \phi$ satisfy the following lemma.

Lemma A.2. *Let M be a sub-Riemannian manifold, equipped with a smooth measure ω, and let $\Omega \subset M$ be an open relatively compact subset whose boundary is smooth and has no characteristic points. Then, as operators on $C_c^\infty(\Omega_{-r_0}^{r_0})$, we have*:

(i) $L I_\Omega = I_\Omega \Delta + \Lambda_\Omega N_\Omega$.

(ii) $L \Lambda_\Omega = \Lambda_\Omega(-N_\Omega^2 + \Delta) + \partial_t I_\Omega N_\Omega - I_\Omega \Delta N_\Omega$.

(iii) *For any $k \in \mathbb{N}$,*

$$L^k I_\Omega = \sum_{j=0}^{k} \frac{\partial^j}{\partial t^j} (\Lambda_\Omega P_{kj} + I_\Omega Q_{kj}) \quad \text{and} \quad L^k \Lambda_\Omega = \sum_{j=0}^{k} \frac{\partial^j}{\partial t^j} (\Lambda_\Omega R_{kj} + I_\Omega S_{kj}).$$

Here we mean that, for any $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$, *the operator* L^k *acts on the functions* $I_\Omega \phi(t, r)$, $\Lambda_\Omega \phi(t, r)$. *Analogously the right-hand side when evaluated in* ϕ *is a function of* (t, r).

Proof. The proof of items (i) and (ii) follows from Proposition 4.2 and the divergence theorem; see [Rizzi and Rossi 2021, Lemma A.2]. We show how to recover the iterative law (94).

Consider the vector $V = (I_\Omega, \Lambda_\Omega)$. Then by items (i) and (ii), we have

$$LV = (LI_\Omega, L\Lambda_\Omega) = VM_{10} + \partial_t VM_{11}. \tag{96}$$

Notice that the operator L^k contains at most k derivatives with respect to t. Therefore we have

$$L^k V = \sum_{j=0}^{k} \partial_t^j (VM_{kj}) \quad \text{for all } k \geq 0.$$

On the other hand, we can evaluate $L^k V$, using (96),

$$L^k V = L(L^{k-1}V) = \sum_{j=0}^{k-1} L\partial_t^j (VM_{k-1,j}) = \sum_{j=0}^{k-1} \partial_t^j (LVM_{k-1,j})$$
$$= \sum_{j=0}^{k-1} \partial_t^j VM_{10}M_{k-1,j} + \sum_{j=0}^{k-1} \partial_t^{j+1} VM_{11}M_{k-1,j}.$$

Reorganizing the sum, we find (94), concluding the proof. □

We want to apply Proposition A.1 to $I_\Omega \phi(t, r)$ for $k \geq 2$, in order to obtain higher-order asymptotics. However, Lemma A.2 shows that $L^k I_\Omega$ for $k \geq 2$, involves time derivatives of $u(t, x)$ which are not well-defined at $\partial\Omega$ as $t \to 0$. Therefore, we consider the following approximation of $I_\Omega \phi$ and $\Lambda_\Omega \phi$, respectively: fix $\varepsilon > 0$ and define, for any $t > 0$, $r \geq 0$,

$$I_\varepsilon \phi(t, r) = = \int_{\Omega_r} (1 - u_\varepsilon(t, x))\phi(x)\, d\omega(x),$$

$$\Lambda_\varepsilon \phi(t, r) = -\partial_r I_\varepsilon \phi(t, r) = \int_{\partial\Omega_r} (1 - u_\varepsilon(t, x))\phi(y)\, d\sigma(y),$$

where $u_\varepsilon(t, x) = e^{t\Delta}\mathbb{1}_{\Omega_\varepsilon}(x)$. We recall that, for any $a \in \mathbb{R}$, $\Omega_a = \{x \in M : \delta(x) > a\}$. Notice that, by the dominated convergence theorem, we have

$$I_\varepsilon \phi(t, 0) \xrightarrow{\varepsilon \to 0} I_\Omega \phi(t, 0) \quad \text{uniformly on } [0, T],$$

and, in addition, Lemma A.2 holds unchanged also for I_ε and Λ_ε.

Lemma A.3. *Let* M *be a compact sub-Riemannian manifold, equipped with a smooth measure* ω, *and let* $\Omega \subset M$ *be an open subset whose boundary is smooth and has no characteristic points. Let* $\psi \in C^\infty([0, \infty))$, $\varepsilon \in (0, r_0)$ *and define*

$$\psi^{(-1)}(r) = \int_0^r \psi(s)\, ds \quad \text{for all } r \geq 0.$$

Then, for any $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$, *the following identities hold:*

(i) $\displaystyle\lim_{t\to 0}\int_0^\infty \frac{\partial^j}{\partial t^j}\Lambda_\varepsilon \phi(t,r)\psi(r)\,dr = \begin{cases} \int_{\Omega_0^\varepsilon} \phi(\psi\circ\delta)\,d\omega & \text{if } j=0, \\ -\int_{\Omega_\varepsilon}\Delta^j(\phi(\psi\circ\delta))\,d\omega & \text{if } j\geq 1, \end{cases}$

(ii) $\displaystyle\lim_{t\to 0}\int_0^\infty \frac{\partial^j}{\partial t^j}I_\varepsilon \phi(t,r)\psi(r)\,dr = \begin{cases} \int_{\Omega_0^\varepsilon} \phi(\psi^{(-1)}\circ\delta)\,d\omega & \text{if } j=0, \\ -\int_{\Omega_\varepsilon}\Delta^j(\phi(\psi^{(-1)}\circ\delta))\,d\omega & \text{if } j\geq 1, \end{cases}$

(iii) $\displaystyle\frac{\partial^j}{\partial t^j}\Lambda_\varepsilon \phi(0,0) = \begin{cases} \int_{\partial\Omega} \phi\,d\sigma & \text{if } j=0, \\ 0 & \text{if } j\geq 1, \end{cases}$

(iv) $\displaystyle\frac{\partial^j}{\partial t^j}I_\varepsilon \phi(0,0) = \begin{cases} d\omega & \text{if } j=0, \\ -\int_{\Omega_\varepsilon}\Delta^j\phi\,d\omega & \text{if } j\geq 1, \end{cases}$

where, we recall, $\Omega_\varepsilon = \{x\in M : \delta(x) > \varepsilon\}$ and $\Omega_0^\varepsilon = \Omega\setminus\Omega_\varepsilon$.

Remark A.4. The only difference with respect to [Rizzi and Rossi 2021, Lemma A.4] is item (iii), which now holds only as $t\to 0$ and not for all positive times.

Proof of Lemma A.3. We claim that, for any $j\geq 1$,

$$\lim_{t\to 0}\int_\Omega \phi(x)\Delta^j u_\varepsilon(t,x)\,d\omega(x) = \int_{\Omega_\varepsilon}\Delta^j\phi(x)\,d\omega(x). \tag{97}$$

Let us prove it by induction: For $j=1$, applying the divergence theorem, we have

$$\int_\Omega \phi\Delta u_\varepsilon\,d\omega = -\int_{\partial\Omega}\phi g(\nabla u_\varepsilon, \nabla\delta)\,d\sigma + \int_{\partial\Omega} u_\varepsilon g(\nabla\phi, \nabla\delta)\,d\sigma + \int_\Omega u_\varepsilon \Delta\phi\,d\omega. \tag{98}$$

Let us discuss the first term in (98): By the divergence theorem applied with respect to the set Ω^c, we have

$$\int_{\partial\Omega}\phi g(\nabla u_\varepsilon, \nabla\delta)\,d\sigma = \int_{\Omega^c}\phi\Delta u_\varepsilon\,d\omega + \int_{\partial\Omega} u_\varepsilon g(\nabla\phi, \nabla\delta)\,d\sigma - \int_{\Omega^c} u_\varepsilon\Delta\phi\,d\omega. \tag{99}$$

Then, using [Jerison and Sánchez-Calle 1986, Theorem 3] and noticing that $d_{\mathrm{SR}}(x,y)\geq\varepsilon$ for any $x\in\Omega_\varepsilon$ and $y\in\Omega^c$, we conclude that in the limit as $t\to 0$, (99) converges to 0. This proves (97) for $j=1$. For $j>1$, proceeding by induction, we conclude. Finally, using the coarea formula (42), we complete the proof of the statement as in the usual argument of [Savo 1998, Lemma 5.6]. □

Remark A.5. In the noncompact case, under the assumption of Theorem 7.3, the above lemma holds. In particular, on the one hand, the divergence theorem holds since ϕ has compact support. On the other hand, notice that the time derivative estimates (87) are enough to ensure that (99) converges to 0 as $t\to 0$, regardless of the compactness of the set of integration. The same is true for $j>1$, where higher-order time derivatives appear.

The next step is to apply the iterated Duhamel's principle (93) to I_ε, which now satisfies its assumptions, then, pass to the limit as $\varepsilon\to 0$. The computations are long but straightforward: we report here the result at order $t^{5/2}$.

Lemma A.6. *Under the same assumptions of Lemma A.3, let* $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$. *Then, as* $t \to 0$, *we have*

$$
I_\Omega\phi(t,0) = 2\mathcal{G}_{1-u}[\phi](t) + \frac{1}{\sqrt{\pi}} \int_0^t \mathcal{G}_{1-u}[N_\Omega\phi](\tau)(t-\tau)^{-1/2}\,d\tau \tag{100}
$$

$$
+ \frac{1}{2\pi} \int_0^t \int_0^\tau \mathcal{G}_{1-u}[N_\Omega^2\phi](\hat{\tau})((\tau-\hat{\tau})(t-\tau))^{-1/2}\,d\hat{\tau}\,d\tau
$$

$$
+ \frac{1}{4\pi^{3/2}} \int_0^t \int_0^\tau \int_0^{\hat{\tau}} \mathcal{G}_{1-u}[N_\Omega^3\phi](s)((\hat{\tau}-s)(\tau-\hat{\tau})(t-\tau))^{-1/2}\,ds\,d\hat{\tau}\,d\tau
$$

$$
+ \frac{1}{4\sqrt{\pi}} \int_0^t \int_{\partial\Omega} (1-u(\tau,\cdot))(4\Delta - N_\Omega^2)\phi\,d\sigma\,(t-\tau)^{1/2}\,d\tau
$$

$$
+ \frac{1}{4\sqrt{\pi}} \int_0^t \mathcal{G}_{1-u}[(6N_\Omega\Delta - N_\Omega^3 - 2\Delta N_\Omega)\phi](\tau)(t-\tau)^{1/2}\,d\tau + O(t^{5/2}),
$$

where $u(t,\cdot) = e^{t\Delta}\mathbb{1}_\Omega$ *and* $\mathcal{G}_u[\phi]$ *is the functional defined in* (60). *We recall that* N_Ω *is the operator defined in* (95).

   The expression (58) is a direct consequence of A.6. Moreover, we can apply it, when the base set is chosen to be Ω^c. Then, evaluating the difference between $I_\Omega\phi(t,0)$ and $I_{\Omega^c}\phi(t,0)$ we obtain the asymptotic equality (66), which is proved in the next lemma. We use the shorthands I, I^c for I_Ω and I_{Ω^c} respectively.

Lemma A.7. *Under the same assumptions of Lemma A.3, let* $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$. *Then, as* $t \to 0$, *we have*

$$
(I\phi - I^c\phi)(t,0) = 2\mathcal{G}_{1-2u}[\phi](t) + \frac{1}{2}\int_{\partial\Omega} N\phi\,d\sigma\,t
$$

$$
+ \frac{1}{2\pi} \int_0^t \int_0^\tau \mathcal{G}_{1-2u}[N^2\phi](\hat{\tau})((\tau-\hat{\tau})(t-\tau))^{-1/2}\,d\hat{\tau}\,d\tau
$$

$$
+ \frac{1}{4\sqrt{\pi}} \int_0^t \int_{\partial\Omega} (1-2u(\tau,\cdot))(4\Delta - N^2)\phi\,d\sigma\,(t-\tau)^{1/2}\,d\tau + O(t^2),
$$

where N *is the operator given by*

$$
N\phi = 2g(\nabla\phi, \nabla\delta) + \phi\Delta\delta \quad \text{for all } \phi \in C_c^\infty(\Omega_{-r_0}^{r_0}),
$$

with $\delta : M \to \mathbb{R}$ *the signed distance function from* $\partial\Omega$.

Proof. Firstly, we apply Lemma A.6 to $I\phi$: we obtain exactly the expression (100), with the operator $N_\Omega = N$. Secondly, for the outside contribution, recall that we have the following equality of smooth functions:

$$
1 - u^c(t,x) = 1 - e^{t\Delta}\mathbb{1}_{\Omega^c}(x) = e^{t\Delta}\mathbb{1}_\Omega(x) = u(t,x) \quad \text{for all } t > 0,\ x \in M.
$$

Therefore, when we apply Lemma A.6 to $I^c\phi$, we replace $1 - u^c(t,\cdot) = 1 - e^{t\Delta}\mathbb{1}_{\Omega^c}$ with the function $u(t,\cdot) = e^{t\Delta}\mathbb{1}_\Omega(\cdot)$. Moreover, the operator N_{Ω^c} defined in (95), for the set Ω^c, is equal to $-N$, since the

inward-pointing normal to Ω^c is $-\nabla\delta$. Therefore, writing the difference of the two contributions, and noticing that Ω and its complement share the boundary, we have

$$(I\phi - I^c\phi)(t, 0) = 2\mathcal{G}_{1-2u}[\phi](t) + \frac{1}{\sqrt{\pi}} \int_0^t \mathcal{G}_1[N\phi](\tau)(t-\tau)^{-1/2} d\tau$$

$$+ \frac{1}{2\pi} \int_0^t \int_0^\tau \mathcal{G}_{1-2u}[N^2\phi](\hat{\tau})((\tau-\hat{\tau})(t-\tau))^{-1/2} d\hat{\tau}\, d\tau$$

$$+ \frac{1}{4\pi^{3/2}} \int_0^t \int_0^\tau \int_0^{\hat{\tau}} \mathcal{G}_1[N^3\phi](s)((\hat{\tau}-s)(\tau-\hat{\tau})(t-\tau))^{-1/2} ds\, d\hat{\tau}\, d\tau \qquad (101)$$

$$+ \frac{1}{4\sqrt{\pi}} \int_0^t \int_{\partial\Omega} (1 - 2u(\tau, \cdot))(4\Delta - N^2)\phi\, d\sigma (t-\tau)^{1/2} d\tau$$

$$+ \frac{1}{4\sqrt{\pi}} \int_0^t \mathcal{G}_1[(6N\Delta - N^3 - 2\Delta N)\phi](\tau)(t-\tau)^{1/2} d\tau + O(t^{5/2}). \quad (102)$$

To conclude, it is enough to notice that the functional $\mathcal{G}_1$ can be explicitly computed:

$$\mathcal{G}_1[\phi](t) = \frac{1}{\sqrt{\pi}} \int_{\partial\Omega} \phi\, d\sigma\, t^{1/2} \quad \text{for all } \phi \in C_c^\infty(\Omega_{-r_0}^{r_0}).$$

Thus, the terms in (101) and (102) are remainder of order $O(t^2)$. □

Applying Lemma A.6 to the sum of $I_\Omega\phi(t, 0)$ and $I_{\Omega^c}\phi(t, 0)$ instead, we obtain (77). The proof of this result is not provided here, as it is similar to the proof of Lemma A.7.

Lemma A.8. *Under the same assumptions of Lemma A.3, let $\phi \in C_c^\infty(\Omega_{-r_0}^{r_0})$. Then, as $t \to 0$, we have*

$$(I\phi + I^c\phi)(t, 0) = \frac{2}{\sqrt{\pi}} \int_{\partial\Omega} \phi\, d\sigma\, t^{1/2} + \frac{1}{\sqrt{\pi}} \int_0^t \mathcal{G}_{1-2u}[N\phi](\tau)(t-\tau)^{-1/2} d\tau$$

$$+ \frac{1}{6\sqrt{\pi}} \int_{\partial\Omega} (4\Delta + N^2)\phi\, d\sigma\, t^{3/2}$$

$$+ \frac{1}{4\pi^{3/2}} \int_0^t \int_0^\tau \int_0^{\hat{\tau}} \mathcal{G}_{1-2u}[N^3\phi](s)((\hat{\tau}-s)(\tau-\hat{\tau})(t-\tau))^{-1/2} ds\, d\hat{\tau}\, d\tau$$

$$+ \frac{1}{4\sqrt{\pi}} \int_0^t \mathcal{G}_{1-2u}[(6N\Delta - N^3 - 2\Delta N)\phi](\tau)(t-\tau)^{1/2} d\tau + O(t^{5/2}).$$

Acknowledgments

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