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Fabrice Baudoin · Nicola Garofalo

Curvature-dimension inequalities and Ricci lower bounds for sub-Riemannian manifolds with transverse symmetries

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Abstract. Let $\mathbb{M}$ be a smooth connected manifold endowed with a smooth measure μ and a smooth locally subelliptic diffusion operator L satisfying $L1 = 0$ and symmetric with respect to μ. Associated with L one has the *carré du champ* Γ and a canonical distance d, with respect to which we suppose that $(\mathbb{M}, d)$ be complete. We assume that $\mathbb{M}$ is also equipped with another first-order differential bilinear form Γ^Z and we assume that Γ and Γ^Z satisfy Hypotheses 1.1, 1.2, and 1.4 below. With these forms we introduce in (1.12) a generalization of the curvature-dimension inequality from Riemannian geometry (see Definition 1.3). In our main results we prove that, using solely (1.12), one can develop a theory which parallels the celebrated works of Yau and Li–Yau on complete manifolds with Ricci curvature bounded from below. We also obtain an analogue of the Bonnet–Myers theorem. In Section 2 we construct large classes of sub-Riemannian manifolds with transverse symmetries which satisfy the generalized curvature-dimension inequality (1.12). Such classes include all Sasakian manifolds whose horizontal Webster–Tanaka–Ricci curvature is bounded from below, all Carnot groups with step two, and wide subclasses of principal bundles over Riemannian manifolds whose Ricci curvature is bounded from below.

Keywords. Sub-Riemannian geometry, curvature dimension inequalities

1. Introduction

In the present paper we introduce a generalization of the curvature-dimension inequality from Riemannian geometry which, as we show, is appropriate for some sub-Riemannian geometries. The central objective of our work is developing a program which, through a systematic use of the curvature-dimension inequality, connects the geometry of the ambient manifold, expressed in terms of lower bounds on a generalization of the Ricci tensor, to global properties of solutions of a certain canonical second-order diffusion (non-elliptic) partial differential operator, a sub-Laplacian, and of its associated heat semigroup.

In Riemannian geometry the Ricci tensor plays a fundamental role. Its connection with the Laplace–Beltrami operator is provided by the celebrated identity of Bochner

F. Baudoin: Department of Mathematics, Purdue University, West Lafayette, IN 47907, USA; e-mail: fbaudoin@purdue.edu

N. Garofalo: Dipartimento d'Ingegneria Civile e Ambientale (DICEA), Università di Padova, via Trieste 63, 35131 Padova, Italy; e-mail: nicola.garofalo@unipd.it

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which states that if $\mathbb{M}$ is an n-dimensional Riemannian manifold with Laplacian Δ, then for any $f \in C^\infty(\mathbb{M})$ one has

$$\Delta(|\nabla f|^2) = 2\|\nabla^2 f\|^2 + 2\langle \nabla f, \nabla(\Delta f)\rangle + 2\,\mathrm{Ric}(\nabla f, \nabla f). \tag{1.1}$$

Consider the following differential forms on functions $f, g \in C^\infty(\mathbb{M})$:

$$\Gamma(f,g) = \frac{1}{2}(\Delta(fg) - f\Delta g - g\Delta f) = (\nabla f, \nabla g),$$
$$\Gamma_2(f,g) = \frac{1}{2}[\Delta\Gamma(f,g) - \Gamma(f,\Delta g) - \Gamma(g,\Delta f)].$$

When $f = g$, we simply write $\Gamma(f) = \Gamma(f,f)$, $\Gamma_2(f) = \Gamma_2(f,f)$. The functional calculus of these forms was introduced and developed in [8]. As an application of Bochner's formula, which in terms of these functionals can be reformulated as

$$\Delta\Gamma(f) = 2\|\nabla^2 f\|^2 + 2\Gamma(f,\Delta f) + 2\,\mathrm{Ric}(\nabla f, \nabla f),$$

one obtains

$$\Gamma_2(f) = \|\nabla^2 f\|_2^2 + \mathrm{Ric}(\nabla f, \nabla f).$$

Using the Cauchy–Schwarz inequality, which gives $\|\nabla^2 f\|_2^2 \ge \frac{1}{n}(\Delta f)^2$, we thus see that the assumption that the Riemannian Ricci tensor on $\mathbb{M}$ is bounded from below by $\rho_1 \in \mathbb{R}$ implies the so-called *curvature-dimension inequality* $\mathrm{CD}(\rho_1, n)$:

$$\Gamma_2(f) \ge \frac{1}{n}(\Delta f)^2 + \rho_1\Gamma(f), \qquad f \in C^\infty(\mathbb{M}). \tag{1.2}$$

In the hands of D. Bakry, M. Ledoux and their co-authors the inequality (1.2) has proven a powerful tool in combination with a systematic use of fine properties of the heat semigroup. Among other things, these authors have succeeded in re-deriving, from a purely analytical perspective, several of the well-known fundamental results which, in Riemannian geometry, are obtained under the assumption that the Ricci curvature is bounded from below (see for instance [5], [9], [36], [39]). It is remarkable that the curvature dimension inequality (1.2) perfectly captures the notion of Ricci curvature lower bound. It was in fact proved by Bakry [5, Proposition 6.2] that *on an n-dimensional Riemannian manifold* $\mathbb{M}$ *the inequality* $\mathrm{CD}(\rho_1, n)$ *implies* $\mathrm{Ric} \ge \rho_1$. In conclusion, $\mathrm{Ric} \ge \rho_1 \Leftrightarrow \mathrm{CD}(\rho_1, n)$.

Inspired by the ideas contained in the above mentioned works, in the present paper we introduce a generalization of the curvature-dimension inequality (1.2) which can be successfully used in sub-Riemannian geometry. At this point, we feel it is important to say a few words concerning the organization of the paper. The essential contribution of the present work is based on ideas and tools which are purely analytical in nature: as mentioned above, we systematically use the heat semigroup to derive new results in sub-Riemannian geometry. On the other hand, an equally important aspect of the present work is the construction of examples from geometry: as the title indicates, the main class studied in this paper is that of sub-Riemannian manifolds with transverse symmetries. We show that this class is quite large, as it incorporates (but is not limited to) examples which are geometrically as diverse as CR manifolds with vanishing Tanaka–Webster torsion (Sasakian manifolds), graded nilpotent Lie groups of step two, and orthonormal frame bundles. To facilitate the perusal of this paper by an audience of analysts we have strived as much as possible to separate the presentation of the analytical part of our work from the geometrical discussion of the examples. With this objective in mind, we have chosen to present the analytical part of the paper in an axiomatic way. By this we mean that all that is asked of a reader less inclined toward geometry is to accept a set of four "abstract" assumptions, which are listed as Hypotheses 1.1, 1.2, Definition 1.3 and Hypothesis 1.4 below. The geometrical relevance, and the motivation, of such assumptions is unraveled in Section 2, where we discuss the examples and we develop the geometric setup.

This being said, we now introduce the relevant setting. We consider a smooth, connected manifold $\mathbb{M}$ endowed with a smooth measure μ and a smooth second-order diffusion operator L with real coefficients satisfying $L1 = 0$, and which is symmetric with respect to μ and non-positive. By this we mean that

$$\int_{\mathbb{M}} fLg\, d\mu = \int_{\mathbb{M}} gLf\, d\mu, \quad \int_{\mathbb{M}} fLf\, d\mu \le 0, \tag{1.3}$$

for all $f, g \in C_0^\infty(\mathbb{M})$. We make the technical assumption that L is locally subelliptic in the sense of [25]. We associate with L the following symmetric, first-order, differential bilinear form:

$$\Gamma(f,g) = \frac{1}{2}(L(fg) - fLg - gLf), \qquad f, g \in C^\infty(\mathbb{M}). \tag{1.4}$$

The expression $\Gamma(f) = \Gamma(f,f)$ is known as the *carré du champ*. Furthermore, using the results in [44], locally in the neighborhood of every point $x \in \mathbb{M}$ we can write

$$L = -\sum_{i=1}^m X_i^* X_i, \tag{1.5}$$

where the vector fields X_i are Lipschitz continuous (such a representation is not unique, but this fact is of no consequence for us). Therefore, for any $x \in \mathbb{M}$ there exists an open neighborhood U_x such that for any $f \in C^\infty(\mathbb{M})$ we have, in U_x,

$$\Gamma(f) = \sum_{i=1}^m (X_i f)^2. \tag{1.6}$$

This shows that $\Gamma(f) \ge 0$ and it actually only involves differentiation of order one.

Furthermore, as is clear from (1.4), the value of $\Gamma(f)(x)$ does not depend on the particular representation (1.5) of L.

With the operator L we can also associate a canonical distance:

$$d(x,y) = \sup\{|f(x) - f(y)| \mid f \in C^\infty(\mathbb{M}),\ \|\Gamma(f)\|_\infty \le 1\}, \qquad x, y \in \mathbb{M}, \tag{1.7}$$

where for a function g on $\mathbb{M}$ we have let $\|g\|_\infty = \operatorname{ess\,sup}_{\mathbb{M}} |g|$. A tangent vector $v \in T_x\mathbb{M}$ is said to be *subunit* for L at x if $v = \sum_{i=1}^m a_i X_i(x)$ with $\sum_{i=1}^m a_i^2 \le 1$ (see [25]). It turns out that the notion of subunit vector for L at x does not depend on the local representation (1.5) of L. A Lipschitz path $\gamma : [0,T] \to \mathbb{M}$ is called *subunit* for L if $\gamma'(t)$ is subunit for

L at $\gamma(t)$ for a.e. $t \in [0, T]$. We then define the *subunit length* of γ as $\ell_s(\gamma) = T$. Given $x, y \in \mathbb{M}$, we set

$$S(x, y) = \{\gamma : [0, T] \to \mathbb{M} \mid \gamma \text{ is subunit for } L,\ \gamma(0) = x,\ \gamma(T) = y\}.$$

In this paper we assume that

$$S(x, y) \neq \emptyset \quad \text{ for all } x, y \in \mathbb{M}.$$

Under this assumption it is easy to verify that

$$d_s(x, y) = \inf\{\ell_s(\gamma) \mid \gamma \in S(x, y)\} \tag{1.8}$$

defines a true distance on $\mathbb{M}$. Furthermore, thanks to [17, Lemma 5.43] we know that

$$d(x, y) = d_s(x, y), \quad x, y \in \mathbb{M},$$

hence we can work indifferently with either one of the distances d or d_s. Throughout this paper we assume that the metric space $(\mathbb{M}, d)$ be complete.

We also suppose that on $\mathbb{M}$ a symmetric, first-order differential bilinear form $\Gamma^Z : C^\infty(\mathbb{M}) \times C^\infty(\mathbb{M}) \to \mathbb{R}$ is given. Hereafter, the term “symmetric first-order differential form” means that $\Gamma^Z(f, g) = \Gamma^Z(g, f)$ and

$$\Gamma^Z(fg, h) = f\Gamma^Z(g, h) + g\Gamma^Z(f, h). \tag{1.9}$$

In particular, we have $\Gamma^Z(1) = 0$, where, as for Γ, we have set $\Gamma^Z(f) = \Gamma^Z(f, f)$. We assume that $\Gamma^Z(f) \geq 0$.

We will work with four general assumptions. The first three will be listed as Hypotheses 1.1, 1.2 and Definition 1.3, the fourth one will be introduced in Hypothesis 1.4 below.

Hypothesis 1.1. *There exists an increasing sequence $h_k \in C_0^\infty(\mathbb{M})$ such that $h_k \nearrow 1$ on $\mathbb{M}$, and*

$$\|\Gamma(h_k)\|_\infty + \|\Gamma^Z(h_k)\|_\infty \to 0 \quad \text{as } k \to \infty.$$

We will also assume that the following commutation relation is satisfied.

Hypothesis 1.2. *For any $f \in C^\infty(\mathbb{M})$ one has*

$$\Gamma(f, \Gamma^Z(f)) = \Gamma^Z(f, \Gamma(f)).$$

Let us notice explicitly that when $\mathbb{M}$ is a Riemannian manifold and μ is the Riemannian volume on $\mathbb{M}$, and $L = \Delta$, then $d(x, y)$ in (1.7) is equal to the Riemannian distance on $\mathbb{M}$. In this situation, if we take $\Gamma^Z \equiv 0$, then Hypotheses 1.1 and 1.2 are fulfilled. In fact, Hypothesis 1.2 is trivially satisfied, whereas Hypothesis 1.1 is equivalent to assuming that $(\mathbb{M}, d)$ is a complete metric space, which we are assuming anyhow. More generally, in all the examples of Section 2, Hypothesis 1.1 is equivalent to assuming that $(\mathbb{M}, d)$ is a complete metric space (the reason is that in those examples $\Gamma + \Gamma^Z$ is the *carré du champ* of the Laplace–Beltrami operator of a Riemannian structure whose completeness is equivalent to the completeness of $(\mathbb{M}, d)$). On the other hand, Hypothesis 1.2 is also satisfied as a consequence of the assumptions about the existence of transverse symmetries that we make.

Before we proceed, we pause to stress that, in the generality in which we work, the bilinear differential form Γ^Z, unlike Γ, is not a priori canonical. Whereas Γ is determined once L is assigned, the form Γ^Z in general is not intrinsically associated with L. However, in the geometric examples described in this paper (see the discussion below and Section 2) the choice of Γ^Z will be natural and even canonical, up to a constant. This is the case, for instance, of the important example of CR Sasakian manifolds. The reader should think of Γ^Z as an orthogonal complement of Γ: the bilinear form Γ represents the square of the length of the gradient in the horizontal directions, whereas Γ^Z represents the square of the length of the gradient along the vertical directions.

Given the sub-Laplacian L and the first-order bilinear forms Γ and Γ^Z on $\mathbb{M}$, we now introduce the following second-order differential forms:

$$\Gamma_2(f,g) = \tfrac{1}{2}[L\Gamma(f,g) - \Gamma(f,Lg) - \Gamma(g,Lf)], \tag{1.10}$$

$$\Gamma_2^Z(f,g) = \tfrac{1}{2}[L\Gamma^Z(f,g) - \Gamma^Z(f,Lg) - \Gamma^Z(g,Lf)]. \tag{1.11}$$

Observe that if $\Gamma^Z \equiv 0$, then $\Gamma_2^Z \equiv 0$ as well. Just as for Γ and Γ^Z, we will write $\Gamma_2(f) = \Gamma_2(f,f)$ and $\Gamma_2^Z(f) = \Gamma_2^Z(f,f)$.

We are ready to introduce the central character of our paper, a generalization of the above mentioned curvature-dimension inequality (1.2).

Definition 1.3. We shall say that $\mathbb{M}$ satisfies the *generalized curvature-dimension inequality* $\mathrm{CD}(\rho_1,\rho_2,\kappa,d)$ with respect to L and Γ^Z if there exist constants $\rho_1 \in \mathbb{R}$, $\rho_2 > 0$, $\kappa \ge 0$, and $0 < d \le \infty$ such that

$$\Gamma_2(f) + \nu\Gamma_2^Z(f) \ge \frac{1}{d}(Lf)^2 + \left(\rho_1 - \frac{\kappa}{\nu}\right)\Gamma(f) + \rho_2\Gamma^Z(f) \tag{1.12}$$

for every $f \in C^\infty(\mathbb{M})$ and every $\nu > 0$.

It is worth observing explicitly that if in Definition 1.3 we choose $L = \Delta$, $\Gamma^Z \equiv 0$, $d = n = \dim(\mathbb{M})$, and $\kappa = 0$, we obtain the Riemannian curvature-dimension inequality $\mathrm{CD}(\rho_1, n)$ of (1.2). Thus, the case of Riemannian manifolds is trivially encompassed by Definition 1.3. We also remark that, changing Γ^Z to $a\Gamma^Z$, where $a > 0$, changes the inequality $\mathrm{CD}(\rho_1,\rho_2,\kappa,d)$ to $\mathrm{CD}(\rho_1,a\rho_2,a\kappa,d)$. We express this fact by saying that the quantity κ/ρ_2 is intrinsic. Hereafter, when we say that $\mathbb{M}$ satisfies the curvature dimension inequality $\mathrm{CD}(\rho_1,\rho_2,\kappa,d)$ (with respect to L and Γ^Z), we will routinely avoid repeating at each occurrence the sentence "for some $\rho_2 > 0$, $\kappa \ge 0$ and $d > 0$". Instead, we will explicitly mention whether $\rho_1 = 0$, or > 0, or simply $\rho_1 \in \mathbb{R}$. The reason for this is that the parameter ρ_1 in (1.12) has a special relevance since, in the geometric examples of Section 2, it represents the lower bound on a sub-Riemannian generalization of the Ricci tensor. Thus, $\rho_1 = 0$ is, in our framework, the counterpart of the Riemannian $\mathrm{Ric} \ge 0$, whereas when $\rho_1 > 0$ (resp. < 0), we are dealing with the counterpart of the case $\mathrm{Ric} > 0$ (resp. Ric bounded from below by a negative constant).

Since, as we have stressed above, we wish to present our results in an axiomatic way, we will also need the following assumption which is necessary to rigorously justify computations on functionals of the heat semigroup. Hereafter, we denote by $P_t = e^{tL}$ the semigroup generated by the diffusion operator L (see the discussion below and Section 4).

Hypothesis 1.4. *The semigroup P_t is stochastically complete, that is, for $t \geq 0$, $P_t 1 = 1$ and for every $f \in C_0^\infty(\mathbb{M})$ and $T \geq 0$, one has*

$$\sup_{t \in [0,T]} \|\Gamma(P_t f)\|_\infty + \|\Gamma^Z(P_t f)\|_\infty < \infty.$$

In the Riemannian setting ($L = \Delta$ and $\Gamma^Z \equiv 0$), Hypothesis 1.4 is satisfied if one assumes the lower bound Ricci $\geq \rho$ for some $\rho \in \mathbb{R}$. This can be derived from Yau [55] and Bakry [4]. It thus follows that, in the Riemannian case, Hypothesis 1.4 is not needed since it can be derived as a consequence of the curvature-dimension inequality $\mathrm{CD}(\rho_1, n)$ of (1.2). In this paper we will prove that, more generally, this situation occurs in the sub-Riemannian setting of our work. As a consequence of the results in Section 2, in Theorem 4.3 we prove that in every sub-Riemannian manifold with transverse symmetries of Yang–Mills type (for the relevant definitions see Sections 2 and 3), Hypothesis 1.4 is not needed since it follows (in a non-trivial way) from the generalized curvature-dimension inequality $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ of Definition 1.3.

In this connection it is worth observing that, even in the abstract framework of the present work, if we assume that $\Gamma^Z = 0$, then Hypothesis 1.4 becomes redundant since it can actually be obtained as a consequence of $\mathrm{CD}(\rho_1, n)$. This can be seen from the results in [3, Chapter 5]. Whether it is possible to generalize this fact to the genuinely non-Riemannian situation of $\Gamma^Z \neq 0$ must be left to a future study. Concerning our axiomatic presentation, we finally mention that, had we chosen to do so, we could have developed our results in an even more abstract setting, as Bakry and Ledoux often do in their work. We could have worked with abstract Markov diffusion generators on measure spaces and replaced Hypotheses 1.1 and 1.4 with the existence of a nice algebra of functions which is dense in the domain of L (see [3, Definition 2.4.2] for the precise properties that should be satisfied by this algebra when $\Gamma^Z = 0$). However, assuming the existence of such an algebra is a strong assumption that may be difficult to verify in some concrete situations.

The above discussion prompts us to underline the distinctive aspect of the theory developed in the present paper: *for the class of complete sub-Riemannian manifolds with transverse symmetries of Yang–Mills type that we study in Section* 3, *all our results are solely deduced from the curvature-dimension inequality* $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ *of* (1.12).

To introduce our results we recall that in their celebrated work [38] Li and Yau, generalizing to the heat equation some fundamental works of Yau (see for instance [54]), obtained various a priori gradient bounds for positive solutions of the heat equation on a complete n-dimensional Riemannian manifold $\mathbb{M}$. When Ric ≥ 0, the Li–Yau inequality states that if $u > 0$ is a solution of $\Delta u - u_t = 0$ in $\mathbb{M} \times (0, \infty)$, then

$$\frac{|\nabla u|^2}{u^2} - \frac{u_t}{u} \leq \frac{n}{2t}. \tag{1.13}$$

Notice that in the flat $\mathbb{R}^n$ the Gauss–Weierstrass kernel $u(x,t)=(4\pi t)^{-n/2}\exp(-|x|^2/4t)$ satisfies (1.13) with equality. The inequality (1.13) was the central tool for obtaining a scale invariant Harnack inequality for the heat equation and optimal off-diagonal upper bounds for the heat kernel on $\mathbb{M}$ (see [38, Corollary 3.1 and Theorem 4.1]). The proof of (1.13) hinges crucially on Bochner's identity (1.1), and on the Laplacian comparison theorem which, for a manifold with Ric ≥ 0, states that, given a base point $x_0 \in \mathbb{M}$, and denoting by $\rho(x)$ the Riemannian distance from x to x_0, we have

$$\Delta\rho(x) \leq \frac{n-1}{\rho(x)} \tag{1.14}$$

outside of the cut-locus of x_0 (and globally in $\mathcal{D}'(\mathbb{M})$). As is well-known (see for instance [19]), the proof of (1.14) exploits the theory of Jacobi fields. In sub-Riemannian geometry the exponential map is not a local diffeomorphism. As a consequence of this obstacle, a general sub-Riemannian comparison theorem such as (1.14) presently represents *terra incognita*.

The main thrust of the present work is that, despite such obstructions, we have succeeded in establishing a sub-Riemannian generalization of the Li–Yau inequalities. In our approach, we completely avoid those tools from geometry that appear typically Riemannian, and instead base our analysis on a systematic use of some entropic inequalities for the heat semigroup that are inspired by [7], [10], [12], and which, as we have stressed above, in the geometric framework of this paper we solely derive from our generalized curvature-dimension inequality CD(ρ_1,ρ_2,κ,d) of (1.12).

More precisely, let $P_t = e^{tL}$ denote the heat semigroup on $\mathbb{M}$ associated with the operator L. It is well-known that P_t is sub-Markovian, i.e., $P_t 1 \leq 1$, and it has a positive and symmetric kernel $p(x,y,t)$. If $f \in C_0^\infty(\mathbb{M})$, the function

$$u(x,t) = P_t f(x) = \int_{\mathbb{M}} p(x,y,t) f(y)\, d\mu(y)$$

solves the Cauchy problem

$$\begin{cases} \frac{\partial u}{\partial t} - Lu = 0 & \text{in } \mathbb{M}\times(0,\infty), \\ u(x,0) = f(x), & x \in \mathbb{M}. \end{cases}$$

For fixed $x \in \mathbb{M}$ and $T > 0$ we introduce the functionals

$$\Phi_1(t) = P_t\big((P_{T-t}f)\Gamma(\ln P_{T-t}f)\big)(x),$$
$$\Phi_2(t) = P_t\big((P_{T-t}f)\Gamma^Z(\ln P_{T-t}f)\big)(x),$$

which are defined for $0 \leq t < T$. The fundamental observation is that, in our framework, the inequality CD(ρ_1,ρ_2,κ,d) of (1.12) leads to the differential inequality

$$\left(-\frac{b'}{2\rho_2}\Phi_1 + b\Phi_2\right)' \geq -\frac{2b'\gamma}{d\rho_2} LP_T f + \frac{b'\gamma^2}{d\rho_2} P_T f, \tag{1.15}$$

where b is any smooth, positive and decreasing function on the time interval $[0,T]$ and

$$\gamma = \frac{d}{4}\left(\frac{b''}{b'} + \frac{\kappa}{\rho_2}\frac{b'}{b} + 2\rho_1\right).$$

Depending on the value of ρ_1, a good choice of the function b leads to a generalized Li–Yau type inequality (see Theorem 6.1 below). In the special case $\rho_1 = 0$ (i.e., our $\mathrm{Ric} \geq 0$), the latter becomes

$$\Gamma(\ln P_t f) + \frac{2\rho_2}{3} t \Gamma^Z(\ln P_t f) \leq \left(1 + \frac{3\kappa}{2\rho_2}\right) \frac{L P_t f}{P_t f} + \frac{d\left(1 + \frac{3\kappa}{2\rho_2}\right)^2}{2t} \tag{1.16}$$

for every sufficiently nice function $f \geq 0$ on $\mathbb{M}$. In the Riemannian case, when $\Gamma^Z \equiv 0$ and $\kappa = 0$, (1.16) is precisely the Li–Yau inequality (1.13), except that our inequality holds for positive solutions of the heat equation of the type $u = P_t f$, i.e., they arise from an initial datum f, whereas in the original Li–Yau inequality (1.13) that limitation is not present.

It is worth emphasizing at this point that, even in the Riemannian case, our approach, based on a systematic use of the entropic inequality (1.15), provides a new and elementary proof of several fundamental results for complete manifolds with $\mathrm{Ric} \geq 0$. In this framework, in fact, besides the already mentioned Li–Yau gradient estimates, with the ensuing scale invariant Harnack inequality and the Liouville theorem of Yau [54], we also obtain an elementary proof of the fundamental monotonicity of Perelman's entropy for the heat equation [43], and of the volume doubling property on Riemannian manifolds (for the statement of this classical result see for instance [18]). For these aspects we refer the reader to the recent note [14]. The reader more oriented toward analysis and pdes might in fact find it somewhat surprising that we can develop the whole local regularity theory for solutions of the relevant heat equation starting from a global object such as the heat semigroup. By this we mean that, at the end of our process, we are able to replace the functions $P_t f$ in (1.16) with *any* positive solution u of the heat equation. This in a sense reverses the way one normally proceeds, starting from local solutions, and then moving from local to global.

We are now ready to provide a brief account of our main results.

(1) *Li–Yau type inequalities* (Theorem 6.1): Assume Hypotheses 1.1, 1.2 and 1.4 hold. If $\mathbb{M}$ satisfies $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ of (1.12) with $\rho_1 \in \mathbb{R}$, then for any $f \in C_0^\infty(\mathbb{M})$, $f \geq 0$, $f \not\equiv 0$, and $t > 0$,

$$\begin{aligned} &\Gamma(\ln P_t f) + \frac{2\rho_2}{3} t \Gamma^Z(\ln P_t f) \\ &\leq \left(1 + \frac{3\kappa}{2\rho_2} - \frac{2\rho_1}{3} t\right) \frac{L P_t f}{P_t f} + \frac{d\rho_1^2}{6} t - \frac{d\rho_1}{2}\left(1 + \frac{3\kappa}{2\rho_2}\right) + \frac{d\left(1 + \frac{3\kappa}{2\rho_2}\right)^2}{2t}. \end{aligned}$$

(2) *Scale-invariant parabolic Harnack inequality* (Theorem 7.1): Assume Hypotheses 1.1, 1.2 and 1.4 hold. If $\mathbb{M}$ satisfies $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ with $\rho_1 \geq 0$, then for every $(x, s), (y, t) \in \mathbb{M} \times (0, \infty)$ with $s < t$ one has

$$u(x, s) \leq u(y, t) \left(\frac{t}{s}\right)^{D/2} \exp\left(\frac{D}{d} \frac{d(x, y)^2}{4(t - s)}\right)$$

for $u(x, t) = P_t f(x)$ with $f \in C^\infty(\mathbb{M})$ such that $f \geq 0$ and bounded. The number $D > 0$, which solely depends on ρ_2, κ and d, is defined in (6.2) below.

(3) *Off-diagonal Gaussian upper bounds* (Theorem 8.1): Assume Hypotheses 1.1, 1.2 and 1.4 hold. If $\mathbb{M}$ satisfies $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ with $\rho_1 \geq 0$, then for all $0 < \varepsilon < 1$ there exists a constant $C(\rho_2, \kappa, d, \varepsilon) > 0$, which tends to ∞ as $\varepsilon \to 0^+$, such that for every $x, y \in \mathbb{M}$ and $t > 0$ one has

$$p(x, y, t) \leq \frac{C(\rho_2, \kappa, d, \varepsilon)}{\mu(B(x, \sqrt{t}))^{1/2} \mu(B(y, \sqrt{t}))^{1/2}} \exp\left(-\frac{d(x, y)^2}{(4+\varepsilon)t}\right).$$

(4) *Liouville type theorem* (Theorem 9.2): Assume Hypotheses 1.1, 1.2 and 1.4 hold. If $\mathbb{M}$ satisfies $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ with $\rho_1 \geq 0$, then there exists no entire bounded solution of $Lf = 0$.

(5) *Bonnet–Myers type theorem* (Theorem 10.1): Assume Hypotheses 1.1, 1.2 and 1.4 hold, and suppose that $\mathbb{M}$ satisfies $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ with $\rho_1 > 0$. Then the metric space $(\mathbb{M}, d)$ is compact in the metric topology, and

$$\operatorname{diam} \mathbb{M} \leq 2\sqrt{3}\pi \sqrt{\frac{\kappa + \rho_2}{\rho_1 \rho_2}\left(1 + \frac{3\kappa}{2\rho_2}\right) d}.$$

Concerning the Gaussian upper bound in (3), we mention that a similar bound was obtained for sub-Laplacians on Lie groups [53]. Our approach is totally different since it does not use the uniform doubling condition on the volume of the metric balls, which is a key assumption in [53]. We should also mention that in the sequel paper [13] we have in fact established a uniform global doubling condition under non-negative lower bound on the sub-Riemannian Ricci tensor ($\rho_1 \geq 0$).

Concerning the sub-Riemannian Bonnet–Myers theorem in (5), we emphasize that, similarly to the Laplacian comparison theorem (1.14), the proof of its classical Riemannian predecessor is based on the theory of Jacobi fields. Our proof of Theorem 10.1 is, instead, purely analytical and exploits in a subtle way some sharp entropic inequalities which, in the case $\rho_1 > 0$, we are able to derive from the inequality $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$.

Having presented the main results of the paper, we now turn to the fundamental question of examples. This aspect is dealt with in Section 2, which is devoted to constructing large classes of sub-Riemannian manifolds to which our general results apply. We begin with a discussion in Section 2.2 of a class of Lie groups which carry a natural CR structure, and which, in our framework, are the 3-dimensional sub-Riemannian CR Sasakian model spaces with constant curvature (see Hughen [33] for a precise meaning of the notion of model spaces). Entropic inequalities on such model spaces were studied in [7], and these inequalities constituted a first motivation for our theory.

Given a $\rho_1 \in \mathbb{R}$ we consider a Lie group $\mathbb{G}(\rho_1)$ whose Lie algebra $\mathfrak{g}$ admits a basis of generators X, Y, Z satisfying the commutation relations

$$[X, Y] = Z, \qquad [X, Z] = -\rho_1 Y, \qquad [Y, Z] = \rho_1 X.$$

The group $\mathbb{G}(\rho_1)$ can be endowed with a natural CR structure θ with respect to which the Reeb vector field is given by $-Z$. A sub-Laplacian on $\mathbb{G}(\rho_1)$ with respect to that structure is thus given by $L = X^2 + Y^2$. The pseudo-hermitian Tanaka–Webster torsion of $\mathbb{G}(\rho_1)$

vanishes (see Definition 2.23 below), and thus $(\mathbb{G}(\rho_1), \theta)$ is a Sasakian manifold. In the smooth manifold $\mathbb{M} = \mathbb{G}(\rho_1)$ with sub-Laplacian L we introduce the differential forms Γ and Γ^Z defined by

$$\Gamma(f, g) = XfXg + YfYg, \quad \Gamma^Z(f, g) = ZfZg.$$

These forms satisfy Hypotheses 1.1 and 1.2. It is worth observing that since $-Z$ is the Reeb vector field of the CR structure θ, the above choice of Γ^Z is canonical. It is also worth remarking at this point that for the CR manifold $(\mathbb{G}(\rho_1), \theta)$ the Tanaka–Webster horizontal sectional curvature is constant and equals ρ_1. Having noted these facts, in Section 2.2 we prove the following proposition.

Proposition 1.5. *The sub-Laplacian L on the Lie group $\mathbb{G}(\rho_1)$ satisfies the generalized curvature-dimension inequality* $\mathrm{CD}(\rho_1, 1/2, 1, 2)$.

The relevance of the model space $\mathbb{G}(\rho_1)$ is illustrated by the Lie groups:

(i) $\mathbb{SU}(2)$;
(ii) the "flat" Heisenberg group $\mathbb{H}^1$;
(iii) $\mathbb{SL}(2, \mathbb{R})$.

In Section 2.2 we note that the Lie groups (i)–(iii) are special instances of the model CR manifold $\mathbb{G}(\rho_1)$ corresponding, respectively, to the cases $\rho_1 = 1$, $\rho_1 = 0$ and $\rho_1 = -1$.

After introducing these motivating examples, in Section 2.3 we turn our attention to the construction of a large class of C^∞ manifolds carrying a natural sub-Riemannian structure for which our generalized curvature-dimension inequality (1.12) holds. As a consequence, in these spaces all the above mentioned results (1)–(6) are valid as well. Let $\mathbb{M}$ be a smooth, connected manifold equipped with a bracket-generating distribution $\mathcal{H}$ of dimension d and a fiberwise inner product g on $\mathcal{H}$. The distribution $\mathcal{H}$ will be referred to as the set of *horizontal directions*.

We denote by $\mathfrak{iso}$ the finite-dimensional Lie algebra of all sub-Riemannian Killing vector fields on $\mathbb{M}$. It is readily seen that $Z \in \mathfrak{iso}$ if and only if:

(a) for every $x \in \mathbb{M}$ and any $u, v \in \mathcal{H}(x)$, $\mathcal{L}_Z g(u, v) = 0$;
(b) if $X \in \mathcal{H}$, then $[Z, X] \in \mathcal{H}$.

In (a) we have denoted by $\mathcal{L}_Z g$ the Lie derivative of g with respect to Z. Our main geometric assumption is the following:

Hypothesis 1.6. *There exists a Lie subalgebra $\mathcal{V} \subset \mathfrak{iso}$ such that for every $x \in \mathbb{M}$,*

$$T_x\mathbb{M} = \mathcal{H}(x) \oplus \mathcal{V}(x).$$

The subbundle of transverse symmetries will be referred to as the set of *vertical directions*. The dimension of $\mathcal{V}$ will be denoted by $\mathfrak{h}$.

The horizontal distribution $\mathcal{H}$ with its fiberwise inner product g plus the Lie algebra $\mathcal{V}$ are the essential data of the construction in Section 2.3. By this we mean that the relevant geometric objects we introduce, namely the sub-Laplacian, the canonical connection ∇ and the tensor $\mathcal{R}$, defined in Section 2.3, solely depend on $(\mathcal{H}, g)$ and $\mathcal{V}$, but not on the choice of the inner product on $\mathcal{V}$. As a consequence, in those situations in which the choice of $\mathcal{V}$ is canonical, our analysis will depend only on the choice of $(\mathcal{H}, g)$. This is the case, for instance, in the basic example of Sasakian manifolds.

Our ultimate objective in Section 2.3 is proving that the smooth manifold $\mathbb{M}$, with a given sub-Riemannian geometry $(\mathcal{H}, g)$ and a vertical distribution of transverse symmetries $\mathcal{V}$, satisfies a generalized curvature-dimension inequality (1.12) as soon as some intrinsic geometric conditions are satisfied. To achieve this, we find it expedient to introduce in Section 2.3.1 a canonical connection ∇. By means of that connection we define in Definition 2.15 a generalization of the Riemannian Ricci tensor, which we denote by $\mathcal{R}$. In Theorem 2.18 we prove two Bochner identities which intertwine the tensor $\mathcal{R}$ with the forms Γ and Γ^Z. With the Bochner identities in hand, in Theorem 2.19 we finally show that, under the geometric assumptions of (2.26), the manifold $\mathbb{M}$ satisfies the generalized curvature-dimension inequality $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$. In Proposition 2.20 we prove that, remarkably, the generalized curvature-dimension inequality implies the geometric bounds (2.26), and therefore: *on any sub-Riemannian manifold with transverse symmetries we have*: $\mathrm{CD}(\rho_1, \rho_2, \kappa, d) \Leftrightarrow$ (2.26) *holds*.

The remaining part of Section 2 is devoted to presenting some basic examples of manifolds which fall within the geometric framework of Section 2.3. In Section 2.4 we prove that all Carnot groups of step two satisfy the curvature-dimension inequality $\mathrm{CD}(0, \rho_2, \kappa, d)$ for appropriate values of ρ_2 and κ (Proposition 2.21). Here, d is the dimension of the bracket-generating layer of their Lie algebra. This result shows, in particular, that in our framework *all* Carnot groups of step two are sub-Riemannian manifolds of non-negative Ricci tensor, since $\rho_1 = 0$. In Section 2.5 we analyze another important class of manifolds which falls within the scope of our work, namely Sasakian manifolds endowed with their CR sub-Laplacian. These are CR manifolds of real hypersurface type for which the Tanaka–Webster pseudo-hermitian torsion vanishes in an appropriate sense. Concerning Sasakian manifolds we prove the following basic result.

Theorem 1.7. *Let* $(\mathbb{M}, \theta)$ *be a complete* CR *manifold with real dimension* $2n + 1$ *and vanishing Tanaka–Webster torsion, i.e., a Sasakian manifold. If for every* $x \in \mathbb{M}$ *the Tanaka–Webster Ricci tensor satisfies the bound*

$$\mathrm{Ric}_x(v, v) \ \geq \rho_1 |v|^2$$

for every horizontal vector $v \in \mathcal{H}_x$*, then for the* CR *sub-Laplacian of* $\mathbb{M}$ *the curvature-dimension inequality* $\mathrm{CD}(\rho_1, d/4, 1, d)$ *holds with* $d = 2n$ *and Hypotheses* 1.1*,* 1.2 *and* 1.4 *are satisfied.*

Thanks to this result, the above listed results (1)–(5) are valid for *all* Sasakian manifolds.

We close this introduction by mentioning that, for general metric measure spaces, a different notion of lower bounds on the Ricci tensor based on the theory of optimal transport has been recently proposed independently by Sturm [51], [52] and by Lott–Villani [40] (see also Ollivier [42]). However, as pointed out by Juillet [34], the remarkable theory developed in those papers does not appear to be suited for sub-Riemannian manifolds. For instance, in that theory the flat Heisenberg group $\mathbb{H}^1$ has curvature $= -\infty$.

Agrachev and Lee [2] have used a notion of Ricci tensor, denoted by $\mathfrak{Ric}$, which was introduced by Agrachev [1]. They study three-dimensional contact manifolds and, under the assumption that the manifold is Sasakian, they prove that a lower bound on $\mathfrak{Ric}$ implies the so-called measure-contraction property. In particular, when $\mathfrak{Ric} \geq 0$, the manifold $\mathbb{M}$ satisfies a global volume growth condition similar to the Riemannian Bishop–Gromov theorem. An analysis shows that, interestingly, our notion of Ricci tensor coincides, up to a scaling factor, with theirs.

We also mention that for three-dimensional contact manifolds, some sub-Riemannian geometric invariants were computed by Hughen in his unpublished Ph.D. dissertation [33]. In particular, with his notation, the CR Sasakian structure corresponds to the case $a_1^2 + a_2^2 = 0$ and, up to a scaling factor, his K is the Tanaka–Webster Ricci curvature. In this connection, the Bonnet–Myers type theorem obtained by Hughen [33, Proposition 3.5] is the exact analogue (with a better constant) of our Theorem 10.1, applied to the case of three-dimensional Sasakian manifolds. Let us finally mention that a Bonnet–Myers type theorem on general three-dimensional CR manifolds was first obtained by Rumin [47]. The methods of Rumin and Hughen are close to each other, as they both rely on the analysis of the second-variation formula for sub-Riemannian geodesics.

2. Examples

In this section we present several classes of sub-Riemannian spaces satisfying the generalized curvature-dimension inequality of Definition 1.3. These examples constitute the central motivation of the present work.

2.1. Riemannian manifolds

As mentioned in the introduction, when $\mathbb{M}$ is an n-dimensional complete Riemannian manifold with Riemannian distance d_R, Levi-Civita connection ∇ and Laplace–Beltrami operator Δ, our main assumptions hold trivially. It suffices in fact to choose $\Gamma^Z = 0$ to satisfy Hypothesis 1.2 in a trivial fashion. Hypothesis 1.1 is also satisfied since it is equivalent to assuming that $(\mathbb{M}, d_R)$ be complete [30] (observe in passing that the distance (1.7) coincides with d_R). Finally, with the choice $\kappa = 0$ the curvature-dimension inequality (1.12) reduces to (1.2), which, as we have shown, is implied by (and in fact equivalent to) the assumption $\mathrm{Ric} \geq \rho_1$.

2.2. Three-dimensional Sasakian models

The purpose of this section is to provide a first basic sub-Riemannian example which fits the framework of the present paper. This example was first studied in [7]. Given $\rho_1 \in \mathbb{R}$, suppose that $\mathbb{G}(\rho_1)$ is a three-dimensional Lie group whose Lie algebra $\mathfrak{g}$ has a basis $\{X, Y, Z\}$ satisfying:

(i) $[X, Y] = Z$,
(ii) $[X, Z] = -\rho_1 Y$,
(iii) $[Y, Z] = \rho_1 X$.

A *sub-Laplacian* on $\mathbb{G}(\rho_1)$ is the left-invariant, second-order differential operator

$$L = X^2 + Y^2. \tag{2.1}$$

In view of (i)–(iii) Hörmander's theorem [32] implies that L is hypoelliptic, although it fails to be elliptic at every point of $\mathbb{G}(\rho_1)$. From (1.4) we find in the present situation

$$\Gamma(f) = \frac{1}{2}(L(f^2) - 2fLf) = (Xf)^2 + (Yf)^2.$$

If we define

$$\Gamma^Z(f, g) = ZfZg,$$

then from (i)–(iii) we easily verify that

$$\Gamma(f, \Gamma^Z(f)) = \Gamma^Z(f, \Gamma(f)).$$

We conclude that Hypothesis 1.2 is satisfied. It is not difficult to show that Hypothesis 1.1 is also fulfilled.

We leave it to the reader to verify using (i)–(iii) that

$$[L, Z] = 0. \tag{2.2}$$

By means of (2.2) we easily find

$$\begin{aligned}\Gamma_2^Z(f) &= \frac{1}{2}L(\Gamma^Z(f)) - \Gamma^Z(f, Lf) = Zf[L, Z]f + (XZf)^2 + (YZf)^2 \\ &= (XZf)^2 + (YZf)^2.\end{aligned}$$

Finally, from definition (1.10) and (i)–(iii) we obtain

$$\begin{aligned}\Gamma_2(f) &= \frac{1}{2}L(\Gamma(f)) - \Gamma(f, Lf) \\ &= \rho_1\Gamma(f) + (X^2f)^2 + (YXf)^2 + (XYf)^2 + (Y^2f)^2 \\ &\quad + 2Yf(XZf) - 2Xf(YZf).\end{aligned}$$

We now notice that

$$(X^2f)^2 + (YXf)^2 + (XYf)^2 + (Y^2f)^2 = \|\nabla_H^2 f\|^2 + \frac{1}{2}\Gamma^Z(f),$$

where we have denoted by

$$\nabla_H^2 f = \begin{pmatrix} X^2f & \frac{1}{2}(XYf + YXf) \\ \frac{1}{2}(XYf + YXf) & Y^2f \end{pmatrix}$$

the symmetrized Hessian of f with respect to the horizontal distribution generated by X, Y. Substituting this information into the above formula we find

$$\Gamma_2(f) = \|\nabla_H^2 f\|^2 + \rho_1\Gamma(f) + \frac{1}{2}\Gamma^Z(f) + 2\big(Yf(XZf) - Xf(YZf)\big).$$

By the above expression for $\Gamma_2^Z(f)$, using the Cauchy–Schwarz inequality we obtain, for every $\nu > 0$,

$$|2Yf(XZf) - 2Xf(YZf)| \le \nu\Gamma_2^Z(f) + \frac{1}{\nu}\Gamma(f).$$

Similarly, one easily finds that

$$\|\nabla_H^2 f\|^2 \ge \tfrac{1}{2}(Lf)^2.$$

Combining these inequalities, we conclude that we have proved the following result.

Proposition 2.1. *For every $\rho_1 \in \mathbb{R}$ the Lie group $\mathbb{G}(\rho_1)$ with the sub-Laplacian L of* (2.1) *satisfies the generalized curvature dimension inequality* CD$(\rho_1, 1/2, 1, 2)$. *More precisely, for all $f \in C^\infty(\mathbb{G}(\rho_1))$ and $\nu > 0$,*

$$\Gamma_2(f) + \nu\Gamma_2^Z(f) \ge \tfrac{1}{2}(Lf)^2 + (\rho_1 - 1/\nu)\Gamma(f) + \tfrac{1}{2}\Gamma^Z(f).$$

Proposition 2.1 provides a basic motivation for Definition 1.3. It is also important to observe at this point that the Lie group $\mathbb{G}(\rho_1)$ can be endowed with a natural CR structure. Denote in fact by $\mathcal{H}$ the subbundle of $T\mathbb{G}(\rho_1)$ generated by the vector fields X and Y. Then the endomorphism J of $\mathcal{H}$ defined by

$$J(Y) = X, \qquad J(X) = -Y$$

satisfies $J^2 = -I$, and thus defines a complex structure on $\mathbb{G}(\rho_1)$. By choosing θ to be the form such that

$$\operatorname{Ker}\theta = \mathcal{H} \quad \text{and} \quad d\theta(X, Y) = 1,$$

we obtain a CR structure on $\mathbb{G}(\rho_1)$ whose Reeb vector field is $-Z$. Thus, the above choice of Γ^Z is canonical.

The pseudo-hermitian Tanaka–Webster torsion of $\mathbb{G}(\rho_1)$ vanishes (see Definition 2.23 below), and thus $(\mathbb{G}(\rho_1), \theta)$ is a Sasakian manifold. It is also easy to verify that for the CR manifold $(\mathbb{G}(\rho_1), \theta)$ the Tanaka–Webster horizontal sectional curvature is constant and equals ρ_1. The following three model spaces correspond respectively to $\rho_1 = 1$, $\rho_1 = 0$ and $\rho_1 = -1$.

Example 2.2. The Lie group $\mathbb{SU}(2)$ is the group of 2×2 complex unitary matrices of determinant 1. Its Lie algebra $\mathfrak{su}(2)$ consists of all 2×2 complex skew-hermitian matrices with trace 0. A basis of $\mathfrak{su}(2)$ is formed by $X = \frac{i}{2}\sigma_1$, $Y = \frac{i}{2}\sigma_2$, $Z = \frac{i}{2}\sigma_3$, where σ_k, $k = 1, 2, 3$, are the Pauli matrices:

$$X = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad Y = \frac{1}{2}\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \quad Z = \frac{1}{2}\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}.$$

One easily verifies

$$[X, Y] = Z, \qquad [X, Z] = -Y, \qquad [Y, Z] = X, \tag{2.3}$$

and thus $\rho_1 = 1$.

Example 2.3. The Heisenberg group $\mathbb{H}$ is the group of 3×3 matrices

$$\begin{pmatrix} 1 & x & z \\ 0 & 1 & y \\ 0 & 0 & 1 \end{pmatrix}, \qquad x, y, z \in \mathbb{R}.$$

The Lie algebra of $\mathbb{H}$ is spanned by the matrices

$$X = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

for which the following commutation relations hold:

$$[X, Y] = Z, \qquad [X, Z] = [Y, Z] = 0.$$

Thus $\rho_1 = 0$ in this case.

Example 2.4. The Lie group $\mathbb{SL}(2)$ is the group of 2×2 real matrices of determinant 1. Its Lie algebra $\mathfrak{sl}(2)$ consists of all 2×2 matrices of trace 0. A basis of $\mathfrak{sl}(2)$ is formed by the matrices

$$X = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad Y = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Z = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

for which the following commutation relations hold:

$$[X, Y] = Z, \qquad [X, Z] = Y, \qquad [Y, Z] = -X. \tag{2.4}$$

Thus $\rho_1 = -1$ in this case.

2.3. Sub-Riemannian manifolds with transverse symmetries

We now turn our attention to a large class of sub-Riemannian manifolds, encompassing the three-dimensional model spaces discussed in the previous section. The central objective of the present section is to prove Theorem 2.19 below. It states that for these sub-Riemannian manifolds the generalized curvature-dimension inequality (1.12) holds under some natural geometric assumptions which, in the Riemannian case, reduce to requiring a lower bound for the Ricci tensor. To achieve this result, we will need to establish some new Bochner type identities. This is done in Theorem 2.18.

Let $\mathbb{M}$ be a smooth, connected manifold. We assume that $\mathbb{M}$ is equipped with a bracket-generating distribution $\mathcal{H}$ of dimension d and a fiberwise inner product g on that distribution. The distribution $\mathcal{H}$ will be referred to as the set of *horizontal directions*.

We denote by $\mathfrak{iso}$ the finite-dimensional Lie algebra of all sub-Riemannian Killing vector fields on $\mathbb{M}$ (see [49]). A vector field $Z \in \mathfrak{iso}$ if the one-parameter flow generated by it locally preserves the sub-Riemannian geometry defined by $(\mathcal{H}, g)$. This amounts to saying that:

(1) for every $x \in \mathbb{M}$, and any $u, v \in \mathcal{H}(x)$, $\mathcal{L}_Z g(u, v) = 0$;
(2) if $X \in \mathcal{H}$, then $[Z, X] \in \mathcal{H}$.

In (1) we have denoted by $\mathcal{L}_Z g$ the Lie derivative of g with respect to Z. Our main geometric assumption is the following:

Hypothesis 2.5. *There exists a Lie subalgebra $\mathcal{V} \subset \mathfrak{iso}$ such that for every $x \in \mathbb{M}$,*

$$T_x\mathbb{M} = \mathcal{H}(x) \oplus \mathcal{V}(x).$$

The distribution $\mathcal{V}$ will be referred to as the set of *vertical directions*. The dimension of $\mathcal{V}$ will be denoted by $\mathfrak{h}$.

The choice of an inner product on the Lie algebra $\mathcal{V}$ naturally endows $\mathbb{M}$ with a Riemannian extension g_R of g that makes the decomposition $\mathcal{H}(x) \oplus \mathcal{V}(x)$ orthogonal. Although g_R will be useful for computations, the geometric objects that we will introduce, like the sub-Laplacian L, the canonical connection ∇ and the "Ricci" tensor $\mathcal{R}$, ultimately will not depend on the choice of the inner product on $\mathcal{V}$.

The Riemannian measure of $(\mathbb{M}, g_R)$ will be denoted by μ; for notational convenience, we will often use the notation $\langle \cdot, \cdot \rangle$ instead of g_R.

Remark 2.6. If the Lie group $\mathbb{V}$ generated by $\mathcal{V}$ acts properly on $\mathbb{M}$, then we have a natural Riemannian submersion $\mathbb{M} \to \mathbb{M}/\mathbb{V}$. In the case of $\mathbb{SU}(2)$ studied in the previous section, we obtain the Hopf fibration $\mathbb{S}^3 \to \mathbb{S}^2$ (see [41]).

The above assumptions imply that, in a sufficiently small neighborhood of every point $x \in \mathbb{M}$, we can find a frame $\{X_1, \dots, X_d, Z_1, \dots, Z_{\mathfrak{h}}\}$ of vector fields such that:

(a) $Z_1, \dots, Z_{\mathfrak{h}} \in \mathcal{V}$;
(b) $\{X_1(x), \dots, X_d(x)\}$ is an orthonormal basis of $\mathcal{H}(x)$;
(c) $\{Z_1(x), \dots, Z_{\mathfrak{h}}(x)\}$ is an orthonormal basis of $\mathcal{V}(x)$;
(d) the following commutation relations hold:

$$[X_i, X_j] = \sum_{\ell=1}^{d} \omega_{ij}^{\ell} X_\ell + \sum_{m=1}^{\mathfrak{h}} \gamma_{ij}^{m} Z_m, \tag{2.5}$$

$$[X_i, Z_m] = \sum_{\ell=1}^{d} \delta_{im}^{\ell} X_\ell, \tag{2.6}$$

for smooth functions ω_{ij}^{ℓ}, γ_{ij}^{m} and δ_{im}^{ℓ} such that

$$\delta_{im}^{\ell} = -\delta_{\ell m}^{i}, \quad i, \ell = 1, \dots, d, \text{ and } m = 1, \dots, \mathfrak{h}. \tag{2.7}$$

We mention explicitly that (2.7) follows from Z_m being sub-Riemannian Killing (see conditions (1) and (2) above). By convention, $\omega_{ij}^{\ell} = -\omega_{ji}^{\ell}$ and $\gamma_{ij}^{m} = -\gamma_{ji}^{m}$.

Definition 2.7. A local frame as in (a)–(d) above will be called an *adapted frame*.

We define the *horizontal gradient* $\nabla_{\mathcal{H}} f$ of a function f as the projection of the Riemannian gradient of f on the horizontal bundle. Similarly, we define the *vertical gradient* $\nabla_{\mathcal{V}} f$ as the projection of the Riemannian gradient of f on the vertical bundle. In an adapted frame,

$$\nabla_{\mathcal{H}} f = \sum_{i=1}^{d} (X_i f) X_i, \qquad \nabla_{\mathcal{V}} f = \sum_{m=1}^{\mathfrak{h}} (Z_m f) Z_m.$$

The canonical sub-Laplacian in this structure is, by definition, the diffusion operator L on $\mathbb{M}$ which is symmetric on $C_0^\infty(\mathbb{M})$ with respect to the measure μ and such that (see (1.4))

$$\Gamma(f,g) = \tfrac{1}{2}(L(fg) - fLg - gLf) = \langle \nabla_{\mathcal{H}} f, \nabla_{\mathcal{H}} g\rangle.$$

It is readily seen that in an adapted frame, one has

$$L = -\sum_{i=1}^{d} X_i^* X_i,$$

where X_i^* is the formal adjoint of X_i with respect to the measure μ. From the commutation relations in an adapted frame, we obtain

$$X_i^* = -X_i + \sum_{k=1}^{d} \omega_{ik}^k,$$

so that in an adapted frame

$$L = \sum_{i=1}^{d} X_i^2 + X_0, \tag{2.8}$$

where

$$X_0 = -\sum_{i,k=1}^{d} \omega_{ik}^k X_i. \tag{2.9}$$

We also note that since $\mathcal{H}$ is supposed to be bracket-generating, from Hörmander's theorem, L is a hypoelliptic operator.

In the present setting, from the very definition of L, one readily recognizes that the canonical bilinear form introduced in (1.4) above is given by

$$\Gamma(f,g) = \langle \nabla_{\mathcal{H}} f, \nabla_{\mathcal{H}} g\rangle.$$

Definition 2.8. We define, for all $f, g \in C^\infty(\mathbb{M})$,

$$\Gamma^Z(f,g) = \langle \nabla_{\mathcal{V}} f, \nabla_{\mathcal{V}} g\rangle.$$

Our first step is verifying that the differential forms Γ and Γ^Z satisfy Hypothesis 1.2 of the introduction. This is the content of the next result.

Lemma 2.9. *For $f, g \in C^\infty(\mathbb{M})$,*

$$\Gamma(f, \Gamma^Z(f)) = \Gamma^Z(f, \Gamma(f)).$$

Proof. This is readily checked in a local adapted frame $\{X_1, \dots, X_d, Z_1, \dots, Z_{\mathfrak{h}}\}$:

$$\begin{aligned}
\Gamma^Z(f, \Gamma(f)) &= 2\sum_{m=1}^{\mathfrak{h}} Z_m f \sum_{i=1}^{d} X_i f Z_m(X_i f)\\
&= 2\sum_{i=1}^{d} X_i f \sum_{m=1}^{\mathfrak{h}} Z_m f X_i(Z_m f) - 2\sum_{i=1}^{d} X_i f \sum_{m=1}^{\mathfrak{h}} Z_m f [X_i, Z_m] f\\
&= \Gamma(f, \Gamma^Z(f)) - 2\sum_{m=1}^{\mathfrak{h}} Z_m f \sum_{i,\ell=1}^{d} \delta_{im}^{\ell} X_i f X_\ell f\\
&= \Gamma(f, \Gamma^Z(f)),
\end{aligned}$$

where in the last two equalities we have used (2.6) and (2.7). □

Another property that will be important for us is that $\mathcal{V}$ is a Lie algebra of symmetries for the sub-Laplacian L.

Lemma 2.10. *For any $Z \in \mathcal{V}$ one has $[L, Z] = 0$.*

Proof. Since Z is a Killing vector field, $[L, Z]$ is a first-order differential operator, and therefore a vector field. Since $Z^* = -Z + c$, where Z^* denotes the formal adjoint of Z and c a constant, we find that $[L, Z]^* = [L, Z]$. Since a symmetric vector field must vanish identically, we obtain the desired conclusion. □

2.3.1. The canonical connection. Our ultimate objective (see Theorem 2.19 in Section 2.3.3) will be to establish natural geometric conditions under which the manifold $\mathbb{M}$, endowed with the above defined sub-Laplacian L, and with the differential bilinear form Γ^Z, satisfies the generalized curvature-dimension inequality $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ of Definition 1.3. A useful ingredient in the realization of this objective is the existence of a canonical connection on $\mathbb{M}$.

Proposition 2.11. *There exists a unique affine connection ∇ on $\mathbb{M}$ with the following properties:*

(i) $\nabla g = 0$*;*
(ii) *if X and Y are horizontal vector fields, then $\nabla_X Y$ is horizontal;*
(iii) *if $Z \in \mathcal{V}$, then $\nabla Z = 0$;*
(iv) *if X, Y are horizontal vector fields and $Z \in \mathcal{V}$, then the torsion vector field $\mathrm{T}(X, Y)$ is vertical and $\mathrm{T}(X, Z) = 0$.*

Proof. If we denote by ∇^R the Riemannian Levi-Civita connection on $\mathbb{M}$, the existence of the connection ∇ follows by prescribing the relations

$$\nabla_Z X = [Z, X], \qquad \nabla_X Y = \pi_{\mathcal{H}}(\nabla_X^R Y), \qquad \nabla Z = 0,$$

where $X, Y \in \mathcal{H}$, $Z \in \mathcal{V}$, and $\pi_{\mathcal{H}}$ the projection onto the horizontal bundle. The uniqueness of ∇ follows in a standard fashion. □

Remark 2.12. The connection ∇ does not depend on the choice of the inner product on $\mathcal{V}$.

Remark 2.13. In the Riemannian case we simply have $\mathcal{H} = T\mathbb{M}$, and ∇ is just the Levi-Civita connection on $\mathbb{M}$.

Remark 2.14. For later use we observe that, in a local adapted frame,

$$\nabla_{X_i} X_j = \sum_{k=1}^{d} \frac{1}{2}(\omega_{ij}^k + \omega_{ki}^j + \omega_{kj}^i) X_k, \tag{2.10}$$

$$\nabla_{Z_m} X_i = -\sum_{\ell=1}^{d} \delta_{im}^{\ell} X_\ell, \tag{2.11}$$

$$\nabla Z_m = 0. \tag{2.12}$$

We also note that, thanks to (2.8) and (2.9), in a local adapted frame we have

$$L = \sum_{i=1}^{d} X_i^2 - \nabla_{X_i} X_i, \quad \text{so that} \quad Lf = \mathrm{div}(\nabla_{\mathcal{H}} f).$$

2.3.2. Generalized Bochner identities. As recalled in the opening of the present paper, at the source of the Riemannian curvature-dimension inequality $\mathrm{CD}(\rho_1, n)$ there is the Bochner identity. It is then only natural that our first step in the formulation of the generalized curvature-dimension inequality in Definition 1.3 above was understanding appropriate versions of the identity of Bochner. This is accomplished in Theorem 2.18 below, which represents the central result of this section. This result contains two Bochner identities: one for the horizontal directions (see (2.17)), and the other for the vertical ones (see (2.18)). One of the essential points of the program laid out in this paper is that to formulate a notion of Ricci tensor that works well for sub-Riemannian spaces, one needs to appropriately intertwine these identities. As a final comment we mention that, as will be clear from the proof of Theorem 2.18, the vertical Bochner formula is incredibly easier than the horizontal one, but this is in the nature of things, and should come as no surprise.

We are ready to introduce the relevant geometric quantities.

Definition 2.15. Let ∇ be the affine connection introduced by Proposition 2.11, and let *Ric* and T be respectively the Ricci and torsion tensors with respect to ∇. For $f \in C^\infty(\mathbb{M})$ we define

$$\mathcal{R}(f) = Ric(\nabla_{\mathcal{H}} f, \nabla_{\mathcal{H}} f) + \sum_{\ell,k=1}^{d} \big(-((\nabla_{X_\ell} T)(X_\ell, X_k) f)(X_k f) + \tfrac{1}{4}(T(X_\ell, X_k) f)^2\big), \tag{2.13}$$

where $\{X_1, \ldots, X_d\}$ is a local frame of horizontal vector fields. We also define the following second-order differential form:

$$\mathcal{S}(f) = -2 \sum_{i=1}^{d} \langle \nabla_{X_i} \nabla_{\mathcal{V}} f, T(X_i, \nabla_{\mathcal{H}} f) \rangle. \tag{2.14}$$

Remark 2.16. The expressions (2.13), (2.14) do not depend on the choice of the frame, so they define intrinsic differential forms on $\mathbb{M}$. Also, since the connection ∇ does not depend on the choice of the inner product on $\mathcal{V}$, it is easy to check that $\mathcal{R}$ and $\mathcal{S}$ do not depend on this choice either. We note explicitly that in the Riemannian case we have $\mathcal{H} = TM$, ∇ is just the Levi-Civita connection of $\mathbb{M}$, and therefore $T \equiv 0$. In that case, $\mathcal{R}(f) = Ric(\nabla f, \nabla f)$, where now Ric is the Riemannian Ricci tensor.

The following lemma provides a useful expression of the differential forms $\mathcal{R}(f)$ and $\mathcal{S}(f)$ in a local adapted frame.

Lemma 2.17. *Let* $\{X_1, \dots, X_d, Z_1, \dots, Z_{\mathfrak{h}}\}$ *be a local adapted frame. Then*

$$\begin{aligned}\mathcal{R}(f) = \sum_{k,\ell=1}^{d} \Big\{ & \Big(\sum_{j=1}^{d} \sum_{m=1}^{\mathfrak{h}} \gamma_{kj}^{m} \delta_{jm}^{\ell} \Big) + \sum_{j=1}^{d} (X_\ell \omega_{kj}^{j} - X_j \omega_{\ell j}^{k}) \\ & + \sum_{i,j=1}^{d} \omega_{ji}^{i} \omega_{kj}^{\ell} - \sum_{i=1}^{d} \omega_{ki}^{i} \omega_{\ell i}^{i} + \frac{1}{2} \sum_{1 \le i < j \le d} (\omega_{ij}^{\ell} \omega_{ij}^{k} - (\omega_{\ell j}^{i} + \omega_{\ell i}^{j})(\omega_{kj}^{i} + \omega_{ki}^{j})) \Big\} X_k f X_\ell f \\ & + \sum_{k=1}^{d} \sum_{m=1}^{\mathfrak{h}} \Big(\sum_{\ell,j=1}^{d} \omega_{j\ell}^{\ell} \gamma_{kj}^{m} + \sum_{1 \le \ell < j \le d} \omega_{\ell j}^{k} \gamma_{\ell j}^{m} - \sum_{j=1}^{d} X_j \gamma_{kj}^{m} \Big) Z_m f X_k f \\ & + \frac{1}{2} \sum_{1 \le \ell < j \le d} \Big(\sum_{m=1}^{\mathfrak{h}} \gamma_{\ell j}^{m} Z_m f \Big)^2, \end{aligned} \tag{2.15}$$

and

$$\mathcal{S}(f) = -2 \sum_{i,j=1}^{d} \sum_{m=1}^{\mathfrak{h}} \gamma_{ij}^{m} (X_j Z_m f)(X_i f). \tag{2.16}$$

Proof. It is a standard but lengthy computation using an adapted frame. □

In the following we denote by $\|\nabla_{\mathcal{H}}^2 f\|^2$ the Hilbert–Schmidt norm of the symmetrized horizontal Hessian of a function f. In a local adapted frame,

$$\begin{aligned} & \|\nabla_{\mathcal{H}}^2 f\|^2 \\ & = \sum_{\ell=1}^{d} \Big(X_\ell^2 f - \sum_{i=1}^{d} \omega_{i\ell}^{\ell} X_i f \Big)^2 + 2 \sum_{1 \le \ell < j \le d} \Big(\frac{X_j X_\ell + X_\ell X_j}{2} f - \sum_{i=1}^{d} \frac{\omega_{ij}^{\ell} + \omega_{i\ell}^{j}}{2} X_i f \Big)^2. \end{aligned}$$

Also, we will write $\|\nabla_{\mathcal{H}} \nabla_{\mathcal{V}} f\|^2 = \sum_{i=1}^{d} \sum_{m=1}^{\mathfrak{h}} (X_i Z_m f)^2$, an expression which is seen to be independent of the local adapted frame. The next theorem constitutes one of the central results of Section 2.3.

Theorem 2.18. *For every* $f \in C^\infty(\mathbb{M})$,

$$\Gamma_2(f) = \|\nabla_{\mathcal{H}}^2 f\|^2 + \mathcal{R}(f) + \mathcal{S}(f) \quad \text{(horizontal Bochner formula)}, \tag{2.17}$$

$$\Gamma_2^Z(f) = \|\nabla_{\mathcal{H}} \nabla_{\mathcal{V}} f\|^2 \quad \text{(vertical Bochner formula)}. \tag{2.18}$$

Proof. It is enough to prove (2.17) and (2.18) in a local adapted frame $\{X_1, \dots, X_d, Z_1, \dots, Z_{\mathfrak{h}}\}$. We begin with the vertical Bochner formula (2.18), which is quite simple: it follows immediately by a direct computation starting from the definition (1.11) of Γ_2^Z, and using the fact that L and Z_m commute (see Lemma 2.10).

The proof of the horizontal Bochner formula (2.17) is not as straightforward. To avoid long and cumbersome computations we will omit the intermediate details and only provide the essential identities. The interested reader should be able to fill in the gaps. Let us preliminarily observe that

$$X_i X_j f = f_{,ij} + \tfrac{1}{2}[X_i, X_j]f,$$

where we have let

$$f_{,ij} = \tfrac{1}{2}(X_i X_j + X_j X_i)f. \tag{2.19}$$

Using (2.5), we find

$$X_i X_j f = f_{,ij} + \frac{1}{2}\sum_{\ell=1}^{d} \omega_{ij}^{\ell} X_\ell f + \frac{1}{2}\sum_{m=1}^{\mathfrak{h}} \gamma_{ij}^{m} Z_m f. \tag{2.20}$$

Now, starting from the definition (1.10) of $\Gamma_2(f)$, we obtain

$$\begin{aligned}\Gamma_2(f) = {} & \sum_{i=1}^{d} X_i f [X_0, X_i] f - 2\sum_{i,j=1}^{d} X_i f [X_i, X_j] X_j f \\ & + \sum_{i,j=1}^{d} X_i f [[X_i, X_j], X_j] f + \sum_{i,j=1}^{d} (X_j X_i f)^2,\end{aligned}$$

where X_0 is defined by (2.9). From (2.20) we have

$$\begin{aligned}\sum_{i,j=1}^{d} (X_j X_i f)^2 = {} & \sum_{i,j=1}^{d} f_{,ij}^2 + \frac{1}{2}\sum_{1\le i<j\le d}\Big(\sum_{\ell=1}^{d}\omega_{ij}^{\ell} X_\ell f\Big)^2 + \frac{1}{2}\sum_{1\le i<j\le d}\Big(\sum_{m=1}^{\mathfrak{h}}\gamma_{ij}^{m} Z_m f\Big)^2 \\ & + \sum_{1\le i<j\le d}\sum_{\ell=1}^{d}\sum_{m=1}^{\mathfrak{h}} \omega_{ij}^{\ell}\gamma_{ij}^{m} Z_m f X_\ell f,\end{aligned}$$

and therefore

$$\begin{aligned}\Gamma_2(f) = {} & \sum_{i,j=1}^{d} f_{,ij}^2 - 2\sum_{i,j=1}^{d} X_i f [X_i, X_j] X_j f + \sum_{i,j=1}^{d} X_i f [[X_i, X_j], X_j] f \\ & + \sum_{i=1}^{d} X_i f [X_0, X_i] f + \frac{1}{2}\sum_{1\le i<j\le d}\Big(\sum_{\ell=1}^{d}\omega_{ij}^{\ell} X_\ell f\Big)^2 + \frac{1}{2}\sum_{1\le i<j\le d}\Big(\sum_{m=1}^{\mathfrak{h}}\gamma_{ij}^{m} Z_m f\Big)^2 \\ & + \sum_{1\le i<j\le d}\sum_{\ell=1}^{d}\sum_{m=1}^{\mathfrak{h}} \omega_{ij}^{\ell}\gamma_{ij}^{m} Z_m f X_\ell f.\end{aligned} \tag{2.21}$$

To complete the proof we need to recognize that the right-hand side in (2.21) coincides with that in (2.17). With this objective in mind, using (2.5) we obtain after a computation

$$\begin{aligned}
\sum_{i,j=1}^{d} f_{,ij}^2 - 2\sum_{i,j=1}^{d} X_i f[X_i,X_j]X_j f = & \sum_{\ell=1}^{d}\Big(f_{,\ell\ell}^2 - 2\Big(\sum_{i=1}^{d}\omega_{i\ell}^{\ell}X_i f\Big) f_{,\ell\ell}\Big) \\
& + 2\sum_{1\le \ell<j\le d}\left(f_{,j\ell}^2 - 2\sum_{1\le \ell<j\le d}\left(\sum_{i=1}^{d}\frac{\omega_{ij}^{\ell}+\omega_{i\ell}^{j}}{2}X_i f\right) f_{,\ell j}\right) \\
& - \sum_{i,j=1}^{d}\sum_{\ell,k=1}^{d}\omega_{ij}^{\ell}\omega_{\ell j}^{k}X_k f X_i f - \sum_{i,j=1}^{d}\sum_{\ell=1}^{d}\sum_{m=1}^{\mathfrak{h}}\omega_{ij}^{\ell}\gamma_{\ell j}^{m} Z_m f X_i f \\
& - 2\sum_{i,j=1}^{d}\sum_{m=1}^{\mathfrak{h}}\gamma_{ij}^{m} Z_m X_j f\ X_i f.
\end{aligned}$$

Completing the squares in the latter expression we find

$$\begin{aligned}
\sum_{i,j=1}^{d} f_{,ij}^2 - 2\sum_{i,j=1}^{d} X_i f[X_i,X_j]X_j f = & \sum_{\ell=1}^{d}\Big(f_{,\ell\ell} - \sum_{i=1}^{d}\omega_{i\ell}^{\ell}X_i f\Big)^2 \\
& + 2\sum_{1\le \ell<j\le d}\left(f_{,j\ell} - \sum_{i=1}^{d}\frac{\omega_{ij}^{\ell}+\omega_{i\ell}^{j}}{2}X_i f\right)^2 - \sum_{\ell=1}^{d}\Big(\sum_{i=1}^{d}\omega_{i\ell}^{\ell}X_i f\Big)^2 \\
& - 2\sum_{1\le \ell<j\le d}\left(\sum_{i=1}^{d}\frac{\omega_{ij}^{\ell}+\omega_{i\ell}^{j}}{2}X_i f\right)^2 - \sum_{i,j,k,\ell=1}^{d}\omega_{ij}^{\ell}\omega_{\ell j}^{k}X_k f X_i f \\
& - \sum_{i,j=1}^{d}\sum_{\ell=1}^{d}\sum_{m=1}^{\mathfrak{h}}\omega_{ij}^{\ell}\gamma_{\ell j}^{m} Z_m f X_i f - 2\sum_{i,j=1}^{d}\sum_{m=1}^{\mathfrak{h}}\gamma_{ij}^{m} X_j Z_m f\ X_i f \\
& - 2\sum_{i,j=1}^{d}\sum_{m=1}^{\mathfrak{h}}\gamma_{ij}^{m}[Z_m,X_j] f X_i f.
\end{aligned}$$

Next, from (2.9) we have

$$\begin{aligned}
\sum_{i=1}^{d} X_i f[X_0,X_i]f = & \sum_{i,j,k,\ell=1}^{d}\omega_{jk}^{k}\omega_{ij}^{\ell}X_\ell f X_i f \\
& + \sum_{i=1}^{d}\sum_{j,k=1}^{d}\sum_{m=1}^{\mathfrak{h}}\omega_{jk}^{k}\gamma_{ij}^{m} Z_m f X_i f + \sum_{i=1}^{d}\sum_{j,k=1}^{d}(X_i\omega_{jk}^{k})X_i f X_j f.
\end{aligned}$$

Using (2.5) we find

$$\begin{aligned}
\sum_{i,j=1}^{d} X_i f[[X_i,X_j],X_j]f = & \sum_{i,j=1}^{d}\sum_{\ell,k=1}^{d}\omega_{ij}^{\ell}\omega_{\ell j}^{k}X_i f X_k f + \sum_{i,j,\ell=1}^{d}\sum_{m=1}^{\mathfrak{h}}\omega_{ij}^{\ell}\gamma_{\ell j}^{m} Z_m f X_i f \\
& + \sum_{i,j=1}^{d}\sum_{m=1}^{\mathfrak{h}}\gamma_{ij}^{m}[Z_m,X_j] f X_i f - \sum_{i,j=1}^{d}\sum_{m=1}^{\mathfrak{h}}(X_j\gamma_{ij}^{m}) Z_m f X_i f \\
& - \sum_{i,j=1}^{d}\sum_{\ell=1}^{d}(X_j\omega_{ij}^{\ell})X_i f X_\ell f.
\end{aligned}$$

Substituting the latter three equations in (2.21) we obtain

$$\Gamma_2(f) = \sum_{\ell=1}^{d}\Big(f_{,\ell\ell} - \sum_{i=1}^{d}\omega_{i\ell}^{\ell}X_i f\Big)^2 + 2\sum_{1\le\ell<j\le d}\left(f_{,j\ell} - \sum_{i=1}^{d}\frac{\omega_{ij}^{\ell}+\omega_{i\ell}^{j}}{2}X_i f\right)^2$$
$$- 2\sum_{i,j=1}^{d}\sum_{m=1}^{\mathfrak{h}}\gamma_{ij}^{m}X_jZ_m f\ X_i f + \mathfrak{M}$$

where we have let

$$\mathfrak{M} = -\sum_{\ell=1}^{d}\Big(\sum_{i=1}^{d}\omega_{i\ell}^{\ell}X_i f\Big)^2 - 2\sum_{1\le\ell<j\le d}\left(\sum_{i=1}^{d}\frac{\omega_{ij}^{\ell}+\omega_{i\ell}^{j}}{2}X_i f\right)^2$$
$$+ \sum_{i,j,k,\ell=1}^{d}\omega_{jk}^{k}\omega_{ij}^{\ell}X_\ell f X_i f - \sum_{i,j,k,\ell=1}^{d}\omega_{ij}^{k}\omega_{kj}^{\ell}X_\ell f X_i f - \sum_{i,j=1}^{d}\sum_{\ell=1}^{d}\sum_{m=1}^{\mathfrak{h}}\omega_{ij}^{\ell}\gamma_{\ell j}^{m}Z_m f X_i f$$
$$- \sum_{i,j=1}^{d}\sum_{m=1}^{\mathfrak{h}}\gamma_{ij}^{m}[Z_m, X_j]f X_i f + \sum_{i=1}^{d}\sum_{j,k=1}^{d}\sum_{m=1}^{\mathfrak{h}}\omega_{jk}^{k}\gamma_{ij}^{m}Z_m f X_i f$$
$$+ \sum_{i=1}^{d}\sum_{j,k=1}^{d}(X_i\omega_{jk}^{k})X_i f X_j f + \sum_{i,j=1}^{d}\sum_{\ell,k=1}^{d}\omega_{ij}^{\ell}\omega_{\ell j}^{k}X_i f X_k f + \sum_{i,j,\ell=1}^{d}\sum_{m=1}^{\mathfrak{h}}\omega_{ij}^{\ell}\gamma_{\ell j}^{m}Z_m f X_i f$$
$$- \sum_{i,j=1}^{d}\sum_{m=1}^{\mathfrak{h}}(X_j\gamma_{ij}^{m})Z_m f X_i f - \sum_{i,j=1}^{d}\sum_{\ell=1}^{d}(X_j\omega_{ij}^{\ell})X_i f X_\ell f$$
$$+ \frac{1}{2}\sum_{1\le i<j\le d}\Big(\sum_{\ell=1}^{d}\omega_{ij}^{\ell}X_\ell f\Big)^2 + \frac{1}{2}\sum_{1\le i<j\le d}\Big(\sum_{m=1}^{\mathfrak{h}}\gamma_{ij}^{m}Z_m f\Big)^2$$
$$+ \sum_{1\le i<j\le d}\sum_{\ell=1}^{d}\sum_{m=1}^{\mathfrak{h}}\omega_{ij}^{\ell}\gamma_{ij}^{m}Z_m f X_\ell f. \tag{2.22}$$

Simplifying the latter expression we obtain

$$\mathfrak{M} = -\sum_{k,\ell=1}^{d}\sum_{i=1}^{d}\omega_{ki}^{i}\omega_{\ell i}^{i}X_k f X_\ell f - \frac{1}{2}\sum_{k,l=1}^{d}\sum_{1\le i<j\le d}(\omega_{\ell j}^{i}+\omega_{\ell i}^{j})(\omega_{kj}^{i}+\omega_{ki}^{j})X_k f X_\ell f$$
$$+ \sum_{k,\ell=1}^{d}\sum_{j=1}^{d}(X_\ell\omega_{kj}^{j} - X_j\omega_{\ell j}^{k})X_k f X_\ell f + \sum_{i,j,k,\ell=1}^{d}\omega_{ji}^{i}\omega_{kj}^{\ell}X_k f X_\ell f$$
$$+ \frac{1}{2}\sum_{k,\ell=1}^{d}\sum_{1\le i<j\le d}\omega_{ij}^{\ell}\omega_{ij}^{k}X_k f X_\ell f + \sum_{k,j=1}^{d}\sum_{m=1}^{\mathfrak{h}}\gamma_{kj}^{m}[X_j, Z_m]f X_k f$$
$$+ \sum_{i=1}^{d}\sum_{j,k=1}^{d}\sum_{m=1}^{\mathfrak{h}}\omega_{jk}^{k}\gamma_{ij}^{m}Z_m f X_i f + \sum_{1\le i<j\le d}\sum_{\ell=1}^{d}\sum_{m=1}^{\mathfrak{h}}\omega_{ij}^{\ell}\gamma_{ij}^{m}Z_m f X_\ell f$$
$$- \sum_{i,j=1}^{d}\sum_{m=1}^{\mathfrak{h}}(X_j\gamma_{ij}^{m})Z_m f X_i f + \frac{1}{2}\sum_{1\le i<j\le d}\Big(\sum_{m=1}^{\mathfrak{h}}\gamma_{ij}^{m}Z_m f\Big)^2. \tag{2.23}$$

At this point, using (2.6), it is easy to recognize in view of (2.13) in Lemma 2.17 that

$$\mathfrak{M} = \mathcal{R}(f).$$

To complete the proof of (2.17) it now suffices to:

- use the equation (2.14) in Lemma 2.17;
- find by a computation that, in a local horizontal frame, the square of the Hilbert–Schmidt norm of the horizontal Hessian $\nabla^2_{\mathcal{H}} f$ is given by

$$\|\nabla^2_{\mathcal{H}} f\|^2 = \sum_{\ell=1}^{d}\Big(f_{,\ell\ell} - \sum_{i=1}^{d}\omega_{i\ell}^{\ell} X_i f\Big)^2 + 2\sum_{1\le \ell<j\le d}\Big(f_{,j\ell} - \sum_{i=1}^{d}\frac{\omega_{ij}^{\ell}+\omega_{i\ell}^{j}}{2} X_i f\Big)^2. \tag{2.24}$$

□

2.3.3. The generalized curvature-dimension inequality. In this final part of Section 2.3 we establish the main result of the whole section, namely Theorem 2.19. This result shows that, under suitable geometric bounds (see (2.26)) which are natural in sub-Riemannian geometry (by this we mean that they are satisfied by large classes of significant examples), the sub-Riemannian manifold $\mathbb{M}$, with its canonical sub-Laplacian L and the Lie subalgebra of transverse symmetries $\mathcal{V}$, satisfies the curvature-dimension inequality (1.12).

We need to introduce the last intrinsic first-order differential quadratic form, which in a local horizontal frame $\{X_1, \dots, X_d\}$ is defined as

$$\mathcal{T}(f) = \sum_{i=1}^{d} \|\mathrm{T}(X_i, \nabla_{\mathcal{H}} f)\|^2.$$

A computation shows that in a local adapted frame,

$$\mathcal{T}(f) = \sum_{j=1}^{d}\sum_{m=1}^{\mathfrak{h}}\Big(\sum_{i=1}^{d}\gamma_{ij}^{m} X_i f\Big)^2. \tag{2.25}$$

It is worth remarking that, as already observed, in the Riemannian case ∇ is the Levi-Civita connection. As a consequence, in that case $\mathcal{T}(f) = 0$ for every $f \in C^\infty(\mathbb{M})$.

Theorem 2.19. *Suppose that there exist constants $\rho_1 \in \mathbb{R}$, $\rho_2 > 0$ and $\kappa \ge 0$ such that for every $f \in C^\infty(\mathbb{M})$,*

$$\begin{cases} \mathcal{R}(f) \ge \rho_1 \Gamma(f) + \rho_2 \Gamma^Z(f), \\ \mathcal{T}(f) \le \kappa \Gamma(f). \end{cases} \tag{2.26}$$

Then the sub-Riemannian manifold $\mathbb{M}$ satisfies the generalized curvature-dimension inequality $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ *of* (1.12) *with respect to the sub-Laplacian L and the differential form Γ^Z.*

Proof. We need to show that for all $f \in C^\infty(\mathbb{M})$ and $\nu > 0$,

$$\Gamma_2(f) + \nu\Gamma_2^Z(f) \ge \frac{1}{d}(Lf)^2 + \Big(\rho_1 - \frac{\kappa}{\nu}\Big)\Gamma(f) + \rho_2 \Gamma^Z(f).$$

Let $\{X_1, \dots, X_d, Z_1, \dots, Z_{\mathfrak{h}}\}$ be a local adapted frame. From (2.8) and (2.9) and the Cauchy–Schwarz inequality we find

$$Lf = \sum_{\ell=1}^{d}\Big(X_\ell^2 f - \sum_{i=1}^{d} \omega_{i\ell}^{\ell} X_i f\Big) \le \sqrt{d}\Big(\sum_{\ell=1}^{d}\Big(X_\ell^2 f - \sum_{i=1}^{d} \omega_{i\ell}^{\ell} X_i f\Big)^2\Big)^{1/2}.$$

This inequality and (2.24) readily give

$$\frac{1}{d}(Lf)^2 \le \|\nabla_{\mathcal{H}}^2 f\|^2.$$

From this estimate and from (2.17) in Theorem 2.18 we obtain

$$\frac{1}{d}(Lf)^2 \le \Gamma_2(f) - \mathcal{R}(f) + \mathcal{S}(f) \le \Gamma_2(f) - \rho_1\Gamma(f) - \rho_2\Gamma^Z(f) + \mathcal{S}(f), \tag{2.27}$$

where in the last inequality we have used the lower bound on $\mathcal{R}(f)$ in (2.26). Using (2.16) and the Cauchy–Schwarz inequality we now find that, for every $\nu > 0$,

$$\begin{aligned}|\mathcal{S}(f)| &\le 2\Big(\sum_{j=1}^{d}\sum_{m=1}^{\mathfrak{h}}\Big(\sum_{i=1}^{d}\gamma_{ij}^m X_i f\Big)^2\Big)^{1/2}\Big(\sum_{j=1}^{d}\sum_{m=1}^{\mathfrak{h}}(X_j Z_m f)^2\Big)^{1/2} \\ &= 2\mathcal{T}(f)^{1/2}\Gamma_2^Z(f)^{1/2} \le \frac{1}{\nu}\mathcal{T}(f) + \nu\Gamma_2^Z(f),\end{aligned}$$

where in the second to the last equality we have used (2.18) and (2.25). Substituting the latter inequality in (2.27) we find

$$\frac{1}{d}(Lf)^2 \le \Gamma_2(f) + \nu\Gamma_2^Z(f) + \frac{1}{\nu}\mathcal{T}(f) - \rho_1\Gamma(f) - \rho_2\Gamma^Z(f).$$

At this point it suffices to use the bound from above on $\mathcal{T}(f)$ in (2.26) to reach the desired conclusion. □

The next result shows that, remarkably, the generalized curvature-dimension inequality (1.12) in Definition 1.3 is equivalent to the geometric bounds (2.26) above.

Theorem 2.20. *Suppose that there exist constants $\rho_1 \in \mathbb{R}$, $\rho_2 > 0$ and $\kappa \ge 0$ such that $\mathbb{M}$ satisfies the generalized curvature-dimension inequality* CD$(\rho_1, \rho_2, \kappa, d)$. *Then $\mathbb{M}$ satisfies the geometric bounds* (2.26). *As a consequence of this fact and of Theorem 2.19 we conclude that*

$$\mathrm{CD}(\rho_1, \rho_2, \kappa, d) \;\Leftrightarrow\; \begin{cases}\mathcal{R}(f) \ge \rho_1\Gamma(f) + \rho_2\Gamma^Z(f),\\ \mathcal{T}(f) \le \kappa\Gamma(f).\end{cases}$$

Proof. Fix $x_0 \in \mathbb{M}$, $u \in \mathcal{H}_{x_0}(\mathbb{M})$ and $v \in \mathcal{V}_{x_0}(\mathbb{M})$. Let also $\nu > 0$. Let $\{X_1, \dots, X_d, Z_1, \dots, Z_{\mathfrak{h}}\}$ be a local adapted frame around x_0. We claim that we can find $f \in C^\infty(\mathbb{M})$ such that:

(i) $\nabla_{\mathcal{H}} f(x_0) = u$;
(ii) $\nabla_{\mathcal{V}} f(x_0) = v$;
(iii) $\nabla_{\mathcal{H}}^2 f(x_0) = 0$;
(iv) $X_j Z_m f(x_0) = \frac{1}{\nu}\sum_{i=1}^{d}\gamma_{ij}^m(x_0)u_i$.

To see this, we denote as before by ∇^R the Levi-Civita connection of the Riemannian metric on $\mathbb{M}$. Since $\{X_1, \dots, X_d, Z_1, \dots, Z_{\mathfrak{h}}\}$ is a local frame, we can find a local chart (U, ϕ) at x_0 such that $\phi(0) = x_0$ and in U we have $X_j = \partial/\partial x_j$, $j = 1, \dots, d$, and $Z_m = \partial/\partial z_m$, $m = 1, \dots, \mathfrak{h}$. We first observe that there exists $f_1 \in C^\infty(\mathbb{M})$ such that

$$\begin{cases} \nabla^R f_1(x_0) = u + v, \\ \nabla^R \nabla^R f_1(x_0) = 0. \end{cases}$$

For an explicit construction of such a function f_1, see for instance [46, proof of Theorem 3.1 and Lemma 3.2]. We can also find $f_2 \in C^\infty(\mathbb{M})$ such that

$$\begin{cases} \nabla^R f_2(x_0) = 0, \\ X_j Z_m f_2(x_0) = \frac{1}{\nu} \sum_{i=1}^d \gamma_{ij}^m(x_0) u_i - X_j Z_m f_1(x_0). \end{cases}$$

Indeed, take the function that in the local coordinates $(x, z) = (x_1, \dots, x_d,\ z_1, \dots, z_{\mathfrak{h}})$ is expressed in the form

$$f_2(x, z) = \sum_{j=1}^d \sum_{m=1}^{\mathfrak{h}} \left(\frac{1}{\nu} \sum_{i=1}^d \gamma_{ij}^m(x_0) u_i - X_j Z_m f_1(x_0) \right) x_j z_m .$$

It is readily verified that it satisfies the above two conditions. We now set $f = f_1 + f_2$. It is clear that f satisfies (i)–(iv) above. Now, using $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ for f, in combination with (i)–(iii) above, we find that at x_0,

$$\Gamma_2(f)(x_0) + \nu \Gamma_2^Z(f)(x_0) \ge \left(\rho_1 - \frac{\kappa}{\nu} \right) \|u\|^2 + \rho_2 \|v\|^2 .$$

But from (2.17) in Theorem 2.18 and (iii) we have

$$\Gamma_2(f)(x_0) = \mathcal{R}(f)(x_0) + \mathcal{S}(f)(x_0).$$

By (2.16) and (iii) we find

$$\begin{aligned} \mathcal{S}(f)(x_0) &= -2 \sum_{i,j=1}^d \sum_{m=1}^{\mathfrak{h}} \gamma_{ij}^m(x_0) X_j Z_m f(x_0) X_i f(x_0) \\ &= -\frac{2}{\nu} \sum_{j=1}^d \sum_{m=1}^{\mathfrak{h}} \sum_{i,\ell=1}^d \gamma_{ij}^m(x_0) \gamma_{\ell j}^m(x_0) u_\ell u_i = -\frac{2}{\nu} \sum_{j=1}^d \sum_{m=1}^{\mathfrak{h}} \left(\sum_{i=1}^d \gamma_{ij}^m(x_0) u_i \right)^2 \\ &= -\frac{2}{\nu} \mathcal{T}(f)(x_0), \end{aligned}$$

where in the last equality we have used (2.25). On the other hand, (2.18) and (iii) give

$$\Gamma_2^Z(f)(x_0) = \|\nabla_{\mathcal{H}} \nabla_{\mathcal{V}} f(x_0)\|^2 = \frac{1}{\nu^2} \sum_{j=1}^d \sum_{m=1}^{\mathfrak{h}} \left(\sum_{i=1}^d \gamma_{ij}^m(x_0) u_i \right)^2 = \frac{1}{\nu^2} \mathcal{T}(f)(x_0),$$

where in the last equality we have used (2.25) again. In conclusion,

$$\begin{aligned}\Gamma_2(f)(x_0) + \nu\Gamma_2^Z(f)(x_0) &= \mathcal{R}(f)(x_0) + \mathcal{S}(f)(x_0) + \nu\|\nabla_{\mathcal{H}}\nabla_{\mathcal{V}} f(x_0)\|^2 \\ &= \mathcal{R}(f)(x_0) - \frac{1}{\nu}\mathcal{T}(f)(x_0).\end{aligned}$$

We thus infer from $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ that

$$\mathcal{R}(f)(x_0) - \frac{1}{\nu}\mathcal{T}(f)(x_0) \geq \left(\rho_1 - \frac{\kappa}{\nu}\right)\|u\|^2 + \rho_2\|v\|^2.$$

We finally note that (2.17) in Lemma 2.17 gives

$$\begin{aligned}\mathcal{R}(f)(x_0) = &\sum_{k,\ell=1}^{d}\Bigg\{\Big(\sum_{j=1}^{d}\sum_{m=1}^{\mathfrak{h}}\gamma_{kj}^m\delta_{jm}^\ell\Big) + \sum_{j=1}^{d}(X_\ell\omega_{kj}^j - X_j\omega_{\ell j}^k) \\ &+ \sum_{i,j=1}^{d}\omega_{ji}^i\omega_{kj}^\ell - \sum_{i=1}^{d}\omega_{ki}^i\omega_{\ell i}^i + \frac{1}{2}\sum_{1\leq i<j\leq d}\Big(\omega_{ij}^\ell\omega_{ij}^k - (\omega_{\ell j}^i + \omega_{\ell i}^j)(\omega_{kj}^i + \omega_{ki}^j)\Big)\Bigg\}u_k u_l \\ &+ \sum_{k=1}^{d}\sum_{m=1}^{\mathfrak{h}}\Big(\sum_{\ell,j=1}^{d}\omega_{j\ell}^\ell\gamma_{kj}^m + \sum_{1\leq\ell<j\leq d}\omega_{\ell j}^k\gamma_{\ell j}^m - \sum_{j=1}^{d}X_j\gamma_{kj}^m\Big)v_m u_k \\ &+ \frac{1}{2}\sum_{1\leq\ell<j\leq d}\Big(\sum_{m=1}^{\mathfrak{h}}\gamma_{\ell j}^m v_m\Big)^2, \\ := &\,\mathcal{R}(u, v),\end{aligned}$$

and that (2.25) gives

$$\mathcal{T}(f)(x_0) = \sum_{j=1}^{d}\sum_{m=1}^{\mathfrak{h}}\Big(\sum_{i=1}^{d}\gamma_{ij}^m u_i\Big)^2 =: \mathcal{T}(u).$$

In conclusion, we have proved that for all $u \in \mathcal{H}_{x_0}(\mathbb{M})$, $v \in \mathcal{V}_{x_0}(\mathbb{M})$ and $\nu > 0$,

$$\mathcal{R}(u, v) - \frac{1}{\nu}\mathcal{T}(u) \geq \left(\rho_1 - \frac{\kappa}{\nu}\right)\|u\|^2 + \rho_2\|v\|^2.$$

By first letting $\nu \to \infty$, we obtain

$$\mathcal{R}(u, v) \geq \rho_1\|u\|^2 + \rho_2\|v\|^2.$$

If instead we let $\nu \to 0$, we find $\mathcal{T}(u) \leq k\|u\|^2$. This completes the proof. □

2.4. Carnot groups of step two

Carnot groups of step two provide a natural reservoir of sub-Riemannian manifolds with transverse symmetries. Let $\mathfrak{g}$ be a graded nilpotent Lie algebra of step two. This means that $\mathfrak{g}$ admits a splitting $\mathfrak{g} = V_1 \oplus V_2$, where $[V_1, V_1] = V_2$ and $[V_1, V_2] = \{0\}$. We endow $\mathfrak{g}$ with an inner product $\langle \cdot, \cdot \rangle$ with respect to which the decomposition $V_1 \oplus V_2$ is orthogonal. We denote by $e_1, \dots, e_d$ an orthonormal basis of V_1 and by $\varepsilon_1, \dots, \varepsilon_{\mathfrak{h}}$ an orthonormal basis of V_2. Let $\mathbb{G}$ be the connected and simply connected graded nilpotent Lie group associated with $\mathfrak{g}$. Left-invariant vector fields in V_2 are seen to be transverse sub-Riemannian Killing vector fields of the horizontal distribution given by V_1. The geometric assumptions of the previous section are thus satisfied.

Let $L_x(y) = xy$ be the operator of left translation on $\mathbb{G}$, and let dL_x be its differential. We denote by $X_j(x) = dL_x(e_j)$, $j = 1, \dots, d$, and $Z_m(x) = dL_x(\varepsilon_m)$, $m = 1, \dots, \mathfrak{h}$, the corresponding system of left-invariant vector fields on $\mathbb{G}$. Using the Baker–Campbell–Hausdorff formula, we see that in exponential coordinates,

$$X_i = \frac{\partial}{\partial x_i} - \frac{1}{2} \sum_{m=1}^{\mathfrak{h}} \sum_{\ell=1}^{d} \gamma_{i\ell}^m x_\ell Z_m$$

where $\gamma_{i\ell}^m = \langle [e_i, e_\ell], \varepsilon_m \rangle$ are the group constants. From the above equation we see that

$$[X_i, X_j] = \sum_{m=1}^{\mathfrak{h}} \gamma_{ij}^m Z_m. \tag{2.28}$$

We note that $\{X_1, \dots, X_d, Z_1, \dots, Z_{\mathfrak{h}}\}$ is a global adapted frame on $\mathbb{G}$.

A canonical sub-Laplacian on $\mathbb{G}$ is given by

$$L = \sum_{i=1}^{d} X_i^2.$$

If we endow $\mathbb{G}$ with a bi-invariant Haar measure μ, then $X_i^* = -X_i$ (see e.g. [27]). Therefore, L is symmetric with respect to μ.

In the present setting we have

$$\Gamma(f) = \sum_{i=1}^{d} (X_i f)^2, \qquad \Gamma^Z(f) = \sum_{m=1}^{\mathfrak{h}} (Z_m f)^2.$$

If we use Lemma 2.17, then we easily see that

$$\mathcal{R}(f) = \frac{1}{4} \sum_{i,j=1}^{d} \Big(\sum_{m=1}^{\mathfrak{h}} \gamma_{ij}^m Z_m f \Big)^2.$$

From this expression it is clear that $\mathcal{R}(f) \geq \rho_2 \Gamma^Z(f)$ with

$$\rho_2 = \inf_{\|z\|=1} \frac{1}{4} \sum_{i,j=1}^{d} \Big(\sum_{m=1}^{\mathfrak{h}} \gamma_{ij}^m z_m \Big)^2. \tag{2.29}$$

Furthermore, from (2.25) one has

$$\mathcal{T}(f) = \sum_{j=1}^{d} \sum_{m=1}^{\mathfrak{h}} \Big(\sum_{i=1}^{d} \gamma_{ij}^{m} X_i f \Big)^2,$$

and therefore $\mathcal{T}(f) \le \kappa \Gamma(f)$ with

$$\kappa = \sup_{\|x\|=1} \sum_{j=1}^{d} \sum_{m=1}^{\mathfrak{h}} \Big(\sum_{i=1}^{d} \gamma_{ij}^{m} x_i \Big)^2. \tag{2.30}$$

From these considerations in view of Theorem 2.19 we immediately obtain

Proposition 2.21. *Let $\mathbb{G}$ be a Carnot group of step two, and let d be the dimension of the horizontal layer of its Lie algebra. Then $\mathbb{G}$ satisfies the generalized curvature-dimension inequality* $\mathrm{CD}(0, \rho_2, \kappa, d)$ *(with respect to any sub-Laplacian L on $\mathbb{G}$) with ρ_2 and κ respectively given by* (2.29) *and* (2.30)*.*

In particular, in our framework, every Carnot group of step two is a *sub-Riemannian manifold with non-negative Ricci tensor*.

2.4.1. Groups of Heisenberg type. A significant class of Carnot groups of step two is that of groups of Heisenberg type. Such groups constitute a generalization of the Heisenberg group and they carry a natural complex structure. Groups of Heisenberg type (or H-type groups) were first introduced by Kaplan [35] in connection with the study of hypoellipticity. They were further developed in [21], where the authors characterized those groups of H-type which arise as the nilpotent component in the Iwasawa decomposition of simple Lie groups of real rank one. In a Carnot group $\mathbb{G}$ of step two, consider the map $J : V_2 \to \mathrm{End}(V_1)$ defined for every $\eta \in V_2$ by

$$\langle J(\eta)\xi, \xi' \rangle = \langle [\xi, \xi'], \eta \rangle, \qquad \xi, \xi' \in V_1, \eta \in V_2.$$

Then $\mathbb{G}$ is said of *H-type* if $J(\eta)$ is an orthogonal map on V_1 for every $\eta \in V_2$ such that $\|\eta\| = 1$. When $\mathbb{G}$ is of H-type we thus have, for $\xi, \xi' \in V_1$, $\eta \in V_2$,

$$\langle J(\eta)\xi, J(\eta)\xi' \rangle = \|\eta\|^2 \langle \xi, \xi' \rangle.$$

The map J induces a complex structure since in every group of H-type one has, for every $\eta, \eta' \in V_2$,

$$J(\eta)J(\eta') + J(\eta')J(\eta) = -2\langle \eta, \eta' \rangle I$$

(see [21]). In particular,

$$J(\eta)^2 = -\|\eta\|^2 I.$$

Since in a Carnot group of step two we always have $[e_i, e_j] = \sum_{s=1}^{\mathfrak{h}} \gamma_{ij}^{s} \varepsilon_s$, we obtain

$$\langle J(\varepsilon_m)e_i, e_j \rangle = \langle [e_i, e_j], \varepsilon_m \rangle = \gamma_{ij}^{m}.$$

When $\mathbb{G}$ is of H-type we thus find that for $z = \sum_{m=1}^{\mathfrak{h}} z_m \varepsilon_m$,

$$\frac{1}{4}\sum_{i,j=1}^{d}\Big(\sum_{m=1}^{\mathfrak{h}} \gamma_{ij}^m z_m\Big)^2 = \frac{1}{4}\sum_{i,j=1}^{d}\langle J(z)e_i, e_j\rangle^2 = \frac{d}{4}\|z\|^2.$$

In view of (2.29) we conclude that if $\mathbb{G}$ is of H-type, then $\rho_2 = d/4$. Also, for $x = \sum_{i=1}^{d} x_i e_i$,

$$\sum_{j=1}^{d}\sum_{m=1}^{\mathfrak{h}}\Big(\sum_{i=1}^{d} \gamma_{ij}^m x_i\Big)^2 = \sum_{j=1}^{d}\sum_{m=1}^{\mathfrak{h}}\langle J(\varepsilon_m)x, e_j\rangle^2 = \sum_{m=1}^{\mathfrak{h}}\|J(\varepsilon_m)x\|^2 = \mathfrak{h}\|x\|^2.$$

In view of (2.30) we conclude $\kappa = \mathfrak{h}$. Combining these considerations with Proposition 2.21, we have thus proved the following result.

Proposition 2.22. *Let $\mathbb{G}$ be a group of H-type. Then $\mathbb{G}$ satisfies the generalized curvature-dimension inequality* CD$(0, d/4, \mathfrak{h}, d)$ *with respect to any sub-Laplacian L.*

2.5. CR Sasakian manifolds

Another interesting class of sub-Riemannian manifolds with transverse symmetries is the class of CR Sasakian manifolds. For all the known results cited in this section we refer the reader to the monograph [23]. Let $\mathbb{M}$ be a non-degenerate CR manifold of real hypersurface type and dimension $d+1$, where $d = 2n$. Let θ be a pseudo-hermitian form on $\mathbb{M}$ with respect to which the Levi form L_θ is positive definite. The kernel of θ determines the horizontal bundle $\mathcal{H}$. Denote now by Z the Reeb vector field on $\mathbb{M}$, i.e., the characteristic direction of θ. It is an immediate consequence of [23, Theorem 1.3, p. 25] that the canonical connection ∇ introduced in Section 2.3.1 coincides with the Tanaka–Webster connection on $\mathbb{M}$. The sub-Laplacian L introduced in Section 2.3 is then the classical CR sub-Laplacian (see [23, Definition 2.1, p. 111]).

As in the Riemannian case, the pseudo-hermitian torsion with respect to ∇ is

$$\mathrm{T}(X, Y) = \nabla_X Y - \nabla_Y X - [X, Y].$$

Definition 2.23. The CR manifold $(\mathbb{M}, \theta)$ is called *Sasakian* if the pseudo-hermitian torsion vanishes, in the sense that

$$T(Z, X) = 0 \quad \text{for every } X \in \mathcal{H}.$$

In every Sasakian manifold the Reeb vector field Z is a sub-Riemannian Killing vector field (see [23, Theorem 1.5, p. 42 and Lemma 1.5, p. 43]). In this situation, the bilinear forms $\mathcal{R}$, $\mathcal{T}$ take a particularly nice form. Indeed, in the Sasakian case, the torsion T of the Tanaka–Webster connection is given, for horizontal vector fields X and Y, by

$$\mathrm{T}(X, Y) = \langle JX, Y\rangle Z,$$

where J is the complex structure on $\mathbb{M}$. Since $\nabla J = 0$, from (2.13) in Definition 2.15 we obtain

$$\mathcal{R}(f) = \mathrm{Ric}(\nabla_{\mathcal{H}} f, \nabla_{\mathcal{H}} f) + \frac{1}{4}\Big(\sum_{l,k=1}^{d}\langle JX_l, X_k\rangle^2\Big)(Zf)^2. \tag{2.31}$$

Since

$$\sum_{l,k=1}^{d} \langle JX_l, X_k\rangle^2 = \sum_{k=1}^{d} \|JX_k\|^2 = d,$$

we conclude from (2.31) that

$$\mathcal{R}(f) = \mathrm{Ric}(\nabla_{\mathcal{H}} f, \nabla_{\mathcal{H}} f) + \frac{d}{4}\Gamma^Z(f).$$

Also, from (2.25),

$$\mathcal{T}(f) = \sum_{i=1}^{d} \langle J\nabla_{\mathcal{H}} f, X_i\rangle^2 = \|J\nabla_{\mathcal{H}} f\|^2 = \Gamma(f).$$

A straightforward consequence of these considerations and of Theorem 2.19 is

Theorem 2.24. *Assume that the Tanaka–Webster Ricci tensor is bounded from below by $\rho_1 \in \mathbb{R}$ on smooth functions, that is, for every $f \in C^\infty(\mathbb{M})$,*

$$\mathrm{Ric}(\nabla_{\mathcal{H}} f, \nabla_{\mathcal{H}} f) \geq \rho_1 \|\nabla_{\mathcal{H}} f\|^2.$$

Then the Sasakian manifold $\mathbb{M}$ satisfies the generalized curvature-dimension inequality $\mathrm{CD}(\rho_1, d/4, 1, d)$ *with $d = 2n$.*

Remark 2.25. The example of CR Sasakian manifolds, together with that of H-type groups studied in Section 2.4.1, suggests the existence of an interesting class of sub-Riemannian manifolds with transverse symmetries. Indeed, returning to the setting and notation of Section 2.3, for $Z \in \mathcal{V}$ consider the map $J(Z)$ defined on the horizontal bundle $\mathcal{H}$ by

$$\langle J(Z)X, Y\rangle = \langle Z, T(X, Y)\rangle.$$

Suppose that $J(Z)$ is orthogonal for every $Z \in \mathcal{V}$ such that $\|Z\| = 1$, and that furthermore $\sum_{k=1}^{d} \nabla_{X_k} J(Z) = 0$. In that case, similarly to the case of groups of H-type and Sasakian manifolds, we can prove that if the horizontal Ricci curvature of the canonical connection ∇ is bounded from below by ρ_1, then $\mathbb{M}$ satisfies $\mathrm{CD}(\rho_1, d/4, \mathfrak{h}, d)$. An example of such a structure is given by the Hopf fibration $\mathbb{S}^7 \to \mathbb{S}^4$ and, more generally, by the so-called 3-Sasakian manifolds (see [15]).

2.6. Principal bundles over Riemannian manifolds

Sub-Riemannian structures with transverse symmetries also naturally arise in the context of principal bundles over Riemannian manifolds. Let $(\mathbb{M}, g)$ be a C^∞ connected Riemannian manifold of dimension d. Let us consider the orthonormal frame bundle $\mathcal{O}(\mathbb{M})$ over $\mathbb{M}$. The kernel of the Levi-Civita connection form defines the distribution $\mathcal{H}$ of horizontal directions. If the Riemannian curvature form is non-degenerate, this distribution is two-step bracket-generating (see for instance [11, Chapter 3]). The set of vertical directions is then given by the vector fields that are tangent to the fibers of the bundle projection. It is easily seen that in that case $\mathcal{V} \simeq \mathfrak{so}_d(\mathbb{R})$, and therefore the vertical bundle is generated by the sub-Riemannian Killing vector fields of the horizontal bundle. We thus have an example of a sub-Riemannian manifold with transverse symmetries. In this example the geometric quantities introduced in Section 2.2 may be interpreted in terms of the geometry of $\mathbb{M}$.

First, let us observe that we can find a globally defined adapted frame. For each $x \in \mathbb{R}^d$ we can define a horizontal vector field H_x on $\mathcal{O}(\mathbb{M})$ by the property that at each point $u \in \mathcal{O}(\mathbb{M})$, $H_x(u)$ is the horizontal lift of $u(x)$ from u. If $(e_1, \dots, e_d)$ is the canonical basis of $\mathbb{R}^d$, then the fundamental horizontal vector fields are defined by

$$H_i = H_{e_i}.$$

Now, for every $M \in \mathfrak{o}_d(\mathbb{R})$ (the space of $d \times d$ skew-symmetric matrices), we can define a vertical vector field V_M on $\mathcal{O}(\mathbb{M})$ by

$$(V_M F)(u) = \lim_{t \to 0} \frac{F(ue^{tM}) - F(u)}{t},$$

where $u \in \mathcal{O}(\mathbb{M})$ and $F : \mathcal{O}(\mathbb{M}) \to \mathbb{R}$. If E_{ij}, $1 \le i < j \le d$, denote the canonical basis of $\mathfrak{o}_d(\mathbb{R})$ (E_{ij} is the matrix whose (i, j)-th entry is $1/2$, (j, i)-th entry is $-1/2$, and all other entries are zero), then the fundamental vertical vector fields are given by

$$V_{ij} = V_{E_{ij}}.$$

It can be shown that we have the following Lie bracket relations:

$$[H_i, H_j] = -2 \sum_{k<l} \Omega_{ij}^{kl} V_{kl}, \qquad [H_i, V_{jk}] = -\delta_{ij} \frac{1}{2} H_k + \delta_{ik} \frac{1}{2} H_j,$$

where $\delta_{ij} = 1$ if $i = j$ and 0 otherwise, and where Ω is the Riemannian curvature form:

$$\Omega(X, Y)(u) = u^{-1} R(\pi_* X, \pi_* Y) u, \qquad X, Y \in \mathrm{T}_u \mathcal{O}(\mathbb{M}),$$

R denoting the Riemannian curvature tensor on $\mathbb{M}$ and π the canonical projection $\mathcal{O}(\mathbb{M}) \to \mathbb{M}$.

In this structure, the sub-Laplacian L is the so-called horizontal Bochner Laplace operator. It is by definition the diffusion operator on $\mathcal{O}(\mathbb{M})$ given by

$$\Delta_{\mathcal{O}(\mathbb{M})} = \sum_{i=1}^{d} H_i^2.$$

Its fundamental property is that it is the lift of the Laplace–Beltrami operator $\Delta_{\mathbb{M}}$ of $\mathbb{M}$. That is, for every smooth $f : \mathbb{M} \to \mathbb{R}$,

$$\Delta_{\mathcal{O}(\mathbb{M})}(f \circ \pi) = (\Delta_{\mathbb{M}} f) \circ \pi.$$

The canonical sub-Riemannian connection ∇ is easily expressed in terms of the Ehresmann bundle connection. Let us recall (see for instance [11, Chapter 3]) that the *Ehresmann connection* form α on $\mathcal{O}(\mathbb{M})$ is the unique skew-symmetric matrix α of one-forms on $\mathcal{O}(\mathbb{M})$ such that:

(1) $\alpha(X) = 0$ if and only if $X \in \mathcal{HO}(\mathbb{M})$;
(2) $V_{\alpha(X)} = X$ if and only if $X \in \mathcal{VO}(\mathbb{M})$,

where $\mathcal{HO}(\mathbb{M})$ denotes the horizontal bundle and $\mathcal{VO}(\mathbb{M})$ the vertical bundle. It is then easily verified that for a vector field Y on $\mathcal{O}(\mathbb{M})$,

$$\nabla_Y H_i = \sum_{k=1}^{d} \alpha_j^k(Y) H_k.$$

Observe that if X, Y are smooth horizontal vector fields then the torsion satisfies

$$\mathrm{T}(X, Y) = V_{\Omega(X,Y)}.$$

Then straightforward computations yield

$$\mathcal{R}(f, f) = \mathrm{Ric}^*(\nabla_{\mathcal{H}} f, \nabla_{\mathcal{H}} f) - \sum_{j,k=1}^{d} V_{(\nabla_{H_j}\Omega)(H_j,H_k)} f H_k f + \tfrac{1}{4}(V_{\Omega(H_j,H_k)} f)^2,$$

where for horizontal vector fields X and Y,

$$\mathrm{Ric}^*(X, Y) = \mathrm{Ric}(\pi_* X, \pi_* Y),$$

and Ric denotes the Ricci tensor of $\mathbb{M}$. In the same vein we have

$$\mathcal{T}(f) = \sum_{i=1}^{d} \|\mathrm{T}(H_i, \nabla_{\mathcal{H}} f)\|^2 = \sum_{i=1}^{d} \|V_{\Omega(H_i,\nabla_{\mathcal{H}} f)}\|^2.$$

We then observe that the expression of $\mathcal{R}$ simplifies if for every horizontal vector field X,

$$\sum_{j=1}^{d} (\nabla_{H_j}\Omega)(H_j, X) = 0.$$

Using the second Bianchi identity, it is seen that this last condition is equivalent to the fact that the Ricci tensor of $\mathbb{M}$ is a *Codazzi tensor*, that is, for any vector fields X, Y, Z on $\mathbb{M}$,

$$(\nabla_X \mathrm{Ric})(Y, Z) = (\nabla_Y \mathrm{Ric})(X, Z).$$

As a conclusion, Theorem 2.19 then yields

Proposition 2.26. *Let* $(\mathbb{M}, g)$ *be a* C^∞ *connected Riemannian manifold of dimension* d*. Assume that:*

(1) Ric *is a Codazzi tensor;*
(2) *there exists* $\rho_1 \geq 0$ *such that* $\mathrm{Ric} \geq \rho_1$*;*
(3) *there exists* $\rho_2 > 0$ *such that for every* $U \in \mathfrak{so}_d(\mathbb{R})$*,*

$$\sum_{i,j=1}^{d} \langle \Omega(H_j, H_k), U\rangle^2 \geq 4\rho_2 \|U\|^2;$$

(4) *there exists* $\kappa \geq 0$ *such that for every horizontal vector field* X*,*

$$\sum_{i=1}^{d} \|\Omega(H_i, X)\|^2 \leq \kappa \|X\|^2,$$

Then the horizontal Bochner operator of $\mathcal{O}(\mathbb{M})$ *satisfies the generalized curvature-dimension inequality* $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$*.*

The previous assumptions are readily satisfied in the case of spaces with constant curvature and, after some standard computations, we obtain the following result.

Corollary 2.27. *Let* $(\mathbb{M}, g)$ *be a* C^∞ *connected Riemannian manifold of dimension* d *and constant curvature* $K \neq 0$. *The sub-Riemannian structure of* $\mathcal{O}(\mathbb{M})$ *satisfies the generalized curvature dimension inequality* $\mathrm{CD}\big((d-1)K, \frac{d}{4}K^2, \frac{d(d-1)}{2}K^2, d\big)$.

Actually, more general principal bundles provide examples of sub-Riemannian structures with transverse symmetries. Let $\pi : (\mathbb{M}, g) \to (\mathbb{M}', g')$ be the projection of a principal fiber bundle with structure group a compact, semisimple Lie group $\mathbb{G}$ of dimension $\mathfrak{h}$ equipped with its bi-invariant metric given by the Cartan–Killing form. We suppose that π is a Riemannian submersion with totally geodesic fibers isometric to $\mathbb{G}$. We denote by θ the one-form of the principal connection corresponding to the horizontal distribution $\mathcal{H}$. If $\mathcal{H}$ is bracket-generating, then we have an example of a sub-Riemannian structure with transverse symmetries.

Let

$$A_X Y = (\tilde{\nabla}_{X_\mathcal{H}} Y_\mathcal{H})_\mathcal{V} + (\tilde{\nabla}_{X_\mathcal{H}} Y_\mathcal{V})_\mathcal{H}$$

be the O'Neill tensor of the submersion. When X and Y are horizontal vector fields we have $\mathrm{T}(X, Y) = -2A_X Y$, where, as usual, T denotes the torsion of the canonical sub-Riemannian connection. As a consequence, A is the skew-symmetrization of $-\frac{1}{2}\mathrm{T}$. The connection form θ is a Yang–Mills connection if for every horizontal vector field X, the vertical component of

$$\sum_{\ell=1}^{d} (\nabla_{X_\ell} T)(X_\ell, X)$$

is zero (see for instance [24, p. 146]). As a consequence of Theorem 2.19, we obtain the following result.

Proposition 2.28. *Assume that:*

(1) θ *is a Yang–Mills connection;*
(2) *there exists* $\rho_1 \geq 0$ *such that* $\mathrm{Ric}' \geq \rho_1$ *where* Ric' *is the Ricci tensor of* $(\mathbb{M}', g')$*;*
(3) *there exists* $\rho_2 > 0$ *such that for every vertical vector field* Z,

$$\sum_{i=1}^{d} \|A_{X_i} Z\|^2 \geq \rho_2 \|Z\|^2;$$

(4) *there exists* $\kappa \geq 0$ *such that for every horizontal vector field* X,

$$\sum_{m=1}^{\mathfrak{h}} \|A_X Z_i\|^2 \leq \kappa \|X\|^2.$$

Then the sub-Riemannian structure on $\mathbb{M}$ *given by the submersion* $\pi : (\mathbb{M}, g) \to (\mathbb{M}', g')$ *satisfies the generalized curvature dimension inequality* $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$.

Remark 2.29. If $\mathbb{G}$ is simple, then by **Ad** invariance,

$$\sum_{i=1}^{d} \|A_{X_i} Z\|^2 = \frac{\|A\|^2}{\mathfrak{h}} \|Z\|^2, \qquad \sum_{m=1}^{\mathfrak{h}} \|A_X Z_i\|^2 \leq \|A\|^2 \|X\|^2.$$

3. Second-derivative estimates

In this section, in the context of sub-Riemannian manifolds with transverse symmetries, we develop some basic tools to obtain bounds on the second derivatives to be used later.

Let $\mathbb{M}$ be a sub-Riemannian manifold with transverse symmetries as in the previous section. If $\{X_1, \dots, X_d\}$ is a local frame of horizontal vector fields, we define the tensor

$$\delta T(V) = \sum_{\ell=1}^{d} (\nabla_{X_\ell} T)(X_\ell, V).$$

Motivated by the examples of the previous section, we make the following definition:

Definition 3.1. The sub-Riemannian manifold $\mathbb{M}$ is said to be *of Yang–Mills type* if for every horizontal vector field X,

$$\delta T(X) = 0.$$

For instance, Riemannian manifolds, CR Sasakian manifolds and Carnot groups of step two are examples of sub-Riemannian manifolds with transverse symmetries of Yang–Mills type.

Proposition 3.2. *Suppose that $\mathbb{M}$ is of Yang–Mills type and there exist constants $\rho_1 \in \mathbb{R}$, $\rho_2 > 0$ and $\kappa \geq 0$ such that*

$$\begin{cases} \mathcal{R}(f) \geq \rho_1 \Gamma(f) + \rho_2 \Gamma^Z(f), \\ \mathcal{T}(f) \leq \kappa \Gamma(f), \end{cases}$$

for every $f \in C^\infty(\mathbb{M})$. Then, for $f \in C^\infty(\mathbb{M})$ and $\nu > 0$,

$$\Gamma(\Gamma(f)) \leq 4\Gamma(f)\left(\Gamma_2(f) + \nu \Gamma_2^Z(f) - \left(\rho_1 - \frac{\kappa}{\nu}\right)\Gamma(f)\right),$$
$$\Gamma(\Gamma^Z(f)) \leq 4\Gamma^Z(f)\Gamma_2^Z(f).$$

Proof. Let $f \in C^\infty(\mathbb{M})$ and $x_0 \in \mathbb{M}$. We assume that $\nabla_{\mathcal{H}} f(x_0) \neq 0$, otherwise the inequalities are straightforward. We can find a local adapted frame $\{X_1, \dots, X_d, Z_1, \dots, Z_{\mathfrak{h}}\}$ in the neighborhood of x_0 such that $X_1 f = 0, \dots, X_d f = \|\nabla_{\mathcal{H}} f\|$. In this frame,

$$\Gamma(\Gamma(f)) = 4\Big(\sum_{i=1}^{d} (X_i X_d f)^2\Big)\Gamma(f),$$

and

$$\|\nabla_{\mathcal{H}}^2 f\|^2 = \sum_{\ell=1}^{d}\Big(X_\ell^2 f - \sum_{i=1}^{d} \omega_{i\ell}^\ell X_i f\Big)^2 + 2\sum_{1\leq \ell < j \leq d}\left(\frac{X_j X_\ell + X_\ell X_j}{2} f - \sum_{i=1}^{d} \frac{\omega_{ij}^\ell + \omega_{i\ell}^j}{2} X_i f\right)^2.$$

By observing that $X_j X_\ell f = 0$ if $\ell \neq d$ and $X_j X_d f = \omega_{jd}^d X_d f + \sum_{m=1}^{\mathfrak{h}} \gamma_{jd}^m Z_m f$ we easily conclude that

$$\Gamma(\Gamma(f)) - 4\|\nabla_{\mathcal{H}}^2 f\|^2 \Gamma(f) \leq 2\Gamma(f) \sum_{\ell=1}^{d} \Big(\sum_{m=1}^{\mathfrak{h}} \gamma_{\ell d}^m Z_m f\Big)^2$$
$$\leq 2\Gamma(f) \sum_{1\leq \ell<j\leq d} \Big(\sum_{m=1}^{\mathfrak{h}} \gamma_{\ell j}^m Z_m f\Big)^2.$$

Now, from (2.17) in Theorem 2.18 we have

$$\Gamma_2(f) = \|\nabla_{\mathcal{H}}^2 f\|^2 + \mathcal{R}(f) + \mathcal{S}(f).$$

From this identity and the proof of Theorem 2.19 we obtain, for every $\nu > 0$,

$$\Gamma_2(f) + \nu \Gamma_2^Z(f) \geq \|\nabla_{\mathcal{H}}^2 f\|^2 - \frac{\kappa}{\nu}\Gamma(f) + \mathcal{R}(f). \tag{3.1}$$

Therefore

$$\Gamma(\Gamma(f)) \leq 4\Gamma(f)\Bigg(\Gamma_2(f) + \nu\Gamma_2^Z(f) + \frac{\kappa}{\nu}\Gamma(f) - \mathcal{R}(f) + \frac{1}{2}\sum_{1\leq \ell<j\leq d}\Big(\sum_{m=1}^{\mathfrak{h}} \gamma_{\ell j}^m Z_m f\Big)^2\Bigg).$$

From the Yang–Mills assumption we have

$$\mathcal{R}(f) - \frac{1}{2}\sum_{1\leq \ell<j\leq d}\Big(\sum_{m=1}^{\mathfrak{h}} \gamma_{\ell j}^m Z_m f\Big)^2$$
$$= \sum_{k,\ell=1}^{d} \Bigg\{ \Big(\sum_{j=1}^{d}\sum_{m=1}^{\mathfrak{h}} \gamma_{kj}^m \delta_{jm}^\ell\Big) + \sum_{j=1}^{d} (X_\ell \omega_{kj}^j - X_j \omega_{\ell j}^k)$$
$$+ \sum_{i,j=1}^{d} \omega_{ji}^i \omega_{kj}^\ell - \sum_{i=1}^{d} \omega_{ki}^i \omega_{\ell i}^i + \frac{1}{2}\sum_{1\leq i<j\leq d} (\omega_{ij}^\ell \omega_{ij}^k - (\omega_{\ell j}^i + \omega_{\ell i}^j)(\omega_{kj}^i + \omega_{ki}^j))\Bigg\} X_k f X_\ell f,$$

and thus

$$\mathcal{R}(f) - \frac{1}{2}\sum_{1\leq \ell<j\leq d}\Big(\sum_{m=1}^{\mathfrak{h}} \gamma_{\ell j}^m Z_m f\Big)^2 \geq \rho_1 \Gamma(f).$$

Putting things together, we conclude that

$$\Gamma(\Gamma(f)) \leq 4\Gamma(f)\Big(\Gamma_2(f) + \nu\Gamma_2^Z(f) - \Big(\rho_1 - \frac{\kappa}{\nu}\Big)\Gamma(f)\Big).$$

The proof of $\Gamma(\Gamma^Z(f)) \leq 4\Gamma^Z(f)\Gamma_2^Z(f)$ is easy and left to the reader. □

In the rest of this section we assume that $\mathbb{M}$ is complete and that there exist constants $\rho_1 \in \mathbb{R}$, $\rho_2 > 0$ and $\kappa \geq 0$ such that (2.26) holds for every $f \in C^\infty(\mathbb{M})$. The completeness of

$\mathbb{M}$ implies that Hypothesis 1.1 is satisfied, that is, there exists a sequence $h_k \in C_0^\infty(\mathbb{M})$ such that $h_k \nearrow 1$ on $\mathbb{M}$, and

$$\|\Gamma(h_k)\|_\infty + \|\Gamma^Z(h_k)\|_\infty \to 0 \quad \text{as } k \to \infty.$$

Following an argument of Strichartz [49, Theorem 7.3, p. 246, and p. 261], this implies that the operators L and $L + L^Z$ are both essentially self-adjoint on the space $C_0^\infty(\mathbb{M})$, where we have let

$$L^Z = -\sum_{m=1}^{\mathfrak{h}} Z_m^* Z_m.$$

We denote by $\mathcal{D}(L)$ the domain of the self-adjoint extension of L.

Lemma 3.3. *The operators L and $L + L^Z$ spectrally commute, that is, for any bounded Borel function $\Psi : (-\infty, 0] \to \mathbb{R}$ and any $f \in L^2(\mathbb{M})$,*

$$\Psi(L)\Psi(L + L^Z)f = \Psi(L + L^Z)\Psi(L)f.$$

Proof. Let $f \in C_0^\infty(\mathbb{M})$. We first observe that

$$\int_{\mathbb{M}} \Gamma^Z(f, Lf)\, d\mu \le 0. \tag{3.2}$$

To see this we note that, thanks to Lemma 2.10,

$$\begin{aligned} 2\int_{\mathbb{M}} \Gamma^Z(f, Lf)\, d\mu &= \int_M L\Gamma^Z(f)\, d\mu - 2\sum_{m=1}^{\mathfrak{h}} \int_{\mathbb{M}} \Gamma(Z_m f)\, d\mu \\ &= -2\sum_{m=1}^{\mathfrak{h}} \int_{\mathbb{M}} \Gamma(Z_m f)\, d\mu \le 0. \end{aligned}$$

Next, we observe that for all $f, g \in C_0^\infty(\mathbb{M})$,

$$0 = \int_{\mathbb{M}} L^Z(fg)\, d\mu = \int_{\mathbb{M}} fL^Z g\, d\mu + \int_{\mathbb{M}} gL^Z f\, d\mu + 2\int_{\mathbb{M}} \Gamma^Z(f, g)\, d\mu.$$

With $f \in C_0^\infty(\mathbb{M})$ and $g = Lf$, this gives

$$-2\int_{\mathbb{M}} \Gamma^Z(f, Lf)\, d\mu = 2\int_{\mathbb{M}} Lf L^Z f\, d\mu.$$

In view of (3.2) this shows that for any $f \in C_0^\infty(\mathbb{M})$,

$$\int_{\mathbb{M}} Lf L^Z f\, d\mu \ge 0.$$

In turn, this implies that for all $f \in C_0^\infty(\mathbb{M})$,

$$\int_{\mathbb{M}} (Lf)^2\, d\mu \le \int_{\mathbb{M}} (Lf + L^Z f)^2\, d\mu. \tag{3.3}$$

But then (3.3) continues to be true for $f \in \mathcal{D}(L + L^Z)$. Let now $f \in \mathcal{D}(L)$ and set

$$\phi(x,t) = LQ_t f(x),$$

where Q_t is the heat semigroup associated with $L + L^Z$. Since L and $L + L^Z$ commute on smooth functions (see Lemma 2.10), we easily see that ϕ solves the heat equation

$$\frac{\partial \phi}{\partial t} = (L + L^Z)\phi$$

with initial condition $\phi(x,0) = Lf(x)$. From (3.3), we see that $\int_{\mathbb{M}} \phi(x,t)^2\, d\mu < \infty$ for every $t \geq 0$. Thus by uniqueness in L^2 of solutions of the heat equation, we conclude that $\phi(x,t) = LQ_t f(x) = Q_t Lf(x)$. By a similar argument, we may prove that for all $f \in L^2(\mathbb{M})$ and $s, t \geq 0$,

$$P_s Q_t f = Q_t P_s f,$$

which implies that L and $L+L^Z$ spectrally commute (see Reed and Simon [45, Chapter 8, Section 5]. □

Lemma 3.4. *There is a constant $C = C(\rho_1, \rho_2, \kappa) > 0$ such that for every smooth function f belonging to $\mathcal{D}(L^2)$,*

$$0 \leq -\int_{\mathbb{M}} \Gamma^Z(f, Lf)\, d\mu \leq C\|f\|^2_{\mathcal{D}(L^2)}, \quad \textit{where} \quad \|f\|^2_{\mathcal{D}(L^2)} = \int_{\mathbb{M}} (f^2 + (L^2 f)^2)\, d\mu.$$

Proof. From Theorem 2.19 we have, for every $\nu > 0$,

$$\Gamma_2(f) + \nu\Gamma_2^Z(f) \geq \left(\rho_1 - \frac{\kappa}{\nu}\right)\Gamma(f) + \rho_2\Gamma^Z(f).$$

Since

$$2\Gamma_2(f) = L\Gamma(f) - 2\Gamma(f, Lf), \quad 2\Gamma_2^Z(f) = L\Gamma^Z(f) - 2\Gamma^Z(f, Lf),$$

we deduce by integration over $\mathbb{M}$ that for $\nu > 0$,

$$\int_{\mathbb{M}} (Lf)^2\, d\mu + \nu \int_{\mathbb{M}} Lf L^Z f\, d\mu \geq \left(\rho_1 - \frac{\kappa}{\nu}\right) \int_{\mathbb{M}} \Gamma(f)\, d\mu + \rho_2 \int_{\mathbb{M}} \Gamma^Z(f)\, d\mu.$$

(One should keep in mind that since $f \in C_0^\infty(\mathbb{M})$, we have $\int_{\mathbb{M}} L\Gamma(f)\, d\mu = \int_{\mathbb{M}} L\Gamma^Z(f)\, d\mu = 0$, and $-\int_{\mathbb{M}} \Gamma(f, Lf)\, d\mu = \int_{\mathbb{M}} (Lf)^2\, d\mu$, $-\int_{\mathbb{M}} \Gamma^Z(f, Lf)\, d\mu = \int_{\mathbb{M}} Lf L^Z f\, d\mu$.) The above inequality can be rewritten as

$$\int_{\mathbb{M}} (Lf)^2\, d\mu + \nu \int_{\mathbb{M}} Lf L^Z f\, d\mu \geq \left(\rho_1 - \frac{\kappa}{\nu}\right) \int_{\mathbb{M}} (-Lf) f\, d\mu + \rho_2 \int_{\mathbb{M}} (-L^Z f) f\, d\mu.$$

From Lemma 2.10, the diffusion operators L and $L + L^Z$ spectrally commute, so by the spectral theorem, there is a measure space (Ω, α), a unitary map $U : L^2_\alpha(\Omega, \mathbb{R}) \to L^2(\mathbb{M})$ and real-valued measurable functions λ and λ^Z on Ω such that for $x \in \Omega$,

$$U^{-1} LUg(x) = -\lambda(x) g(x), \quad U^{-1} L^Z U g(x) = -\lambda^Z(x) g(x).$$

From the previous inequality, we obtain

$$\|\lambda U^{-1} f\|^2_{L^2_\alpha} + \nu\langle \lambda U^{-1} f, \lambda^Z U^{-1} f\rangle_{L^2_\alpha} \geq \left(\rho_1 - \frac{\kappa}{\nu}\right)\langle \lambda U^{-1} f, U^{-1} f\rangle_{L^2_\alpha} + \rho_2\langle \lambda^Z U^{-1} f, U^{-1} f\rangle_{L^2_\alpha}.$$

Since this holds for every smooth and compactly supported function f, we deduce that for every $\nu > 0$, almost everywhere with respect to α,

$$\lambda^2(x) + \nu\lambda^Z(x)\lambda(x) \geq \left(\rho_1 - \frac{\kappa}{\nu}\right)\lambda(x) + \rho_2\lambda^Z(x).$$

In particular, by choosing $\nu = \rho_2(\lambda(x)+1)^{-1}$, we obtain the following inequality for the spectral measures:

$$\frac{\rho_2\lambda^Z}{\lambda+1} \leq -\left(\rho_1 - \frac{\kappa}{\rho_2}\right)\lambda + \left(1 + \frac{\kappa}{\rho_2}\right)\lambda^2. \tag{3.4}$$

As a consequence, for any $f \in \mathcal{D}(L^2)$,

$$\rho_2 \int_{\mathbb{M}} (-L^Z f) f\, d\mu \leq -\left(\rho_1 - \frac{\kappa}{\rho_2}\right)\left(\int_{\mathbb{M}} (-Lf) f\, d\mu + \int_{\mathbb{M}} (Lf)^2\, d\mu\right) + \left(1 + \frac{\kappa}{\rho_2}\right)\left(\int_{\mathbb{M}} (Lf)^2\, d\mu + \int_{\mathbb{M}} (-Lf)(L^2 f)\, d\mu\right). \tag{3.5}$$

By denoting $\mathbf{R} = \rho_2(-L + \mathrm{Id})^{-1}$, we also deduce from (3.4) that for every $f \in \mathcal{D}(L)$,

$$\rho_2 \int_{\mathbb{M}} (-L^Z f)(\mathbf{R} f)\, d\mu \leq -\left(\rho_1 - \frac{\kappa}{\rho_2}\right) \int_{\mathbb{M}} -f Lf\, d\mu + \left(1 + \frac{\kappa}{\rho_2}\right) \int_{\mathbb{M}} (Lf)^2\, d\mu.$$

By using now the above inequality with $-Lf + f$ instead of f, and applying (3.5), we obtain the desired inequality. □

Remark 3.5. The previous proof also shows the following inclusion of domains:

$$\mathcal{D}(L^2) \subset \mathcal{D}(L + L^Z) \subset \mathcal{D}(L).$$

As a consequence of Lemma 3.4, we obtain the following useful a priori bounds.

Proposition 3.6. *There exists a positive constant $C = C(\rho_1, \rho_2, \kappa) > 0$ such that for every smooth function f belonging to $\mathcal{D}(L^2)$,*

$$\int_{\mathbb{M}} \Gamma^Z(f)\, d\mu \leq C\|f\|^2_{\mathcal{D}(L^2)}, \qquad \int_{\mathbb{M}} \Gamma_2^Z(f)\, d\mu \leq C\|f\|^2_{\mathcal{D}(L^2)},$$
$$\int_{\mathbb{M}} \big(\Gamma_2(f) + \Gamma_2^Z(f) - (\rho_1 - \kappa)\Gamma(f)\big)\, d\mu \leq C\|f\|^2_{\mathcal{D}(L^2)}.$$

Proof. Let $f \in C_0^\infty(\mathbb{M})$. According to Lemma 3.4, we have

$$\int_{\mathbb{M}} \Gamma_2^Z(f)\, d\mu = -\int_{\mathbb{M}} \Gamma^Z(f, Lf)\, d\mu \le C_1 \|f\|^2_{\mathcal{D}(L^2)}.$$

Then

$$\int_{\mathbb{M}} \Gamma_2(f)\, d\mu = -\int_{\mathbb{M}} \Gamma(f, Lf)\, d\mu = \int_{\mathbb{M}} (Lf)^2\, d\mu \le \|f\|^2_{\mathcal{D}(L^2)},$$
$$\int_{\mathbb{M}} (Lf)^2\, d\mu + \nu \int_{\mathbb{M}} Lf L^Z f\, d\mu \ge \left(\rho_1 - \frac{\kappa}{\nu}\right) \int_{\mathbb{M}} \Gamma(f,f)\, d\mu + \rho_2 \int_{\mathbb{M}} \Gamma^Z(f,f)\, d\mu,$$

which implies

$$\int_{\mathbb{M}} \Gamma^Z(f)\, d\mu \le C_2 \|f\|^2_{\mathcal{D}(L^2)}.$$

Putting things together, we conclude that for $f \in C_0^\infty(\mathbb{M})$,

$$\int_{\mathbb{M}} \Gamma^Z(f)\, d\mu \le C\|f\|^2_{\mathcal{D}(L^2)}, \qquad \int_{\mathbb{M}} \Gamma_2^Z(f)\, d\mu \le C\|f\|^2_{\mathcal{D}(L^2)},$$
$$\int_{\mathbb{M}} \big(\Gamma_2(f) + \Gamma_2^Z(f) - (\rho_1 - \kappa)\Gamma(f)\big)\, d\mu \le C\|f\|^2_{\mathcal{D}(L^2)}.$$

The inequalities are then extended to the smooth functions of $\mathcal{D}(L^2)$ by using the essential self-adjointness of L which implies the density of $C_0^\infty(\mathbb{M})$ in $\mathcal{D}(L^2)$, and the same arguments as in Bakry [4, 5]. The details are left to the reader. □

4. The heat semigroup and parabolic comparison theorems

We now return to the general framework described in the introduction. Hereafter, $\mathbb{M}$ will be a C^∞ connected manifold endowed with a smooth measure μ and a smooth, locally subelliptic operator L satisfying $L1 = 0$ and (1.3). We denote by $\Gamma(f)$ the quadratic differential form defined by (1.4), and by $d(x, y)$ the associated canonical distance (1.7). As mentioned in the introduction, we assume throughout that $(\mathbb{M}, d)$ is a complete metric space. Furthermore, we assume that $\mathbb{M}$ is endowed with another smooth bilinear differential form, denoted Γ^Z, satisfying (1.9). In particular, $\Gamma^Z(1) = 0$. As stated in the introduction, we assume that $\Gamma^Z(f) \ge 0$ for every $f \in C^\infty(\mathbb{M})$.

From (1.3) we see that, as an operator defined on $C_0^\infty(\mathbb{M})$, L is symmetric with respect to the measure μ and non-positive: $\langle Lf, f\rangle \le 0$ for $f \in C_0^\infty(\mathbb{M})$.

Then, following an argument of Strichartz [49, Theorem 7.3, p. 246, and p. 261], by using the completeness of $(\mathbb{M}, d)$, we conclude that L is essentially self-adjoint on $C_0^\infty(\mathbb{M})$. As a consequence, L admits a unique self-adjoint extension (its Friedrichs extension), still denoted by L. The domain of this extension will be denoted by $\mathcal{D}(L)$.

Hereafter, for $1 \le p \le \infty$ we will write $L^p(\mathbb{M})$ instead of $L^p(\mathbb{M}, \mu)$. If $L = -\int_0^\infty \lambda\, dE_\lambda$ denotes the spectral decomposition of L in $L^2(\mathbb{M})$, then by definition, the heat semigroup $(P_t)_{t\ge 0}$ is given by $P_t = \int_0^\infty e^{-\lambda t} dE_\lambda$. It is a one-parameter family of bounded operators on $L^2(\mathbb{M})$. Since the quadratic form $\mathcal{Q}(f) = -\langle f, Lf\rangle$ is a Dirichlet form in the sense of Fukushima [29], we deduce that $(P_t)_{t\geq 0}$ is a sub-Markov semigroup: it transforms positive functions into positive functions and satisfies

$$P_t 1 \leq 1. \tag{4.1}$$

This property implies in particular

$$\|P_t f\|_{L^1(\mathbb{M})} \leq \|f\|_{L^1(\mathbb{M})}, \qquad \|P_t f\|_{L^\infty(\mathbb{M})} \leq \|f\|_{L^\infty(\mathbb{M})}, \tag{4.2}$$

and therefore by the Riesz–Thorin theorem,

$$\|P_t f\|_{L^p(\mathbb{M})} \leq \|f\|_{L^p(\mathbb{M})}, \quad 1 \leq p \leq \infty. \tag{4.3}$$

From the spectral definition of P_t, it is clear that for all $t > 0$ and $f \in L^2(\mathbb{M})$, $P_t f \in \mathcal{D}_\infty(L) = \bigcap_{k\geq 1} \mathcal{D}(L^k)$. Moreover, the following can be shown as in [37]:

Proposition 4.1. *The unique solution of the Cauchy problem*

$$\begin{cases} \frac{\partial u}{\partial t} - Lu = 0, \\ u(x,0) = f(x), \quad f \in L^p(\mathbb{M}),\ p < \infty, \end{cases}$$

that satisfies $\|u(\cdot,t)\|_p < \infty$ is given by $u(x,t) = P_t f(x)$.

Due to the hypoellipticity of L the function $(x,t) \mapsto P_t f(x)$ is smooth on $\mathbb{M} \times (0,\infty)$ and

$$P_t f(x) = \int_{\mathbb{M}} p(x,y,t) f(y)\, d\mu(y), \qquad f \in C_0^\infty(\mathbb{M}),$$

where $p(x,y,t) > 0$ is the so-called heat kernel associated to P_t. It is smooth and symmetric, i.e.,

$$p(x,y,t) = p(y,x,t).$$

By the semigroup property, for all $x, y \in \mathbb{M}$ and $s, t > 0$ we have

$$\begin{aligned} p(x,y,t+s) &= \int_{\mathbb{M}} p(x,z,t) p(z,y,s)\, d\mu(z) \\ &= \int_{\mathbb{M}} p(x,z,t) p(y,z,s)\, d\mu(z) = P_s(p(x,\cdot,t))(y). \end{aligned} \tag{4.4}$$

We first establish a global comparison theorem in L^2.

Proposition 4.2. *Suppose that $\mathbb{M}$ satisfies Hypothesis 1.1. Let $T > 0$ and let $u, v : \mathbb{M} \times [0,T] \to \mathbb{R}$ be smooth functions such that:*

(i) *$u(\cdot,t) \in L^2(\mathbb{M})$ for every $t \in [0,T]$, and $\int_0^T \|u(\cdot,t)\|_2\, dt < \infty$;*
(ii) *$\int_0^T \|\sqrt{\Gamma(u)(\cdot,t)}\|_p\, dt < \infty$ for some $1 \leq p \leq \infty$;*
(iii) *$v(\cdot,t) \in L^q(\mathbb{M})$ for every $t \in [0,T]$, and $\int_0^T \|v(\cdot,t)\|_q\, dt < \infty$ for some $1 \leq q \leq \infty$.*

If

$$Lu + \frac{\partial u}{\partial t} \geq v \quad \text{on } \mathbb{M} \times [0, T],$$

then

$$P_T u(\cdot, T)(x) \geq u(x, 0) + \int_0^T P_s v(\cdot, s)(x)\, ds.$$

Proof. Let $f, g \in C_0^\infty(\mathbb{M})$ with $f, g \geq 0$. We claim that

$$\int_{\mathbb{M}} g P_T(f u(\cdot, T))\, d\mu - \int_{\mathbb{M}} g f u(x, 0)\, d\mu \geq -\|\sqrt{\Gamma(f)}\|_\infty \int_0^T \int_{\mathbb{M}} (P_t g)\sqrt{\Gamma(u)}\, d\mu\, dt$$
$$- \|\sqrt{\Gamma(f)}\|_\infty \int_0^T \|\sqrt{\Gamma(P_t g)}\|_2 \|u(\cdot, t)\|_2\, dt + \int_{\mathbb{M}} g \int_0^T P_t(f v(\cdot, t))\, d\mu\, dt, \tag{4.5}$$

where for every $1 \leq p \leq \infty$ and a measurable F, we have let $\|F\|_p = \|F\|_{L^p(\mathbb{M})}$. To establish (4.5) we consider the function

$$\phi(t) = \int_{\mathbb{M}} g P_t(f u(\cdot, t))\, d\mu.$$

Differentiating ϕ we find

$$\begin{aligned}
\phi'(t) &= \int_{\mathbb{M}} g P_t\left(L(fu) + f\frac{\partial u}{\partial t}\right) d\mu \\
&= \int_{\mathbb{M}} g P_t\left((Lf)u + 2\Gamma(f, u) + f Lu + f\frac{\partial u}{\partial t}\right) d\mu \\
&\geq \int_{\mathbb{M}} g P_t\big((Lf)u + 2\Gamma(f, u)\big)\, d\mu + \int_{\mathbb{M}} g P_t(f v)\, d\mu.
\end{aligned}$$

Since

$$\begin{aligned}
\int_{\mathbb{M}} g P_t((Lf)u)\, d\mu &= \int_{\mathbb{M}} (P_t g)(Lf) u\, d\mu = -\int_{\mathbb{M}} \Gamma(f, u(P_t g))\, d\mu \\
&= -\left(\int_{\mathbb{M}} \big(P_t g \Gamma(f, u) + u\Gamma(f, P_t g)\big)\, d\mu\right),
\end{aligned}$$

we obtain

$$\phi'(t) \geq \int_{\mathbb{M}} P_t g \Gamma(f, u)\, d\mu - \int_{\mathbb{M}} u\Gamma(f, P_t g)\, d\mu + \int_{\mathbb{M}} g P_t(f v)\, d\mu.$$

Now, we can bound

$$\left|\int_{\mathbb{M}} (P_t g)\Gamma(f, u)\, d\mu\right| \leq \|\sqrt{\Gamma(f)}\|_\infty \int_{\mathbb{M}} (P_t g)\sqrt{\Gamma(u)}\, d\mu,$$

and for a.e. $t \in [0, T]$ the integral on the right-hand side is finite in view of the assumption (ii) above. We have thus obtained

$$\phi'(t) \ge -\|\sqrt{\Gamma(f)}\|_\infty \int_{\mathbb{M}} (P_t g)\sqrt{\Gamma(u)}\, d\mu - \int_{\mathbb{M}} u\Gamma(f, P_t g)\, d\mu + \int_{\mathbb{M}} g P_t(f v(\cdot, t))\, d\mu.$$

As a consequence,

$$\begin{aligned}
&\int_{\mathbb{M}} g P_T(f u(\cdot, T))\, d\mu - \int_{\mathbb{M}} g f u(x, 0)\, d\mu \\
&\quad\ge -\|\sqrt{\Gamma(f)}\|_\infty \int_0^T \int_{\mathbb{M}} (P_t g)\sqrt{\Gamma(u)}\, d\mu\, dt - \int_0^T \int_{\mathbb{M}} u\Gamma(f, P_t g)\, d\mu\, dt \\
&\qquad + \int_0^T \int_{\mathbb{M}} g P_t(f v(\cdot, t))\, d\mu\, dt \\
&\quad\ge -\|\sqrt{\Gamma(f)}\|_\infty \int_0^T \int_{\mathbb{M}} (P_t g)\sqrt{\Gamma(u)}\, d\mu\, dt - \int_0^T \|u(\cdot, t)\|_2 \|\Gamma(f, P_t g)\|_2\, dt \\
&\qquad + \int_{\mathbb{M}} g \int_0^T P_t(f v(\cdot, t))\, dt\, d\mu \\
&\quad\ge -\|\sqrt{\Gamma(f)}\|_\infty \int_0^T \int_{\mathbb{M}} (P_t g)\sqrt{\Gamma(u)}\, d\mu\, dt \\
&\qquad - \|\sqrt{\Gamma(f)}\|_\infty \int_0^T \|u(\cdot, t)\|_2 \|\sqrt{\Gamma(P_t g)}\|_2\, dt + \int_{\mathbb{M}} g \int_0^T P_t(f v(\cdot, t))\, dt\, d\mu,
\end{aligned}$$

which proves (4.5). Let now $h_k \in C_0^\infty(\mathbb{M})$ be a sequence as in Hypothesis 1.1. Using h_k in place of f in (4.5), and letting $k \to \infty$, gives

$$\int_{\mathbb{M}} g P_T(u(\cdot, T))\, d\mu - \int_{\mathbb{M}} g u(x, 0)\, d\mu \ge \int_{\mathbb{M}} g \int_0^T P_t(v(\cdot, t))\, dt\, d\mu.$$

We observe that the assumption on v and Minkowski's integral inequality guarantee that the function $x \mapsto \int_0^T P_t(v(\cdot, t))(x)\, dt$ belongs to $L^q(\mathbb{M})$. We have in fact

$$\begin{aligned}
\left(\int_{\mathbb{M}} \left| \int_0^T P_t(v(\cdot, t))\, dt \right|^q d\mu \right)^{1/q} &\le \int_0^T \left| \int_{\mathbb{M}} |P_t(v(\cdot, t))|^q\, d\mu \right|^{1/q} dt \\
&\le \int_0^T \left| \int_{\mathbb{M}} |v(\cdot, t)|^q\, d\mu \right|^{1/q} dt \le T^{1/q'} \left(\int_0^T \int_{\mathbb{M}} |v(\cdot, t)|^q\, d\mu\, dt \right)^{1/q} < \infty.
\end{aligned}$$

Since this must hold for every non-negative $g \in C_0^\infty(\mathbb{M})$, we conclude that

$$P_T(u(\cdot, T))(x) \ge u(x, 0) + \int_0^T P_s(v(\cdot, s))(x)\, ds,$$

which completes the proof. □

The next theorem shows that Hypothesis 1.4 is redundant on complete sub-Riemannian manifolds with transverse symmetries of Yang–Mills type if the sub-Laplacian L satisfies the generalized curvature dimension inequality.

Theorem 4.3. *Let L be the sub-Laplacian on a complete sub-Riemannian manifold with transverse symmetries of Yang–Mills type. Suppose that L satisfies* $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ *for some $\rho_1 \in \mathbb{R}$. Then Hypothesis 1.4 is satisfied.*

Proof. Let $f \in C_0^\infty(\mathbb{M})$ and consider the functional

$$\Phi(t) = \sqrt{\Gamma^Z(P_{T-t} f)}.$$

We first assume that $\Gamma^Z(P_t f)(x) > 0$ for all $(x,t) \in \mathbb{M} \times [0,T]$. From Proposition 3.6 we have $\Phi(t) \in L^2(\mathbb{M})$. Moreover $\Gamma(\Phi)(t) = \frac{\Gamma(\Gamma^Z(P_{T-t}f))}{4\Gamma^Z(P_{T-t}f)}$. So Proposition 3.2 yields $\Gamma(\Phi)(t) \le \Gamma_2^Z(P_{T-t} f)$. Therefore, again from Proposition 3.6, we deduce that $\Gamma(\Phi)(t) \in L^1(\mathbb{M})$. Next, we easily compute that

$$\frac{\partial \Phi}{\partial t} + L\Phi = \frac{\Gamma_2^Z(P_{T-t} f)}{\sqrt{\Gamma^Z(P_{T-t} f)}} - \frac{\Gamma(\Gamma^Z(P_{T-t} f))}{4\Gamma^Z(P_{T-t} f)^{3/2}}.$$

Thus, Proposition 3.2 implies that

$$\frac{\partial \Phi}{\partial t} + L\Phi \ge 0.$$

We can then use Proposition 4.2 to infer that

$$\sqrt{\Gamma^Z(P_T f)} \le P_T\big(\sqrt{\Gamma^Z(f)}\big).$$

This implies that for every $t \ge 0$, $\Gamma^Z(P_t f) \in L^p(\mathbb{M})$ for every $1 \le p \le \infty$. If $\Gamma^Z(P_t f)(x)$ vanishes for all $(x,t) \in \mathbb{M} \times [0,T]$, we consider the functional

$$\Phi(t) = g_\varepsilon(\Gamma^Z(P_{T-t} f)),$$

where, for $0 < \varepsilon < 1$,

$$g_\varepsilon(y) = \sqrt{y + \varepsilon^2} - \varepsilon.$$

Since $\Phi(t) \in L^2(\mathbb{M})$, an argument similar to that above (the details are left to the reader) shows that

$$g_\varepsilon(\Gamma^Z(P_T f)) \le P_T(g_\varepsilon(\Gamma^Z(f))).$$

Letting $\varepsilon \to 0$, we conclude that

$$\sqrt{\Gamma^Z(P_T f)} \le P_T\big(\sqrt{\Gamma^Z(f)}\big).$$

Proving that $(x,t) \mapsto \Gamma(P_t f)(x)$ is bounded is similar. For $\alpha \in \mathbb{R}$, we consider the functional

$$\Psi(t) = e^{-\alpha(T-t)}\big(\sqrt{\Gamma(P_{T-t} f)} + \Gamma^Z(P_{T-t} f)\big),$$

and first assume that $(x,t) \mapsto \Gamma(P_t f)(x)$ does not vanish on $\mathbb{M} \times [0,T]$. From the previous inequality, Proposition 3.6 and Proposition 3.2, it is seen that $\Psi(t) \in L^2(\mathbb{M})$ and $\sqrt{\Gamma(\Psi)(t)} \in L^1(\mathbb{M}) + L^2(\mathbb{M})$. Moreover,

$$\frac{\partial \Psi}{\partial t} + L\Psi = e^{-\alpha(T-t)}\left(\frac{\Gamma_2(P_{T-t}f)}{\sqrt{\Gamma(P_{T-t}f)}} - \frac{\Gamma(\Gamma(P_{T-t}f))}{4\Gamma(P_{T-t}f)^{3/2}} + 2\Gamma_2^Z(P_{T-t}f)\right) + \alpha\Phi.$$

According to Proposition 3.2, for all $f \in C^\infty(\mathbb{M})$ and $\nu > 0$ we have

$$\Gamma(\Gamma(f)) \leq 4\Gamma(f)\left(\Gamma_2(f) + \nu\Gamma_2^Z(f) - \left(\rho_1 - \frac{\kappa}{\nu}\right)\Gamma(f)\right).$$

Choosing $\nu = 2\sqrt{\Gamma(f)}$ gives

$$\frac{\Gamma_2(f)}{\sqrt{\Gamma(f)}} - \frac{\Gamma(\Gamma(f))}{4\Gamma(f)^{3/2}} + 2\Gamma_2^Z(f) \geq \rho_1\sqrt{\Gamma(f)} - \frac{\kappa}{2}.$$

We deduce that

$$\frac{\partial \Psi}{\partial t} + L\Psi \geq e^{-\alpha(T-t)}\big((\alpha+\rho_1)\sqrt{\Gamma(P_{T-t}f)} + \alpha\Gamma^Z(P_{T-t}f)\big) - \frac{\kappa}{2}e^{-\alpha(T-t)}.$$

Therefore, by choosing α large enough we obtain

$$\frac{\partial \Psi}{\partial t} + L\Psi \geq -\frac{\kappa}{2}e^{-\alpha(T-t)}.$$

As a consequence of Proposition 4.2, we find

$$\sqrt{\Gamma(P_T f)} + \Gamma^Z(P_T f) \leq e^{\alpha T}\big(P_T(\sqrt{\Gamma}(f)) + P_T(\Gamma^Z(f))\big) + \frac{\kappa}{2}e^{\alpha T}\int_0^T (P_s 1)\, ds.$$

Since $P_s 1 \leq 1$, we conclude that

$$\sqrt{\Gamma(P_T f)} + \Gamma^Z(P_T f) \leq e^{\alpha T}\big(P_T(\sqrt{\Gamma}(f)) + P_T(\Gamma^Z(f))\big) + \frac{\kappa}{2}Te^{\alpha T}.$$

This implies that $(x,t) \mapsto \Gamma(P_t f)(x) + \Gamma^Z(P_t f)(x) \in L^\infty(\mathbb{M} \times [0,T])$. If $(x,t) \mapsto \Gamma(P_t f)(x)$ does vanish somewhere on $\mathbb{M} \times [0,T]$, then we consider the C^∞ approximation of the square root as above.

We now prove that $P_t 1 = 1$, that is, P_t is stochastically complete. A first consequence of the fact that for all $f \in C_0^\infty(\mathbb{M})$ and $T \geq 0$, $(x,t) \mapsto \Gamma(P_t f)(x) + \Gamma^Z(P_t f)(x)$ is in $L^\infty(\mathbb{M} \times [0,T])$, is that in Proposition 4.2 we can now allow u to be in L^1. More precisely, under the assumptions of Proposition 4.2 with (i) replaced by: $u(\cdot,t) \in L^1(\mathbb{M})$ for every $t \in [0,T]$ and $\int_0^T \|u(\cdot,t)\|_1\, dt < \infty$, we still have the conclusion

$$P_T(u(\cdot,T))(x) \geq u(x,0) + \int_0^T P_s(v(\cdot,s))(x)\, ds.$$

The proof is identical to that of Proposition 4.2. With the notation of that proof, $\Gamma(P_{\cdot}g) \in L^\infty([0,T]\times\mathbb{M})$ is used to obtain the bound

$$\left|\int_0^T \int_{\mathbb{M}} u\Gamma(f, P_t g)\, d\mu\, dt\right| \le \|\sqrt{\Gamma(f)}\|_\infty \int_0^T \|\sqrt{\Gamma(P_t g)}\|_\infty \|u(\cdot,t)\|_1\, dt.$$

This leads to an inequality replacing (4.5):

$$\begin{aligned}\int_{\mathbb{M}} g P_T(fu(\cdot,T))\, d\mu - \int_{\mathbb{M}} gfu(x,0)\, d\mu \ge -\|\sqrt{\Gamma(f)}\|_\infty \int_0^T \int_{\mathbb{M}} (P_t g)\sqrt{\Gamma(u)}\, d\mu\, dt \\ - \|\sqrt{\Gamma(f)}\|_\infty \int_0^T \|\sqrt{\Gamma(P_t g)}\|_\infty \|u(\cdot,t)\|_1\, dt + \int_{\mathbb{M}} g \int_0^T P_t(fv(\cdot,t))\, d\mu\, dt. \qquad (4.6)\end{aligned}$$

From this point on, the argument proceeds exactly as in the conclusion of the proof of Proposition 4.2.

With this L^1 comparison result in hand, we can now come back to the stochastic completeness problem. Let $f \in C_0^\infty(\mathbb{M})$ and consider the functional

$$u(x,t) = e^{\alpha(T-t)}\big(\Gamma(P_{T-t}f)(x) + \Gamma^Z(P_{T-t}f)(x)\big).$$

We have

$$\begin{aligned}&Lu(x,t) = e^{\alpha(T-t)}\big(L\Gamma(P_{T-t}f)(x) + L\Gamma^Z(P_{T-t}f)(x)\big),\\ &\frac{\partial u}{\partial t}(x,t) = -\alpha u(x,t) - 2e^{\alpha(T-t)}\big(\Gamma(P_{T-t}f, LP_{T-t})(x) + \Gamma^Z(P_{T-t}f, LP_{T-t})(x)\big).\end{aligned}$$

Therefore

$$Lu(x,t) + \frac{\partial u}{\partial t}(x,t) = -\alpha u(x,t) + 2e^{\alpha(T-t)}\big(\Gamma_2(P_{T-t}f)(x) + \Gamma_2^Z(P_{T-t}f)(x)\big).$$

By using now the inequality $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ with $\nu = 1$, we obtain

$$Lu(x,t) + \frac{\partial u}{\partial t}(x,t) \ge e^{\alpha(T-t)}\big((2(\rho_1-\kappa)-\alpha)\Gamma(P_{T-t}f)(x) + (2\rho_2-\alpha)\Gamma^Z(P_{T-t}f)(x)\big).$$

By choosing $\alpha \le 2\min\{\rho_2, \rho_1 - \kappa\}$, we thus get

$$Lu(x,t) + \frac{\partial u}{\partial t}(x,t) \ge 0,$$

and by using the L^1 version of Proposition 4.5 we conclude that

$$\Gamma(P_t f) + \Gamma^Z(P_t f) \le e^{-\alpha t}\big(P_t\Gamma(f) + P_t\Gamma^Z(f)\big). \qquad (4.7)$$

We are now ready for the final argument leading to the stochastic completeness. Let $f, g \in C_0^\infty(\mathbb{M})$. By (1.3) and (1.4) we have

$$\int_{\mathbb{M}} (P_t f - f) g \, d\mu = \int_0^t \int_{\mathbb{M}} \left(\frac{\partial}{\partial s} P_s f \right) g \, d\mu \, ds = \int_0^t \int_{\mathbb{M}} (L P_s f) g \, d\mu \, ds$$
$$= - \int_0^t \int_{\mathbb{M}} \Gamma(P_s f, g) \, d\mu \, ds.$$

By means of the Cauchy–Schwarz inequality and (4.7), we find

$$\left| \int_{\mathbb{M}} (P_t f - f) g \, d\mu \right| \le \left(\int_0^t e^{-\alpha s/2} \, ds \right) \sqrt{\|\Gamma(f)\|_\infty + \|\Gamma^Z(f)\|_\infty} \int_{\mathbb{M}} \Gamma(g)^{1/2} \, d\mu. \tag{4.8}$$

We now apply (4.8) with $f = h_k$, where h_k is the sequence whose existence is postulated in Hypothesis 1.1, and then let $k \to \infty$. By Beppo Levi's monotone convergence theorem we have $P_t h_k(x) \nearrow P_t 1(x)$ for every $x \in \mathbb{M}$. We conclude that the left-hand side of (4.8) converges to $\int_{\mathbb{M}} (P_t 1 - 1) g \, d\mu$. Since in view of Hypothesis 1.1 the right-hand side converges to zero, we reach the conclusion

$$\int_{\mathbb{M}} (P_t 1 - 1) g \, d\mu = 0, \qquad g \in C_0^\infty(\mathbb{M}).$$

It follows that $P_t 1 = 1$. □

We point out that the stochastic completeness of the heat semigroup is classically equivalent to uniqueness in the Cauchy problem for initial data in $L^\infty(\mathbb{M})$. Following the classical approach (see for instance [31, Theorem 8.18]), we in fact obtain:

Proposition 4.4. *Suppose that $\mathbb{M}$ satisfies Hypotheses 1.1 and 1.4. Then for every $f \in L^\infty(\mathbb{M})$ the Cauchy problem*

$$\begin{cases} Lu - u_t = 0 & \text{in } \mathbb{M} \times (0, \infty), \\ u(x, 0) = f(x), & f \in L^\infty(\mathbb{M}), \end{cases}$$

has a unique bounded solution, given by $u(x, t) = P_t f(x)$.

We state the following L^∞ global parabolic comparison theorem that will be easier to use than Proposition 4.2 because it does not require a priori bounds on the derivatives.

Proposition 4.5. *Suppose that $\mathbb{M}$ satisfies Hypothesis 1.4. Let $T > 0$. Let $u, v : \mathbb{M} \times [0, T] \to \mathbb{R}$ be smooth functions such that for every $T > 0$, $\sup_{t \in [0,T]} \|u(\cdot, t)\|_\infty < \infty$ and $\sup_{t \in [0,T]} \|v(\cdot, t)\|_\infty < \infty$. If*

$$Lu + \frac{\partial u}{\partial t} \ge v \quad \text{on } \mathbb{M} \times [0, T],$$

then

$$P_T(u(\cdot, T))(x) \ge u(x, 0) + \int_0^T P_s(v(\cdot, s))(x) \, ds.$$

Proof. Let $(X_t^x)_{t\ge 0}$ be the diffusion Markov process with semigroup $(P_t)_{t\ge 0}$ and started at $x \in \mathbb{M}$ (see for instance [29, Chapter 7] for the construction of that process). From $P_t 1 = 1$, we deduce that $(X_t^x)_{t\ge 0}$ has an infinite lifetime. Then, for $t \ge 0$,

$$u(X_t^x, t) = u(x, 0) + \int_0^t \left(Lu + \frac{\partial u}{\partial t} \right)(X_s^x, s)\, ds + M_t,$$

where $(M_t)_{t\ge 0}$ is a local martingale. From the assumption one obtains

$$u(X_t^x, t) \ge u(x, 0) + \int_0^t v(X_s^x, s)\, ds + M_t.$$

Let now $(T_n)_{n\in\mathbb{N}}$ be an increasing sequence of stopping times such that almost surely $T_n \to \infty$ and $(M_{t\wedge T_n})_{t\ge 0}$ is a martingale. From the previous inequality, we find

$$\mathbb{E}(u(X_{t\wedge T_n}^x, t\wedge T_n)) \ge u(x, 0) + \mathbb{E}\left(\int_0^{t\wedge T_n} v(X_s^x, s)\, ds \right).$$

By using the dominated convergence theorem, we deduce that

$$\mathbb{E}(u(X_t^x, t)) \ge u(x, 0) + \mathbb{E}\left(\int_0^t v(X_s^x, s)\, ds \right),$$

which yields the conclusion. □

For later use, we also record the following gradient bounds that are consequences of Hypothesis 1.4.

Corollary 4.6. *Suppose that L satisfies $\mathrm{CD}(\rho_1, \rho_2, \kappa, d)$ for some $\rho_1 \in \mathbb{R}$ and Hypothesis 1.4 is satisfied. There exists $\alpha \in \mathbb{R}$ ($\alpha \le 2\min\{\rho_2, \rho_1 - \kappa\}$ will do) such that for every $f \in C_0^\infty(\mathbb{M})$,*

$$\Gamma(P_t f) + \Gamma^Z(P_t f) \le e^{-\alpha t}\big(P_t \Gamma(f) + P_t \Gamma^Z(f)\big). \tag{4.9}$$

As a consequence, for every $f \in C_0^\infty(\mathbb{M})$ and $1 \le p \le \infty$,

$$\|\Gamma(P_t f)\|_{L^p(\mathbb{M})} \le e^{-\alpha t}(\|\Gamma(f)\|_{L^p(\mathbb{M})} + \|\Gamma^Z(f)\|_{L^p(\mathbb{M})}), \quad t \ge 0, \tag{4.10}$$

$$\|\Gamma^Z(P_t f)\|_{L^p(\mathbb{M})} \le e^{-\alpha t}(\|\Gamma(f)\|_{L^p(\mathbb{M})} + \|\Gamma^Z(f)\|_{L^p(\mathbb{M})}), \quad t \ge 0. \tag{4.11}$$

Proof. The proof is identical to that of (4.7) except that we now use Proposition 4.5. □

5. Entropic variational inequalities

Our objective in this section is to prove a fundamental variational inequality which will play a pervasive role in our study (see Theorem 5.2). We begin with some preliminary results. Henceforth, we write $C_b^\infty(\mathbb{M}) = C^\infty(\mathbb{M}) \cap L^\infty(\mathbb{M})$.

Lemma 5.1. *Let $f \in C_b^\infty(\mathbb{M})$, $f > 0$ and $T > 0$, and consider the functions*

$$\phi_1(x,t) = (P_{T-t}f)(x)\Gamma(\ln P_{T-t}f)(x),$$
$$\phi_2(x,t) = (P_{T-t}f)(x)\Gamma^Z(\ln P_{T-t}f)(x),$$

defined on $\mathbb{M} \times (-\infty, T)$. Then

$$L\phi_1 + \frac{\partial\phi_1}{\partial t} = 2(P_{T-t}f)\Gamma_2(\ln P_{T-t}f).$$

If furthermore Hypothesis 1.2 is valid, then

$$L\phi_2 + \frac{\partial\phi_2}{\partial t} = 2(P_{T-t}f)\Gamma_2^Z(\ln P_{T-t}f).$$

Proof. Let for simplicity $g(x,t) = P_{T-t}f(x)$. A simple computation gives

$$\frac{\partial\phi_1}{\partial t} = g_t\Gamma(\ln g) + 2g\Gamma\left(\ln g, \frac{g_t}{g}\right).$$

On the other hand,

$$L\phi_1 = Lg\Gamma(\ln g) + gL\Gamma(\ln g) + 2\Gamma(g, \Gamma(\ln g)).$$

Combining these equations we obtain

$$L\phi_1 + \frac{\partial\phi_1}{\partial t} = gL\Gamma(\ln g) + 2\Gamma(g, \Gamma(\ln g)) + 2g\Gamma\left(\ln g, \frac{g_t}{g}\right).$$

From (1.10) we see that

$$2g\Gamma_2(\ln g) = g(L\Gamma(\ln g) - 2\Gamma(\ln g, L(\ln g))) = gL\Gamma(\ln g) - 2g\Gamma(\ln g, L(\ln g)).$$

Observing that $L(\ln g) = -\Gamma(g)/g^2 - g_t/g$, we conclude that

$$L\phi_1 + \frac{\partial\phi_1}{\partial t} = 2(P_{T-t}f)\Gamma_2(\ln P_{T-t}f).$$

In the same vein, we obtain

$$L\phi_2 + \frac{\partial\phi_2}{\partial t} = gL\Gamma^Z(\ln g) + 2\Gamma(g, \Gamma^Z(\ln g)) + 2g\Gamma^Z\left(\ln g, \frac{g_t}{g}\right).$$

On the other hand, this time using (1.11), we find

$$\begin{aligned} 2g\Gamma_2^Z(\ln g) &= g\big(L\Gamma^Z(\ln g) - 2\Gamma^Z(\ln g, L(\ln g))\big) \\ &= gL\Gamma^Z(\ln g) + 2g\Gamma^Z\left(\ln g, \frac{\Gamma(g)}{g^2}\right) + 2g\Gamma^Z\left(\ln g, \frac{g_t}{g}\right). \end{aligned}$$

From this last equation it is now clear that if Hypothesis 1.2 is valid, then

$$L\phi_2 + \frac{\partial\phi_2}{\partial t} = 2g\Gamma_2^Z(\ln g).$$

This concludes the proof. □

We now turn to our most important variational inequality. Given $f \in C_b^\infty(\mathbb{M})$ and $\varepsilon > 0$, we let $f_\varepsilon = f + \varepsilon$.

Suppose that $T > 0$, and let $x \in \mathbb{M}$ be given. For a function $f \in C_b^\infty(\mathbb{M})$ with $f \geq 0$ we define, for $t \in [0, T]$,

$$\Phi_1(t) = P_t\big((P_{T-t} f_\varepsilon)\Gamma(\ln P_{T-t} f_\varepsilon)\big),$$
$$\Phi_2(t) = P_t\big((P_{T-t} f_\varepsilon)\Gamma^Z(\ln P_{T-t} f_\varepsilon)\big).$$

Theorem 5.2. *Suppose that Hypotheses 1.1, 1.2 and 1.4 are satisfied and the curvature-dimension inequality (1.12) holds for some $\rho_1 \in \mathbb{R}$. Let $a, b \in C^1([0,T],[0,\infty))$ and $\gamma \in C((0,T),\mathbb{R})$ be such that $a' + 2\rho_1 a - 2\kappa a^2/b - 4a\gamma/d$, $b' + 2\rho_2 a$, $a\gamma$, $a\gamma^2$ are continuous functions on $[0,T]$. Given $f \in C_0^\infty(\mathbb{M})$ with $f \geq 0$, we have*

$$\begin{aligned}
a(T)P_T(f_\varepsilon\Gamma(\ln f_\varepsilon)) &+ b(T)P_T(f_\varepsilon\Gamma^Z(\ln f_\varepsilon)) - a(0)(P_T f_\varepsilon)\Gamma(\ln P_T f_\varepsilon) - b(0)\Gamma^Z(\ln P_T f_\varepsilon)\\
&\geq \int_0^T \left(a' + 2\rho_1 a - 2\kappa\frac{a^2}{b} - \frac{4a\gamma}{d}\right)\Phi_1\, ds + \int_0^T (b' + 2\rho_2 a)\Phi_2\, ds\\
&\quad + \left(\frac{4}{d}\int_0^T a\gamma\, ds\right) L P_T f_\varepsilon - \left(\frac{2}{d}\int_0^T a\gamma^2 ds\right) P_T f_\varepsilon.
\end{aligned}$$

Proof. Let $f \in C^\infty(\mathbb{M})$ with $f \geq 0$. Consider the function

$$\phi(x,t) = a(t)(P_{T-t} f)(x)\Gamma(\ln P_{T-t} f)(x) + b(t)(P_{T-t} f)(x)\Gamma^Z(\ln P_{T-t} f)(x).$$

Applying Lemma 5.1 and the curvature-dimension inequality (1.12), we obtain

$$\begin{aligned}
L\phi + \frac{\partial\phi}{\partial t} &= a'(P_{T-t} f)\Gamma(\ln P_{T-t} f) + b'(P_{T-t} f)\Gamma^Z(\ln P_{T-t} f)\\
&\quad + 2a(P_{T-t} f)\Gamma_2(\ln P_{T-t} f) + 2b(P_{T-t} f)\Gamma_2^Z(\ln P_{T-t} f)\\
&\geq \left(a' + 2\rho_1 a - 2\kappa\frac{a^2}{b}\right)(P_{T-t} f)\Gamma(\ln P_{T-t} f)\\
&\quad + (b' + 2\rho_2 a)(P_{T-t} f)\Gamma^Z(\ln P_{T-t} f) + \frac{2a}{d}(P_{T-t} f)(L(\ln P_{T-t} f))^2.
\end{aligned}$$

But

$$(L(\ln P_{T-t} f))^2 \geq 2\gamma L(\ln P_{T-t} f) - \gamma^2$$

and

$$L(\ln P_{T-t} f) = \frac{L P_{T-t} f}{P_{T-t} f} - \Gamma(\ln P_{T-t} f).$$

Therefore,

$$\begin{aligned}
L\phi + \frac{\partial\phi}{\partial t} &\geq \left(a' + 2\rho_1 a - 2\kappa\frac{a^2}{b} - \frac{4a\gamma}{d}\right)(P_{T-t} f)\Gamma(\ln P_{T-t} f)\\
&\quad + (b' + 2\rho_2 a)(P_{T-t} f)\Gamma^Z(\ln P_{T-t} f) + \frac{4a\gamma}{d} L P_{T-t} f - \frac{2a\gamma^2}{d} P_{T-t} f.
\end{aligned}$$

If now $f \in C_0^\infty(\mathbb{M})$ with $f \geq 0$, we obtain the same differential inequality with f_ε instead of f throughout. Now we apply Proposition 4.5 to reach the desired conclusion. □

The following corollary is of particular importance.

Corollary 5.3. *Under the assumptions of Theorem 5.2, let $b : [0, T] \to [0, \infty)$ be a non-increasing C^2 function such that, with*

$$\gamma := \frac{d}{4}\left(\frac{b''}{b'} + \frac{\kappa}{\rho_2}\frac{b'}{b} + 2\rho_1\right), \tag{5.1}$$

the functions $b'\gamma, b'\gamma^2$ are continuous on $[0, T]$. Then, for $f \in C_0^\infty(\mathbb{M})$,

$$\begin{aligned}
-\frac{b'(T)}{2\rho_2} P_T(f_\varepsilon\Gamma(\ln f_\varepsilon)) + b(T)P_T(f_\varepsilon\Gamma^Z(\ln f_\varepsilon)) \\
+ \frac{b'(0)}{2\rho_2}(P_T f_\varepsilon)\Gamma(\ln P_T f_\varepsilon) - b(0)\Gamma^Z(\ln P_T f_\varepsilon) \\
\geq -\left(\frac{2}{d\rho_2}\int_0^T b'\gamma\, ds\right) L P_T f_\varepsilon + \left(\frac{1}{d\rho_2}\int_0^T b'\gamma^2\, ds\right) P_T f_\varepsilon.
\end{aligned} \tag{5.2}$$

Proof. We choose $a : [0, T] \to [0, \infty)$ of class C^1 so that $b' + 2\rho_2 a = 0$. With this choice, and with γ defined by (5.1), we obtain

$$a' + 2\rho_1 a - 2\kappa\frac{a^2}{b} - \frac{4a\gamma}{d} = 0.$$

Applying Theorem 5.2 with these a, b and γ yields the desired conclusion. □

6. Li–Yau type estimates

In this section, we extend the celebrated Li–Yau inequality [38] to the heat semigroup associated with the subelliptic operator L. Let us mention that, in this setting, related inequalities were obtained by Cao–Yau [16]. However, these authors work locally and the geometry of the manifold does not enter their study. Instead, our analysis is based on the entropic inequalities established in Section 5, and so it hinges crucially on our curvature-dimension inequality (1.12). As shown in the discussion of the examples in Section 2, this inequality is deeply connected to the sub-Riemannian geometry of the manifold. We have mentioned in the introduction that, even when specialized to the Riemannian case, the ideas in this section provide a new, more elementary approach to the Li–Yau inequalities. For this aspect we refer the reader to [14].

Theorem 6.1 (Gradient estimate). *Assume that Hypotheses 1.1, 1.2 and 1.4 hold and the curvature-dimension inequality (1.12) is satisfied for some $\rho_1 \in \mathbb{R}$. Let $f \in C_0^\infty(\mathbb{M})$ with $f \geq 0$, $f \not\equiv 0$. Then for $t > 0$,*

$$\begin{aligned}
\Gamma(\ln P_t f) + \frac{2\rho_2}{3} t\Gamma^Z(\ln P_t f) \\
\leq \left(1 + \frac{3\kappa}{2\rho_2} - \frac{2\rho_1}{3}t\right)\frac{LP_t f}{P_t f} + \frac{d\rho_1^2}{6}t - \frac{\rho_1 d}{2}\left(1 + \frac{3\kappa}{2\rho_2}\right) + \frac{d\left(1 + \frac{3\kappa}{2\rho_2}\right)^2}{2t}.
\end{aligned}$$

Proof. We apply Corollary 5.3, in which we choose $b(t) = (T-t)^3$. With this choice, (5.1) gives

$$\gamma(t) = \frac{d}{2}\left(\rho_1 - \frac{1}{T-t}\left(1+\frac{3\kappa}{2\rho_2}\right)\right),$$

and thus $b'\gamma, b'\gamma^2 \in C([0,t]), \mathbb{R})$. Simple calculations give

$$\int_0^T b'(t)\gamma(t)\,dt = -\frac{\rho_1 d}{2}T^3 + \frac{3d}{4}\left(1+\frac{3\kappa}{2\rho_2}\right)T^2,$$
$$\int_0^T b'(t)\gamma(t)^2\,dt = -\frac{3d^2}{16}\left(\frac{4\rho_1^2}{3}T^3 + 4\left(1+\frac{3\kappa}{2\rho_2}\right)^2 T - 4\rho_1\left(1+\frac{3\kappa}{2\rho_2}\right)T^2\right).$$

Using the last two equations in (5.2) and letting $\varepsilon \to 0$, by the arbitrariness of $T > 0$ we obtain the desired conclusion. □

Remark 6.2. We notice that if $\rho_1 \geq \rho_1'$, then trivially

$$\mathrm{CD}(\rho_1,\rho_2,\kappa,d) \;\Rightarrow\; \mathrm{CD}(\rho_1',\rho_2,\kappa,d).$$

As a consequence, if (1.12) holds with some $\rho_1 > 0$, then also $\mathrm{CD}(0,\rho_2,\kappa,d)$ is true. Therefore, when $\rho_1 > 0$, Theorem 6.1 gives in particular, for $f \in C_0^\infty(\mathbb{M})$ with $f \geq 0$,

$$\Gamma(\ln P_t f) + \frac{2\rho_2}{3}t\Gamma^Z(\ln P_t f) \leq \left(1+\frac{3\kappa}{2\rho_2}\right)\frac{LP_t f}{P_t f} + \frac{d\left(1+\frac{3\kappa}{2\rho_2}\right)^2}{2t}. \tag{6.1}$$

However, this inequality is not optimal when $\rho_1 > 0$. It leads to an optimal Harnack inequality only when $\rho_1 = 0$. Sharper bounds in the case $\rho_1 > 0$ will be obtained in (10.4) of Proposition 10.2 below by a different choice of the function $b(t)$ of Corollary 5.3.

Remark 6.3. Throughout the remainder of the paper, the symbol D will always mean

$$D = d\left(1+\frac{3\kappa}{2\rho_2}\right). \tag{6.2}$$

With this notation, as the left-hand side of (6.1) is always non-negative, and $LP_t f = \partial_t P_t f$, when $\rho_1 \geq 0$ we obtain

$$\partial_t(\ln(t^{D/2}P_t f(x))) \geq 0. \tag{6.3}$$

Integrating (6.3) from $t < 1$ to 1 leads to the following diagonal bound for the heat kernel:

$$p(x,x,t) \leq \frac{1}{t^{D/2}}p(x,x,1). \tag{6.4}$$

The constant $D/2$ in (6.4) is not optimal in general, as the example of the heat semigroup on a Carnot group shows. In that case, in fact, one can argue as in [27] to show that the heat kernel $p(x, y, t)$ is homogeneous of degree $-Q/2$ with respect to the non-isotropic group dilations, where Q indicates the corresponding homogeneous dimension of the group. From that homogeneity of $p(x, y, t)$, one obtains the estimate

$$p(x, x, t) \leq \frac{1}{t^{Q/2}} p(x, x, 1),$$

which, unlike (6.4), is best possible. In the sub-Riemannian setting it does not seem easy to obtain sharp geometric constants by using only the curvature-dimension inequality (1.12). This aspect is quite different from the Riemannian case, for which the $\mathrm{CD}(\rho_1, n)$ inequality (1.2) does provide sharp geometric constants (see [6], [36]). However, in that case our bound (6.4) is sharp as well, since if $d = n = \dim(\mathbb{M})$ and $\kappa = 0$, then (6.2) gives $D = n$.

7. A parabolic Harnack inequality

In this section we generalize the celebrated Harnack inequality of [38] to solutions of the heat equation $Lu - u_t = 0$ on $\mathbb{M}$ which are of the form $u(x, t) = P_t f(x)$ for some $f \in C_b^\infty(\mathbb{M})$, $f \geq 0$. Theorem 7.1 below should be seen as a generalization of [38, Theorem 2.2(i)] in the case of a zero potential q. See also [16], where the authors deal with subelliptic operators on a compact manifold. As already mentioned, these authors do not obtain bounds which depend on the sub-Riemannian geometry of the underlying manifold.

Theorem 7.1. *Assume Hypotheses 1.1, 1.2 and 1.4 hold and the curvature-dimension inequality (1.12) is satisfied for some $\rho_1 \geq 0$. Given $(x, s), (y, t) \in \mathbb{M} \times (0, \infty)$ with $s < t$, for any $f \in C_b^\infty(\mathbb{M})$, $f \geq 0$, one has*

$$P_s f(x) \leq P_t f(y) \left(\frac{t}{s}\right)^{D/2} \exp\left(\frac{D}{d} \frac{d(x, y)^2}{4(t - s)}\right). \tag{7.1}$$

Proof. Let $f \in C_0^\infty(\mathbb{M})$ be as in the statement, and for every $(x, t) \in \mathbb{M} \times (0, \infty)$ consider $u(x, t) = P_t f(x)$. Since $Lu = \frac{\partial u}{\partial t}$, in terms of u the inequality (6.1) can be reformulated as

$$\Gamma(\ln u) + \frac{2\rho_2}{3} t \Gamma^Z(\ln u) \leq \left(1 + \frac{3\kappa}{2\rho_2}\right) \frac{\partial \log u}{\partial t} + \frac{d\left(1 + \frac{3\kappa}{2\rho_2}\right)^2}{2t}.$$

Recalling (6.2), this implies in particular,

$$-\frac{\partial \ln u}{\partial t} \leq -\frac{d}{D} \Gamma(\ln u) + \frac{D}{2t}. \tag{7.2}$$

We now fix $(x, s), (y, t) \in \mathbb{M} \times (0, \infty)$ with $s < t$. Let $\gamma(\tau)$, $0 \leq \tau \leq T$, be a subunit path such that $\gamma(0) = y$, $\gamma(T) = x$ (for the definition of a subunit path see the introduction or [25]). Consider the path in $\mathbb{M} \times (0, \infty)$ defined by

$$\alpha(\tau) = \left(\gamma(\tau), t + \frac{s - t}{T} \tau\right), \qquad 0 \leq \tau \leq T,$$

so that $\alpha(0) = (y, t)$, $\alpha(T) = (x, s)$. We have

$$\ln \frac{u(x,s)}{u(y,t)} = \int_0^T \frac{d}{d\tau} \ln u(\alpha(\tau))\, d\tau$$
$$\leq \int_0^T \left[\Gamma(\ln u(\alpha(\tau)))^{1/2} - \frac{t-s}{T} \frac{\partial \ln u}{\partial t}(\alpha(\tau)) \right] d\tau.$$

Applying (7.2) for any $\epsilon > 0$ we find

$$\log \frac{u(x,s)}{u(y,t)} \leq T^{1/2} \left(\int_0^T \Gamma(\ln u)(\alpha(\tau))\, d\tau \right)^{1/2} - \frac{t-s}{T} \int_0^T \frac{\partial \ln u}{\partial t}(\alpha(\tau))\, d\tau$$
$$\leq \frac{1}{2\epsilon} T + \frac{\epsilon}{2} \int_0^T \Gamma(\ln u)(\alpha(\tau))\, d\tau - \frac{d}{D} \frac{t-s}{T} \int_0^T \Gamma(\ln u)(\alpha(\tau))\, d\tau$$
$$- \frac{D(s-t)}{2T} \int_0^T \frac{d\tau}{t + \frac{s-t}{T}\tau}.$$

If we now choose $\epsilon > 0$ such that

$$\frac{\epsilon}{2} = \frac{d}{D} \frac{t-s}{T},$$

the above inequality yields

$$\log \frac{u(x,s)}{u(y,t)} \leq \frac{D}{d} \frac{\ell_s(\gamma)^2}{4(t-s)} + \frac{D}{2} \ln \left(\frac{t}{s} \right),$$

where we have denoted by $\ell_s(\gamma)$ the subunit length of γ. If we now minimize over all subunit paths joining y to x, and we exponentiate, we obtain

$$u(x,s) \leq u(y,t) \left(\frac{t}{s} \right)^{D/2} \exp\left(\frac{D}{d} \frac{d(x,y)^2}{4(t-s)} \right).$$

This proves (7.1) when $f \in C_0^\infty(\mathbb{M})$. We can then extend the result to $f \in C_b^\infty(\mathbb{M})$ by considering the approximations $h_n P_\tau f \in C_0^\infty(\mathbb{M})$, where $h_n \in C_0^\infty(\mathbb{M})$, $h_n \geq 0$, $h_n \to 1$, and let $n \to \infty$ and $\tau \to 0$. □

The following is an important consequence of Theorem 7.1.

Corollary 7.2. *Suppose that Hypotheses 1.1, 1.2 and 1.4 are valid, and the curvature-dimension inequality (1.12) is satisfied for some $\rho_1 \geq 0$. Let $p(x, y, t)$ be the heat kernel on $\mathbb{M}$. Then for all $x, y, z \in \mathbb{M}$ and $0 < s < t < \infty$,*

$$p(x,y,s) \leq p(x,z,t) \left(\frac{t}{s} \right)^{D/2} \exp\left(\frac{D}{d} \frac{d(y,z)^2}{4(t-s)} \right).$$

Proof. Fix $\tau > 0$ and $x \in \mathbb{M}$. By the hypoellipticity of $L - \partial_t$, we know that $p(x, \cdot, \cdot + \tau) \in C^\infty(\mathbb{M} \times (-\tau, \infty))$ (see [26]). From (4.4) we have

$$p(x,y,s+\tau) = P_s(p(x,\cdot,\tau))(y), \qquad p(x,z,t+\tau) = P_t(p(x,\cdot,\tau))(z).$$

Since we cannot apply Theorem 7.1 directly to $u(y,t) = P_t(p(x,\cdot,\tau))(y)$, we consider $u_n(y,t) = P_t(h_n p(x,\cdot,\tau))(y)$, where $h_n \in C_0^\infty(\mathbb{M})$, $0 \le h_n \le 1$, and $h_n \nearrow 1$. From (7.1) we find

$$P_s(h_n p(x,\cdot,\tau))(y) \le P_t(h_n p(x,\cdot,\tau))(z)\left(\frac{t}{s}\right)^{D/2} \exp\left(\frac{D}{d}\frac{d(y,z)^2}{4(t-s)}\right).$$

Letting $n \to \infty$, by Beppo Levi's monotone convergence theorem we obtain

$$p(x,y,s+\tau) \le p(x,z,t+\tau)\left(\frac{t}{s}\right)^{D/2} \exp\left(\frac{D}{d}\frac{d(y,z)^2}{4(t-s)}\right).$$

The desired conclusion follows by letting $\tau \to 0$. □

8. Off-diagonal Gaussian upper bounds for $p(x,y,t)$

Suppose that the assumptions of Theorem 7.1 are in force. Fix $x \in \mathbb{M}$ and $t > 0$. Applying Corollary 7.2 to $(y,t) \mapsto p(x,y,t)$, for every $y \in B(x,\sqrt{t})$ we find

$$p(x,x,t) \le 2^{D/2} e^{D/(4d)}\ p(x,y,2t) = C(\rho_2,\kappa,d)p(x,y,2t).$$

Integration over $B(x,\sqrt{t})$ gives

$$p(x,x,t)\mu(B(x,\sqrt{t})) \le C(\rho_2,\kappa,d)\int_{B(x,\sqrt{t})} p(x,y,2t)\,d\mu(y) \le C(\rho_2,\kappa,d),$$

where we have used $P_t 1 \le 1$. This gives the diagonal upper bound

$$p(x,x,t) \le \frac{C(\rho_2,\kappa,d)}{\mu(B(x,\sqrt{t}))}. \tag{8.1}$$

The aim of this section is to establish the following off-diagonal upper bound for the heat kernel. Before doing so, let us observe that from the general theory of Markov semigroups, if the volume doubling property is assumed, then the diagonal bound (8.1) implies an off-diagonal bound (see for instance [20]). However, in our framework, the volume doubling property is only proved in the sequel paper [13] which relies on the results of the present paper. Therefore, and we think this is of independent interest, to prove the off-diagonal upper bound, we completely bypass the use of uniform volume estimates and instead rely in an essential way on the scale invariant parabolic Harnack inequality.

Theorem 8.1. *Assume that Hypotheses 1.1, 1.2 and 1.4 hold and the curvature-dimension inequality (1.12) is satisfied for some $\rho_1 \ge 0$. For any $0 < \epsilon < 1$ there exists a constant $C(\rho_2,\kappa,d,\epsilon) > 0$, which tends to ∞ as $\epsilon \to 0^+$, such that for all $x, y \in \mathbb{M}$ and $t > 0$,*

$$p(x,y,t) \le \frac{C(d,\kappa,\rho_2,\epsilon)}{\mu(B(x,\sqrt{t}))^{1/2}\mu(B(y,\sqrt{t}))^{1/2}} \exp\left(-\frac{d(x,y)^2}{(4+\epsilon)t}\right).$$

Proof. We adapt an idea of [16] concerning the case of a compact manifold without boundary. Since here we allow $\mathbb{M}$ to be non-compact, we need to take care of this aspect. Corollary 4.6 will prove crucial in this connection. Given $T > 0$ and $\alpha > 0$ we fix $0 < \tau \le (1+\alpha)T$. For a function $\psi \in C_0^\infty(\mathbb{M})$ with $\psi \ge 0$, in $\mathbb{M} \times (0,\tau)$ we consider the function

$$f(y,t) = \int_{\mathbb{M}} p(y,z,t)p(x,z,T)\psi(z)\,d\mu(z), \qquad x \in \mathbb{M}.$$

Since $f = P_t(p(x,\cdot,T)\psi)$, it satisfies the Cauchy problem

$$\begin{cases} Lf - f_t = 0 & \text{in } \mathbb{M}\times(0,\tau),\\ f(z,0) = p(x,z,T)\psi(z), & z \in \mathbb{M}. \end{cases}$$

Notice that by the hypoellipticity of $L - \partial_t$ we know $y \mapsto p(x,y,T)$ is in $C^\infty(\mathbb{M})$, and therefore $p(x,\cdot,T)\psi \in L^\infty(\mathbb{M})$. Moreover, (4.3) gives

$$\|P_t(p(x,\cdot,T)\psi)\|^2_{L^2(\mathbb{M})} \le \|p(x,\cdot,T)\psi\|^2_{L^2(\mathbb{M})} = \int_{\mathbb{M}} p(x,z,T)^2\psi(z)\,d\mu(z) < \infty,$$

and therefore

$$\int_0^\tau \int_{\mathbb{M}} f(y,t)^2\,d\mu(z)\,dt \le \tau \int_{\mathbb{M}} p(x,z,T)^2\psi(z)\,d\mu(z)\,dt < \infty. \tag{8.2}$$

Invoking (4.9) of Corollary 4.6 we have

$$\Gamma(f)(z,t) \le e^{-\alpha t}\big(P_t\Gamma(p(x,\cdot,T)\psi)(z) + P_t\Gamma^Z(p(x,\cdot,T)\psi)(z)\big).$$

This allows us to conclude that

$$\int_0^\tau \int_{\mathbb{M}} \Gamma(f)(z,t)^2\,d\mu(z)\,dt < \infty. \tag{8.3}$$

We now consider a function $g \in C^1([0,(1+\alpha)T], \mathrm{Lip}_d(\mathbb{M})) \cap L^\infty(\mathbb{M}\times(0,(1+\alpha)T))$ such that

$$-\frac{\partial g}{\partial t} \ge \frac{1}{2}\Gamma(g) \qquad \text{on } \mathbb{M}\times(0,(1+\alpha)T). \tag{8.4}$$

Since

$$\left(L - \frac{\partial}{\partial t}\right) f^2 = 2f\left(L - \frac{\partial}{\partial t}\right) f + 2\Gamma(f) = 2\Gamma(f),$$

multiplying this identity by $h_n(y)^2 e^{g(y,t)}$, where h_n is a sequence as in Hypothesis 1.1, and integrating by parts, we obtain

$$\begin{aligned}
0 &= 2\int_0^\tau \int_{\mathbb{M}} h_n^2 e^g \Gamma(f)\, d\mu(y)\, dt - \int_0^\tau \int_{\mathbb{M}} h_n^2 e^g \left(L - \frac{\partial}{\partial t}\right) f^2\, d\mu(y)\, dt \\
&= 2\int_0^\tau \int_{\mathbb{M}} h_n^2 e^g \Gamma(f)\, d\mu(y)\, dt + 4\int_0^\tau \int_{\mathbb{M}} h_n e^g f \Gamma(h_n, f)\, d\mu(y)\, dt \\
&\quad + 2\int_0^\tau \int_{\mathbb{M}} h_n^2 e^g f \Gamma(f, g)\, d\mu(y)\, dt - \int_0^\tau \int_{\mathbb{M}} h_n e^g f^2 \frac{\partial g}{\partial t}\, d\mu(y)\, dt \\
&\quad - \int_{\mathbb{M}} h_n e^g f^2\, d\mu(y)\Big|_{t=0} + \int_{\mathbb{M}} h_n e^g f^2\, d\mu(y)\Big|_{t=\tau} \\
&\geq 2\int_0^\tau \int_{\mathbb{M}} h_n^2 e^g \left(\Gamma(f) + \frac{f^2}{4}\Gamma(g) + f\Gamma(f, g)\right) d\mu(y)\, dt \\
&\quad + 4\int_0^\tau \int_{\mathbb{M}} h_n e^g f \Gamma(h_n, f)\, d\mu(y)\, dt + \int_{\mathbb{M}} h_n e^g f^2\, d\mu(y)\Big|_{t=\tau} \\
&\quad - \int_{\mathbb{M}} h_n e^g f^2\, d\mu(y)\Big|_{t=0},
\end{aligned}$$

where in the last inequality we have made use of the assumption (8.4) on g. From this we deduce that

$$\int_{\mathbb{M}} h_n e^g f^2\, d\mu(y)\Big|_{t=\tau} \leq \int_{\mathbb{M}} h_n e^g f^2\, d\mu(y)\Big|_{t=0} - 4\int_0^\tau \int_{\mathbb{M}} h_n e^g f \Gamma(h_n, f)\, d\mu(y)\, dt.$$

We now claim that

$$\lim_{n\to\infty} \int_0^\tau \int_{\mathbb{M}} h_n e^g f \Gamma(h_n, f)\, d\mu(y)\, dt = 0.$$

To see this we apply the Cauchy–Schwarz inequality, which gives

$$\begin{aligned}
&\left|\int_0^\tau \int_{\mathbb{M}} h_n e^g f \Gamma(h_n, f)\, d\mu(y)\, dt\right| \\
&\quad \leq \left(\int_0^\tau \int_{\mathbb{M}} h_n^2 e^g f^2 \Gamma(h_n)\, d\mu(y)\, dt\right)^{1/2} \left(\int_0^\tau \int_{\mathbb{M}} e^g \Gamma(f)\, d\mu(y)\, dt\right)^{1/2} \\
&\quad \leq \left(\int_0^\tau \int_{\mathbb{M}} e^g f^2 \Gamma(h_n)\, d\mu(y) dt\right)^{1/2} \left(\int_0^\tau \int_{\mathbb{M}} e^g \Gamma(f)\, d\mu(y)\, dt\right)^{1/2} \to 0
\end{aligned}$$

as $n \to \infty$, thanks to (8.2), (8.3). With the claim in hand we now let $n \to \infty$ in the above inequality, obtaining

$$\int_{\mathbb{M}} e^{g(y,\tau)} f(y, \tau)^2\, d\mu(y) \leq \int_{\mathbb{M}} e^{g(y,0)} f(y, 0)^2\, d\mu(y). \tag{8.5}$$

At this point we fix $x \in \mathbb{M}$ and for $0 < t \leq \tau$ consider the indicator function $\mathbf{1}_{B(x,\sqrt{t})}$ of the ball $B(x, \sqrt{t})$. Let $\psi_k \in C_0^\infty(\mathbb{M})$, $\psi_k \geq 0$, be a sequence such that $\psi_k \to \mathbf{1}_{B(x,\sqrt{t})}$ in $L^2(\mathbb{M})$ with supp $\psi_k \subset B(x, 100\sqrt{t})$. Slightly abusing the notation we now set

$$f(y,s) = P_s(p(x,\cdot,T)\mathbf{1}_{B(x,\sqrt{t})})(y) = \int_{B(x,\sqrt{t})} p(y,z,s)p(x,z,T)\,d\mu(z).$$

Thanks to the symmetry $p(x, y, s) = p(y, x, s)$, we have

$$f(x,T) = \int_{B(x,\sqrt{t})} p(x,z,T)^2\,d\mu(z). \tag{8.6}$$

Applying (8.5) to $f_k(y, s) = P_s(p(x, \cdot, T)\psi_k)(y)$, we find

$$\int_{\mathbb{M}} e^{g(y,\tau)} f_k(y,\tau)^2\,d\mu(y) \leq \int_{\mathbb{M}} e^{g(y,0)} f_k(y,0)^2\,d\mu(y). \tag{8.7}$$

At this point we observe that as $k \to \infty$,

$$\begin{aligned}&\left|\int_{\mathbb{M}} e^{g(y,\tau)} f_k(y,\tau)^2\,d\mu(y) - \int_{\mathbb{M}} e^{g(y,\tau)} f(y,\tau)^2\,d\mu(y)\right| \\ &\quad\leq 2\|e^{g(\cdot,\tau)}\|_{L^\infty(\mathbb{M})}\|p(x,\cdot,T)\|_{L^2(\mathbb{M})}\|p(x,\cdot,\tau)\|_{L^\infty(B(x,110\sqrt{t}))}\|\psi_k - \mathbf{1}_{B(x,\sqrt{t})}\|_{L^2(\mathbb{M})} \\ &\qquad\to 0.\end{aligned}$$

By similar considerations we find

$$\begin{aligned}&\left|\int_{\mathbb{M}} e^{g(y,0)} f_k(y,0)^2\,d\mu(y) - \int_{\mathbb{M}} e^{g(y,0)} f(y,0)^2\,d\mu(y)\right| \\ &\quad\leq 2\|e^{g(\cdot,0)}\|_{L^\infty(\mathbb{M})}\|p(x,\cdot,T)\|_{L^\infty(B(x,110\sqrt{t}))}\|\psi_k - \mathbf{1}_{B(x,\sqrt{t})}\|_{L^2(\mathbb{M})} \to 0.\end{aligned}$$

Letting $k \to \infty$ in (8.7) we thus conclude that the same inequality holds with f_k replaced by $f(y,s) = P_s(p(x,\cdot,T)1_{B(x,\sqrt{t})})(y)$. This implies in particular the basic estimate

$$\begin{aligned}&\inf_{z\in B(x,\sqrt{t})} e^{g(z,\tau)} \int_{B(x,\sqrt{t})} f(z,\tau)^2\,d\mu(z) \\ &\quad\leq \int_{B(x,\sqrt{t})} e^{g(z,\tau)} f(z,\tau)^2\,d\mu(z) \leq \int_{\mathbb{M}} e^{g(z,\tau)} f(z,\tau)^2\,d\mu(z) \\ &\quad\leq \int_{\mathbb{M}} e^{g(z,0)} f(z,0)^2\,d\mu(z) = \int_{B(y,\sqrt{t})} e^{g(z,0)} p(x,z,T)^2\,d\mu(z) \\ &\quad\leq \sup_{z\in B(y,\sqrt{t})} e^{g(z,0)} \int_{B(y,\sqrt{t})} p(x,z,T)^2\,d\mu(z).\end{aligned} \tag{8.8}$$

Now we choose in (8.8)

$$g(y,t) = g_x(y,t) = -\frac{d(x,y)^2}{2((1+2\alpha)T - t)}.$$

Using $\Gamma(d) \leq 1$, one can easily check that (8.4) is satisfied for this g. Taking into account that

$$\inf_{z \in B(x,\sqrt{t})} e^{g_x(z,\tau)} = \inf_{z \in B(x,\sqrt{t})} x e^{-\frac{d(x,z)^2}{2((1+2\alpha)T-\tau)}} \geq e^{\frac{-t}{2((1+2\alpha)T-\tau)}},$$

if we now choose $\tau = (1+\alpha)T$, then from the previous inequality and from (8.6) we conclude that

$$\int_{B(x,\sqrt{t})} f(z,(1+\alpha)T)^2\, d\mu(z) \leq \left(\sup_{z \in B(y,\sqrt{t})} e^{-\frac{d(x,z)^2}{2(1+2\alpha)T}+\frac{t}{2\alpha T}} \right) \int_{B(y,\sqrt{t})} p(x,z,T)^2\, d\mu(z). \tag{8.9}$$

We now apply Theorem 7.1, which gives, for every $z \in B(x,\sqrt{t})$,

$$f(x,T)^2 \leq f(z,(1+\alpha)T)^2 (1+\alpha)^{d(1+\frac{3\kappa}{2\rho_2})} e^{\frac{t(1+\frac{3\kappa}{2\rho_2})}{2\alpha T}}.$$

Integrating this inequality on $B(y,\sqrt{t})$ we find

$$\begin{aligned}\left(\int_{B(y,\sqrt{t})} p(x,z,T)^2\, d\mu(z) \right)^2 &= f(x,T)^2 \\ &\leq \frac{(1+\alpha)^{d(1+\frac{3\kappa}{2\rho_2})} e^{\frac{t(1+\frac{3\kappa}{2\rho_2})}{2\alpha T}}}{\mu(B(x,\sqrt{t}))} \int_{B(x,\sqrt{t})} f(z,(1+\alpha)T)^2\, d\mu(z).\end{aligned}$$

If we now use (8.9) in the last inequality we obtain

$$\int_{B(y,\sqrt{t})} p(x,z,T)^2\, d\mu(z) \leq \frac{(1+\alpha)^{d(1+\frac{3\kappa}{2\rho_2})} e^{\frac{t(1+\frac{3\kappa}{2\rho_2})}{2\alpha T}}}{\mu(B(x,\sqrt{t}))} \left(\sup_{z \in B(y,\sqrt{t})} e^{-\frac{d(x,z)^2}{2(1+2\alpha)T}+\frac{t}{2\alpha T}} \right).$$

Choosing $T = (1+\alpha)t$ in this inequality we find

$$\begin{aligned}&\int_{B(y,\sqrt{t})} p(x,z,(1+\alpha)t)^2\, d\mu(z) \\ &\quad \leq \frac{(1+\alpha)^{d(1+\frac{3\kappa}{2\rho_2})} e^{\frac{1+\frac{3\kappa}{2\rho_2}}{2\alpha(1+\alpha)}+\frac{1}{2\alpha(1+\alpha)}}}{\mu(B(x,\sqrt{t}))} \left(\sup_{z \in B(y,\sqrt{t})} e^{-\frac{d(x,z)^2}{2(1+2\alpha)(1+\alpha)t}+\frac{1}{2\alpha(1+\alpha)}} \right).\end{aligned} \tag{8.10}$$

We now apply Corollary 7.2 to obtain, for every $z \in B(y,\sqrt{t})$,

$$p(x,y,t)^2 \leq p(x,z,(1+\alpha)t)^2 (1+\alpha)^{d(1+\frac{3\kappa}{2\rho_2})} \exp\left(\frac{1+\frac{3\kappa}{2\rho_2}}{2\alpha} \right).$$

Integrating this inequality over $z \in B(y,\sqrt{t})$, we have

$$\mu(B(y,\sqrt{t}))\, p(x,y,t)^2 \leq (1+\alpha)^{d(1+\frac{3\kappa}{2\rho_2})} e^{\frac{1+\frac{3\kappa}{2\rho_2}}{2\alpha}} \int_{B(y,\sqrt{t})} p(x,z,(1+\alpha)t)^2\, d\mu(z).$$

Combining this inequality with (8.10) we conclude that

$$p(x,y,t) \le \frac{(1+\alpha)^{d(1+\frac{3\kappa}{2\rho_2})} e^{\frac{(1+\frac{3\kappa}{2\rho_2})(2+\alpha)}{4\alpha(1+\alpha)}+\frac{3}{4\alpha(1+\alpha)}}}{\mu(B(x,\sqrt{t}))^{1/2}\mu(B(y,\sqrt{t}))^{1/2}} \left(\sup_{z\in B(y,\sqrt{t})} e^{-\frac{d(x,z)^2}{2(1+2\alpha)(1+\alpha)t}} \right).$$

If now $x \in B(y,\sqrt{t})$, then

$$d(x,z)^2 \ge (d(x,y)-\sqrt{t})^2 > d(x,y)^2 - t,$$

and therefore

$$\sup_{z\in B(y,\sqrt{t})} e^{-\frac{d(x,z)^2}{2(1+2\alpha)(1+\alpha)t}} \le e^{\frac{1}{2(1+2\alpha)(1+\alpha)}} e^{-\frac{d(x,y)^2}{2(1+2\alpha)(1+\alpha)t}}.$$

If instead $x \notin B(y,\sqrt{t})$, then for every $\delta > 0$ we have

$$d(x,z)^2 \ge (1-\delta)d(x,y)^2 - (1+\delta^{-1})t.$$

Choosing $\delta = \alpha/(\alpha+1)$ we find

$$d(x,z)^2 \ge \frac{d(x,y)^2}{1+\alpha} - (2+\alpha^{-1})t,$$

and therefore

$$\sup_{z\in B(y,\sqrt{t})} e^{-\frac{d(x,z)^2}{2(1+2\alpha)(1+\alpha)t}} \le e^{-\frac{d(x,y)^2}{2(1+2\alpha)(1+\alpha)^2 t}+\frac{2+\alpha^{-1}}{2(1+2\alpha)(1+\alpha)}}$$

For any $\epsilon > 0$ we now choose $\alpha > 0$ such that $2(1+2\alpha)(1+\alpha)^2 = 4+\epsilon$ to reach the desired conclusion. □

9. A generalization of Yau's Liouville theorem

In his seminal 1975 paper [54], by using gradient estimates, Yau proved his celebrated Liouville theorem that there exists no non-constant positive harmonic function on a complete Riemannian manifold with non-negative Ricci curvature. The aim of this section is to extend Yau's theorem to the sub-Riemannian setting of this paper. An interesting point to keep in mind here is that, even in the Riemannian setting, our approach gives a new proof of Yau's theorem which is not based on delicate tools from Riemannian geometry such as the Laplacian comparison theorem (1.14) for the geodesic distance. However, due to the nature of our proof at the moment we are only able to deal with harmonic functions bounded from two sides, whereas in [54] the author is able to treat functions satisfying a one-side bound. In the sequel paper [13] we remove this restriction.

We begin with a Harnack type inequality for the operator L.

Theorem 9.1. *Assume that Hypotheses 1.1, 1.2 and 1.4 hold and the curvature-dimension inequality (1.12) is satisfied for some $\rho_1 \geq 0$. Let $0 \leq f \leq M$ be a harmonic function on $\mathbb{M}$. Then there exists a constant $C = C(\rho_2, \kappa, d) > 0$ such that for any $x_0 \in \mathbb{M}$ and $r > 0$,*

$$\sup_{B(x_0,r)} f \leq C \inf_{B(x_0,r)} f.$$

Proof. We know that $f \in C_b^\infty(\mathbb{M})$ and $f \geq 0$. Applying Theorem 7.1 to the function $u(x,t) = P_t f(x)$, for $x, y \in B(x_0, r)$ we obtain

$$P_s f(x) \leq P_t f(y) \left(\frac{t}{s}\right)^{D/2} \exp\left(\frac{Dr^2}{d(t-s)}\right), \qquad 0 < s < t < \infty.$$

Now observe that, thanks to the assumption $Lf = 0$, the functions $u(x,t) = P_t f(x)$ and $v(x,t) = f(x)$ solve the same Cauchy problem on $\mathbb{M}$. By Proposition 4.4 we must have $P_t f(x) = f(x)$ for every $x \in \mathbb{M}$ and every $t > 0$. Therefore, if we take $s = r^2$, $t = 2r^2$, the above inequality gives

$$f(x) \leq \left(\sqrt{2}\, e^{1/d}\right)^D f(y), \qquad x, y \in B(x_0, r). \qquad \square$$

Theorem 9.2 (of Cauchy–Liouville type). *Under the assumptions of Theorem 9.1, there exist no bounded solutions to $Lf = 0$ on $\mathbb{M}$ other than the constants.*

Proof. Suppose $a \leq f \leq b$ on $\mathbb{M}$. Consider the function $g = f - \inf_{\mathbb{M}} f$. Clearly, $0 \leq g \leq M = b - a$. If we apply Theorem 9.1 to g we find, for any $x_0 \in \mathbb{M}$ and $r > 0$,

$$\sup_{B(x_0,r)} g \leq C \inf_{B(x_0,r)} g.$$

Letting $r \to \infty$ yields $\sup_{\mathbb{M}} f = \inf_{\mathbb{M}} f$, hence $f \equiv \text{const}$. $\square$

10. A sub-Riemannian Bonnet–Myers theorem

Let $(\mathbb{M}, g)$ be a complete, connected Riemannian manifold of dimension $n \geq 2$. It is well-known that if for some $\rho_1 > 0$ the Ricci tensor of $\mathbb{M}$ satisfies the bound

$$\mathrm{Ric} \geq (n-1)\rho_1, \tag{10.1}$$

then $\mathbb{M}$ is compact, with a finite fundamental group, and $\mathrm{diam}(\mathbb{M}) \leq \pi/\sqrt{\rho_1}$. This is the celebrated Myers theorem, which strengthens Bonnet's theorem. Like the latter, Myers' theorem is usually proved by using Jacobi vector fields (see e.g. [18, Theorem 2.12]).

A different approach is based on the curvature-dimension inequality $\mathrm{CD}((n-1)\rho_1, n)$, which—as we have seen—follows from (10.1) (see (1.2)). When $n > 2$, Ledoux [36] (see also [9]) uses ingenious non-linear methods, based on the study of the partial differential equation

$$c(f^{p-1} - f) = -\Delta f, \qquad 1 \leq p \leq \frac{2n}{n-2},$$

to deduce from $\mathrm{CD}((n-1)\rho_1, n)$ the Sobolev inequality

$$\frac{n}{(n-2)\rho_1^2}\left[\left(\int_{\mathbb{M}} |f|^p \, d\mu\right)^{2/p} - \int_{\mathbb{M}} f^2 \, d\mu\right] \le \int_{\mathbb{M}} \Gamma(f) \, d\mu, \qquad f \in C_0^\infty(\mathbb{M}), \tag{10.2}$$

where μ is the Riemannian measure. By a simple iteration procedure, Ledoux deduces from (10.2) that the diameter of $\mathbb{M}$ is finite and bounded by $\pi/\sqrt{\rho_1}$. The non-linear methods in [36] seem difficult to extend to the framework of the present paper.

A weaker version of the Myers theorem was proved by Bakry [5] by using linear methods only. We have been able to suitably adapt his approach, based on entropy-energy inequalities (a strong form of log-Sobolev inequalities). In this section we establish the following sub-Riemannian Bonnet–Myers compactness theorem.

Theorem 10.1. *Assume that Hypotheses 1.1, 1.2 and 1.4 hold and the curvature-dimension inequality (1.12) is satisfied for some $\rho_1 > 0$. Then the metric space $(\mathbb{M}, d)$ is compact and*

$$\operatorname{diam} \mathbb{M} \le \frac{\pi}{\sqrt{\rho_1}} 2\sqrt{3} \sqrt{\left(\frac{\kappa}{\rho_2} + 1\right) D} = 2\sqrt{3}\,\pi \sqrt{\frac{\rho_2 + \kappa}{\rho_1 \rho_2}\left(1 + \frac{3\kappa}{2\rho_2}\right) d}.$$

The proof of Theorem 10.1 will be accomplished in several steps. In the remainder of this section we will tacitly assume the hypothesis of Theorem 10.1.

10.1. Global heat kernel bounds

Our first result is the following large-time exponential decay for the heat kernel.

Proposition 10.2. *Let $0 < \nu < \rho_1\rho_2/(\rho_2 + \kappa)$. There exist $t_0, C_1 > 0$ such that for every $f \in C_0^\infty(\mathbb{M})$ with $f \ge 0$,*

$$\left| \frac{\partial}{\partial t} \ln P_t f(x) \right| \le C_1 e^{-\nu t}, \qquad x \in \mathbb{M},\ t \ge t_0.$$

Proof. In Corollary 5.3, we choose

$$b(t) = (e^{-\alpha t} - e^{-\alpha T})^\beta, \qquad 0 \le t \le T,$$

with $\beta > 2$ and $\alpha > 0$. With this choice a simple computation gives

$$\gamma(t) = \frac{d}{4}\left(2\rho_1 - \alpha\beta - \alpha\beta\frac{\kappa}{\rho_2} - e^{-\alpha T}\left(\alpha(\beta-1) + \frac{\alpha\beta\kappa}{\rho_2}\right) b(t)^{-1/\beta}\right).$$

Keeping in mind that $b(T) = b'(T) = 0$ and $b(0) = (1 - e^{-\alpha T})^\beta$, $b'(0) = -\alpha\beta(1 - e^{-\alpha T})^{\beta-1}$, we deduce from (5.2) that

$$\begin{aligned} -&\frac{\alpha\beta(1-e^{-\alpha T})^{\beta-1}}{2\rho_2}\Gamma(\ln P_T f) - (1-e^{-\alpha T})^\beta \Gamma^Z(\ln P_T f) \\ &\quad \ge -\frac{2}{d\rho_2}\left(\int_0^T b'(t)\gamma(t)\,dt\right)\frac{LP_T f}{P_T f} + \frac{1}{d\rho_2}\left(\int_0^T b'(t)\gamma(t)^2\,dt\right). \end{aligned} \tag{10.3}$$

Now,

$$\int_0^T b'(t)\gamma(t)\,dt = -\frac{d}{4}\left(2\rho_1-\alpha\beta-\alpha\beta\frac{\kappa}{\rho_2}\right)(1-e^{-\alpha T})^{\beta} + \frac{d}{4}\frac{1}{1-1/\beta}\left(\alpha\beta-\alpha+\alpha\beta\frac{\kappa}{\rho_2}\right)e^{-\alpha T}(1-e^{-\alpha T})^{\beta-1},$$

$$\int_0^T b'(t)\gamma(t)^2\,dt = -\frac{d^2}{16}\left(2\rho_1-\alpha\beta-\alpha\beta\frac{\kappa}{\rho_2}\right)^2(1-e^{-\alpha T})^{\beta} + \frac{d^2}{8}\frac{(2\rho_1-\alpha\beta-\alpha\beta\kappa/\rho_2)(\alpha\beta-\alpha+\alpha\beta\kappa/\rho_2)}{1-1/\beta}e^{-\alpha T}(1-e^{-\alpha T})^{\beta-1} - \frac{d^2}{16}\frac{(\alpha\beta-\alpha+\alpha\beta\kappa/\rho_2)^2}{1-2/\beta}e^{-2\alpha T}(1-e^{-\alpha T})^{\beta-2}.$$

If we choose

$$\alpha = \frac{2\rho_1\rho_2}{\beta(\rho_2+\kappa)},$$

then

$$2\rho_1-\alpha\beta-\alpha\beta\frac{\kappa}{\rho_2}=0, \qquad \alpha\beta-\alpha+\alpha\beta\frac{\kappa}{\rho_2}=2\rho_1-\alpha,$$

and from (10.3) we obtain

$$0 \le \frac{\rho_1}{\rho_2+\kappa}\Gamma(\ln P_T f) + (1-e^{-\alpha T})\Gamma^Z(\ln P_T f) \le \frac{d(2\rho_1-\alpha)}{2\rho_2(1-1/\beta)}e^{-\alpha T}\frac{LP_T f}{P_T f} + \frac{d(2\rho_1-\alpha)^2}{16\rho_2(1-2/\beta)}\frac{e^{-2\alpha T}}{1-e^{-\alpha T}}. \tag{10.4}$$

Noting that $2\rho_1-\alpha=\frac{2\rho_1}{\beta(\rho_2+\kappa)}((\beta-1)\rho_2+\beta\kappa)>0$, and that $\beta>2$ implies $\alpha<\frac{\rho_1\rho_2}{\rho_2+\kappa}$, (10.4) gives in particular the desired lower bound for $\frac{\partial}{\partial t}\ln P_t f(x)$ with $\nu=\alpha$.

The upper bound is more delicate. We fix $0<\eta=\frac{2\rho_1\rho_2}{\beta(\rho_2+\kappa)}$, and with $\gamma=2\beta\rho_1\rho_2$ we now choose in (10.3)

$$\alpha = \frac{2\rho_1\rho_2-\gamma e^{-\eta T}}{\beta(\rho_2+\kappa)} = \eta - \frac{\gamma e^{-\eta T}}{\beta(\rho_2+\kappa)}.$$

Clearly, $\alpha>0$ provided that T is sufficiently large. This choice gives

$$2\rho_1-\alpha\beta-\alpha\beta\frac{\kappa}{\rho_2}=\frac{\gamma e^{-\eta T}}{\rho_2}, \qquad \alpha\beta-\alpha+\alpha\beta\frac{\kappa}{\rho_2}=2\rho_1-\alpha-\frac{\gamma e^{-\eta T}}{\rho_2}.$$

We thus have

$$\int_0^T b'(t)\gamma(t)\,dt = -\frac{d}{4}e^{-\alpha T}(1-e^{-\alpha T})^{\beta-1}\left\{\frac{\gamma(1-e^{-\alpha T})e^{-(\eta-\alpha)T}}{\rho_2} - \frac{\beta}{\beta-1}\left(2\rho_1-\alpha-\frac{\gamma e^{-\eta T}}{\rho_2}\right)\right\}.$$

Noting that $e^{-(\eta-\alpha)T} = e^{-\frac{\gamma T e^{-\eta T}}{\beta(\rho_2+\kappa)}} \to 1$ and $\alpha \to \frac{2\rho_1\rho_2}{\beta(\rho_2+\kappa)}$ as $T \to \infty$, we obtain

$$\frac{\gamma(1-e^{-\alpha T})e^{-(\eta-\alpha)T}}{\rho_2} - \frac{\beta}{\beta-1}\left(2\rho_1 - \alpha - \frac{\gamma e^{-\eta T}}{\rho_2}\right) \to \frac{\gamma}{\rho_2} - \frac{\beta}{\beta-1}\left(2\rho_1 - \frac{2\rho_1\rho_2}{\beta(\rho_2+\kappa)}\right).$$

Since by our choice of γ we have $\frac{\gamma}{\rho_2} - \frac{\beta}{\beta-1}\left(2\rho_1 - \frac{2\rho_1\rho_2}{\beta(\rho_2+\kappa)}\right) > 0$, it is clear that

$$\int_0^T b'(t)\gamma(t)\,dt \le -\frac{d}{8}\left(\frac{\gamma}{\rho_2} - \frac{\beta}{\beta-1}\left(2\rho_1 - \frac{2\rho_1\rho_2}{\beta(\rho_2+\kappa)}\right)\right)e^{-\alpha T}(1-e^{-\alpha T})^{\beta-1}$$

provided that T is large enough. We also have

$$\int_0^T b'(t)\gamma(t)^2\,dt = -\frac{d^2}{16}e^{-2\alpha T}(1-e^{-\alpha T})^{\beta-2}\left\{\frac{\beta}{\beta-2}\left(2\rho_1 - \alpha - \frac{\gamma e^{-\eta T}}{\rho_2}\right)^2 \right.$$
$$\left. + \frac{\gamma^2}{\rho_2^2}(1-e^{-\alpha T})^2 e^{-2(\eta-\alpha)T} - 2\frac{\gamma}{\rho_2}\frac{\beta}{\beta-1}(1-e^{-\alpha T})\left(2\rho_1 - \alpha - \frac{\gamma e^{-\eta T}}{\rho_2}\right)e^{-(\eta-\alpha)T}\right\}.$$

Using our choice of γ we see that if we let $T \to \infty$, the quantity in curly brackets converges to

$$\frac{\beta}{\beta-2}4\rho_1^2\left(\frac{(\beta-1)\rho_2+\beta\kappa}{\beta(\rho_2+\kappa)}\right)^2 + 4\beta^2\rho_1^2 - \frac{8\beta^2\rho_1^2}{\beta-1}\frac{(\beta-1)\rho_2+\beta\kappa}{\beta(\rho_2+\kappa)}.$$

This quantity is strictly positive provided that

$$\frac{2\beta}{\beta-1}\frac{(\beta-1)\rho_2+\beta\kappa}{\beta(\rho_2+\kappa)} < \frac{1}{\beta-2}\left(\frac{(\beta-1)\rho_2+\beta\kappa}{\beta(\rho_2+\kappa)}\right)^2 + \beta,$$

and this last inequality is true, as one finds by applying the inequality $2xy \le x^2 + y^2$. Consequently, from (10.3) we deduce the desired upper bound for $\frac{\partial}{\partial t}\ln P_t f(x)$. □

Proposition 10.3. *Let $0 < \nu < \frac{\rho_1\rho_2}{\kappa+\rho_2}$. There exist $t_0, C_2 > 0$ such that for every $f \in C_0^\infty(\mathbb{M})$ with $f \ge 0$,*

$$e^{-C_2 e^{-\nu t} d(x,y)} \le \frac{P_t f(x)}{P_t f(y)} \le e^{C_2 e^{-\nu t} d(x,y)}, \qquad x, y \in \mathbb{M},\ t \ge t_0.$$

Proof. If we combine (10.4) (in which we take $\alpha = \nu$) with the upper bound of Proposition 10.2, we see that for $x \in \mathbb{M}$ and $t \ge t_0$,

$$\Gamma(\ln P_t f)(x) \le C_2^2 e^{-2\nu t}$$

with $C_2 = \sqrt{d(2\rho_1 - \nu)/2\rho_2(1-\beta^{-1})}$. We infer that the function $u(x) = C_2^{-1}e^{\nu t}\ln P_t f(x)$, which belongs to $C^\infty(\mathbb{M})$, is such that $\|\Gamma(u)\|_\infty \le 1$. From (1.7) we obtain

$$|u(x) - u(y)| \le d(x,y), \qquad x, y \in \mathbb{M}.$$

This implies the desired conclusion. □

If we now fix $x \in \mathbb{M}$, and denote by $p(x, \cdot, t)$ the heat kernel with singularity at $(x, 0)$, then according to Proposition 10.2, for $t \geq t_0$ we obtain

$$\left| \frac{\partial \ln p(x, y, t)}{\partial t} \right| \leq C_1 \exp(-\nu t) \tag{10.5}$$

with $0 < \nu < \frac{\rho_1 \rho_2}{\kappa + \rho_2}$. This shows that $\ln p(\cdot, \cdot, t)$ converges as $t \to \infty$. Let us call this limit $\ln p_\infty$. Moreover, from Proposition 10.3 the limit $\ln p_\infty(x, \cdot)$ is a constant $C(x)$. By the symmetry property, $p(x, y, t) = p(y, x, t)$, so that $C(x)$ actually does not depend on x. We deduce that the measure μ is finite. We may then as well suppose that μ is a probability measure, in which case $p_\infty = 1$. We assume this from now on.

We can now prove a global and explicit upper bound for the heat kernel $p(x, y, t)$.

Proposition 10.4. *For $x, y \in \mathbb{M}$ and $t > 0$,*

$$p(x, y, t) \leq \frac{1}{\left(1 - e^{-\frac{2\rho_1 \rho_2 t}{3(\rho_2 + \kappa)}}\right)^{\frac{d}{2}\left(1 + \frac{3\kappa}{2\rho_2}\right)}}.$$

Proof. We apply (10.4) with $\beta = 3$ to obtain

$$\begin{aligned} \frac{\rho_1}{\rho_2 + \kappa} \Gamma(\ln P_t f) + (1 - e^{-\alpha t}) \Gamma^Z(\ln P_t f) \leq{}& \frac{\rho_1}{2\rho_2} \frac{2\rho_2 + 3\kappa}{\rho_2 + \kappa} e^{-\alpha t} \frac{L P_t f}{P_t f} \\ &+ \frac{d\rho_1^2}{12\rho_2} \left(\frac{2\rho_2 + 3\kappa}{\rho_2 + \kappa} \right)^2 \frac{e^{-2\alpha t}}{1 - e^{-\alpha t}}, \end{aligned} \tag{10.6}$$

where $\alpha = \frac{2\rho_1 \rho_2}{3(\rho_2 + \kappa)}$. We deduce

$$\frac{\partial \ln P_t f}{\partial t} \geq -\frac{d\rho_1}{6} \frac{2\rho_2 + 3\kappa}{\rho_2 + \kappa} \frac{e^{-\alpha t}}{1 - e^{-\alpha t}}.$$

By integrating from t to ∞, we obtain

$$-\ln p(x, y, t) \geq -\frac{d}{2} \left(1 + \frac{3\kappa}{2\rho_2} \right) \ln(1 - e^{-\alpha t}).$$

This gives the desired conclusion. □

10.2. Diameter bound

In this subsection we conclude the proof of Theorem 10.1 by showing that $\operatorname{diam} \mathbb{M}$ is bounded. The idea is to show that the operator L satisfies an entropy-energy inequality. Such inequalities have been extensively studied by Bakry (see [5, Chapters 4 and 5]). To simplify the computations, in what follows we denote by D the number defined in (6.2), and we set

$$\alpha = \frac{2\rho_1 \rho_2}{3(\rho_2 + \kappa)}.$$

Proposition 10.5. *For $f \in L^2(\mathbb{M})$ such that $\int_{\mathbb{M}} f^2\, d\mu = 1$, we have*

$$\int_{\mathbb{M}} f^2 \ln f^2\, d\mu \le \Phi\left(\int_{\mathbb{M}} \Gamma(f)\, d\mu\right),$$

where

$$\Phi(x) = D\left[\left(1+\frac{2}{\alpha D}x\right)\ln\left(1+\frac{2}{\alpha D}x\right) - \frac{2}{\alpha D}x\ln\left(\frac{2}{\alpha D}x\right)\right].$$

Proof. From Proposition 10.4, for every $f \in L^2(\mathbb{M})$ we have

$$\|P_t f\|_\infty \le \frac{1}{(1-e^{-\alpha t})^{D/2}}\|f\|_2.$$

Therefore, from Davies' theorem [22, Theorem 2.2.3], for $f \in L^2(\mathbb{M})$ such that $\int_{\mathbb{M}} f^2\, d\mu = 1$, we obtain

$$\int_{\mathbb{M}} f^2 \ln f^2\, d\mu \le 2t\int_{\mathbb{M}} \Gamma(f)\, d\mu - D\ln(1-e^{-\alpha t}), \qquad t > 0.$$

By minimizing the right-hand side over t, we obtain

$$\int_{\mathbb{M}} f^2 \ln f^2\, d\mu \le -\frac{2}{\alpha}x\ln\left(\frac{2x}{2x+\alpha D}\right) + D\ln\left(\frac{2x+\alpha D}{\alpha D}\right),$$

where $x = \int_{\mathbb{M}} \Gamma(f)\, d\mu$. It is now easy to check that the right-hand side is $\Phi(x)$. □

With Proposition 10.5 in hand, we can finally complete the proof of Theorem 10.1.

Proposition 10.6.

$$\operatorname{diam}\mathbb{M} \le 2\sqrt{2}\sqrt{\frac{D}{\alpha}}\pi = 2\sqrt{3}\pi\sqrt{\frac{\rho_2+\kappa}{\rho_1\rho_2}\left(1+\frac{3\kappa}{2\rho_2}\right)d}.$$

Proof. The function Φ that appears in Proposition 10.5 enjoys the following properties:

- $\Phi'(x)/x^{1/2}$ and $\Phi(x)/x^{3/2}$ are integrable on $(0,\infty)$;
- Φ is concave;
- $\frac{1}{2}\int_0^\infty \frac{\Phi(x)}{x^{3/2}}dx = \int_0^\infty \frac{\Phi'(x)}{\sqrt{x}}dx = -2\int_0^\infty \sqrt{x}\Phi''(x)dx < \infty$.

We can therefore apply the beautiful Theorem 5.4 of [5] to deduce that the diameter of $\mathbb{M}$ is finite and

$$\operatorname{diam}\mathbb{M} \le -2\int_0^\infty \sqrt{x}\,\Phi''(x)\, dx.$$

Since $\Phi''(x) = -\frac{2D}{x(2x+\alpha D)}$, a routine calculation shows

$$-2\int_0^\infty \sqrt{x}\,\Phi''(x)\, dx = \frac{\pi}{\sqrt{\rho_1}}2\sqrt{3}\sqrt{\left(\frac{\kappa}{\rho_2}+1\right)D}.$$ □

Remark 10.7. The constant $2\sqrt{3}\pi\sqrt{\frac{\rho_2+\kappa}{\rho_1\rho_2}\left(1+\frac{3\kappa}{2\rho_2}\right)d}$ is not sharp. For instance, if $\mathbb{M}$ is a Riemannian manifold, we can take $d = n = \dim(\mathbb{M})$, $\kappa = 0$, and we thus obtain

$$\operatorname{diam}\mathbb{M} \le 2\sqrt{3}\pi\sqrt{\frac{n}{\rho_1}},$$

whereas it is known from the classical Bonnet–Myers theorem that

$$\operatorname{diam}\mathbb{M} \le \pi\sqrt{\frac{n-1}{\rho_1}}.$$

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References

[1] Agrachev, A.: Geometry of optimal control problems and Hamiltonian systems. In: Nonlinear and Optimal Control Theory, Lecture Notes in Math. 1932, Springer, 1–59 (2008) Zbl 1170.49035 MR 2410710

[2] Agrachev, A., Lee, P.: Generalized Ricci curvature bounds on three-dimensional contact sub-Riemannian manifolds. Math. Ann. **360**, 209–253 (2014) Zbl 1327.53032 MR 3263162

[3] Ané, C., Blachère, S., Chafaï, D., Fougères, P., Gentil, I., Malrieu, F., Roberto, C., Scheffer, G.: Sur les inégalités de Sobolev logarithmiques. Panoramas Synthèses 10, Soc. Math. France, Paris (2000) Zbl 0982.46026 MR 1845806

[4] Bakry, D.: Un critère de non-explosion pour certaines diffusions sur une variété riemannienne complète. C. R. Acad. Sci. Paris Sér. I Math. **303**, 23–26 (1986) Zbl 0589.60069 MR 0849620

[5] Bakry, D.: L'hypercontractivité et son utilisation en théorie des semigroupes. In: Lectures on Probability Theory (Saint-Flour, 1992), Lecture Notes in Math. 1581, Springer, 1–114 (1994) Zbl 0856.47026 MR 1307413

[6] Bakry, D.: Functional inequalities for Markov semigroups. In: Probability Measures on Groups: Recent Directions and Trends, Tata Inst. Fund. Res., Mumbai, 91–147 (2006) Zbl 1148.60057 MR 2213477

[7] Bakry, D., Baudoin, F., Bonnefont, M., Qian, B.: Subelliptic Li–Yau estimates on three dimensional model spaces. In: Potential Theory and Stochastics in Albac, Aurel Cornea Memorial Volume, Theta, Bucharest, 115–122 (2009) Zbl 1199.35051 MR 2213477

[8] Bakry, D., Emery, M.: Diffusions hypercontractives. In: Séminaire de probabilités, XIX, 1983/84, Lecture Notes in Math. 1123, Springer, 177–206 (1985) Zbl 0561.60080 MR 0889476

[9] Bakry, D., Ledoux, M.: Sobolev inequalities and Myers's diameter theorem for an abstract Markov generator. Duke Math. J. **85**, 253–270 (1996) Zbl 0870.60071 MR 1412446

[10] Bakry, D., Ledoux, M.: A logarithmic Sobolev form of the Li–Yau parabolic inequality. Revista Mat. Iberoamer. **22**, 683–702 (2006) Zbl 1116.58024 MR 22947946

[11] Baudoin, F.: An Introduction to the Geometry of Stochastic Flows. Imperial College Press, London (2004) Zbl 1085.60002 MR 2154760

[12] Baudoin, F., Bonnefont, M.: The subelliptic heat kernel on $\mathbb{SU}(2)$: Representations, asymptotics and gradient bounds. Math. Z. **263**, 647–672 (2009) Zbl 1189.58009 MR 2545862

[13] Baudoin, F., Bonnefont, M., Garofalo, N.: A sub-Riemannian curvature-dimension inequality, volume doubling property and the Poincaré inequality. Math. Ann. **358**, 833–860 (2014) Zbl 06290722 MR 3175142

[14] Baudoin, F., Garofalo, N.: Perelman's entropy and doubling property on Riemannian manifolds. J. Geom. Anal. **21**, 1119–1131 (2011) Zbl 1238.58024 MR 2836593

[15] Boyer, C. P., Galicki, K.: 3-Sasakian manifolds. In: Surveys in Differential Geometry: Essays on Einstein Manifolds, Int. Press, Boston, MA, 123–184 (1999) Zbl 1008.53047 MR 1798609

[16] Cao, H. D., Yau, S. T.: Gradient estimates, Harnack inequalities and estimates for heat kernels of the sum of squares of vector fields. Math. Z. **211**, 485–504 (1992) Zbl 0808.58037 MR 1190224

[17] Carlen, E., Kusuoka, S., Stroock, D.: Upper bounds for symmetric Markov transition functions. Ann. Inst. H. Poincaré Probab. Statist. **23**, no. 2, suppl., 245–287 (1987) Zbl 0634.60066 MR 0898496

[18] Chavel, I.: Riemannian Geometry: a Modern Introduction. Cambridge Tracts in Math. 108, Cambridge Univ. Press (1993) Zbl 0819.53001 MR 1271141

[19] Chow, B., Lu, P., Ni, L.: Hamilton's Ricci Flow. Grad. Stud. Math. 77, Amer. Math. Soc., Providence, RI and Science Press, New York (2006) Zbl 1118.53001 MR 2274812

[20] Coulhon, T., Sikora, A.: Gaussian heat kernel bounds via Phragmén–Lindelöf theorem. Proc. London Math. Soc. **96**, 507–544 (2008) Zbl 1148.35009 MR 2396848

[21] Cowling, M., Dooley, A. H., Korányi, A., Ricci, F.: H-type groups and Iwasawa decompositions. Adv. Math. **87**, 1–41 (1991) Zbl 0761.22010 MR 1102963

[22] Davies, E. B.: Heat Kernels and Spectral Theory. Cambridge Tracts in Math. 92, Cambridge Univ. Press, Cambridge (1989) Zbl 0699.35006 MR 1103113

[23] Dragomir, S., Tomassini, G.: Differential Geometry and Analysis on CR Manifolds. Progr. Math. 246, Birkhäuser (2006) Zbl 1099.32008 MR 2214654

[24] Falcitelli, M., Ianus, S., Pastore, A. M.: Riemannian Submersions and Related Topics. World Sci., River Edge, NJ (2004) Zbl 1067.53016 MR 2110043

[25] Fefferman, C., Phong, D. H.: Subelliptic eigenvalue problems. In: Conference on Harmonic Analysis in Honor of Antoni Zygmund, Vol. I, II (Chicago, IL, 1981), Wadsworth Math. Ser., Wadsworth, Belmont, CA, 590–606 (1983) Zbl 0503.35071 MR 0730094

[26] Fefferman, C. L., Sánchez-Calle, A.: Fundamental solutions for second order subelliptic operators. Ann. of Math. (2) **124**, 247–272 (1986) Zbl 0613.35002 MR 0855295

[27] Folland, G.: Subelliptic estimates and function spaces on nilpotent Lie groups. Ark. Mat. **13**, 161–207 (1975) Zbl 0312.35026 MR 0494315

[28] Friedman, A.: Partial Differential Equations of Parabolic Type. Dover (2008)

[29] Fukushima, M., Oshima, Y., Takeda, M.: Dirichlet Forms and Symmetric Markov Processes. de Gruyter Stud. Math. 19, de Gruyter (1994) Zbl 1227.31001 MR 2778606

[30] Greene, R., Wu, H.: Function Theory on Manifolds which Possess a Pole. Lecture Notes in Math. 699, Springer (1979) Zbl 0414.53043 MR 0521983

[31] Grigor'yan, A.: Heat Kernel and Analysis on Manifolds. AMS/IP Stud. Adv. Math. 47, Amer. Math. Soc., Providence, RI and Int. Press, Boston, MA (2009) Zbl 1206.58008 MR 2569498

[32] Hörmander, L.: Hypoelliptic second-order differential equations. Acta Math. **119**, 147–171 (1967) Zbl 0156.10701 MR 0222474

[33] Hughen, K.: The geometry of sub-Riemannian three-manifolds. Duke Univ. preprint (1995)

[34] Juillet, N.: Geometric inequalities and generalized Ricci bounds in the Heisenberg group. Int. Math. Res. Notices **2009**, 2347–2373 Zbl 1176.53053 MR 2520783

[35] Kaplan, A.: Fundamental solutions for a class of hypoelliptic PDE generated by composition of quadratic forms. Trans. Amer. Math. Soc. **258**, 147–153 (1980) Zbl 0393.35015 MR 0554324

[36] Ledoux, M.: The geometry of Markov diffusion generators. Ann. Fac. Sci. Toulouse Math. (6) **9**, 305–366 (2000) Zbl 0980.60097 MR 1813804

[37] Li, P.: Uniqueness of L^1 solutions for the Laplace equation and the heat equation on Riemannian manifolds. J. Differential Geom. **20**, 447–457 (1984) Zbl 0561.53045 MR 0788288

[38] Li, P., Yau, S. T.: On the parabolic kernel of the Schrödinger operator. Acta Math. **156**, 153–201 (1986) Zbl 0611.58045 MR 0834612

[39] Li, X. D.: Liouville theorems for symmetric diffusion operators on complete Riemannian manifolds. J. Math. Pures Appl. **84**, 1295–1361 (2005) Zbl 1082.58036 MR 2170766

[40] Lott, J., Villani, C.: Ricci curvature for metric-measure spaces via optimal transport. Ann. of Math. **169**, 903–991 (2009) Zbl 1178.53038 MR 2480619

[41] Montgomery, R.: A Tour of sub-Riemannian Geometries, their Geodesics and Applications. Math. Surveys Monogr. 91, Amer. Math. Soc. (2002) Zbl 1044.53022 MR 1867362

[42] Ollivier, Y.: Ricci curvature of Markov chains on metric spaces. J. Funct. Anal. **256**, 810–864 (2009) Zbl 1181.53015 MR 2484937

[43] Perelman, G.: The entropy formula for the Ricci flow and its geometric applications. arXiv:math/0211159, 39 pp. (2002) Zbl 1130.53001

[44] Phillips, R. S., Sarason, L.: Elliptic-parabolic equations of the second order. J. Math. Mech. **17**, 891–917 (1967/1968) Zbl 0163.34402 MR 0219868

[45] Reed, M., Simon, B.: Methods of Modern Mathematical Physics. Functional Analysis. 2nd ed., Academic Press, New York (1980) Zbl 0459.46001 MR 0751959

[46] von Renesse, M.-K., Sturm, K.-T.: Transport inequalities, gradient estimates, entropy, and Ricci curvature. Comm. Pure Appl. Math. **58**, 923–940 (2005) Zbl 1078.53028 MR 2142879

[47] Rumin, M.: Formes différentielles sur les variétés de contact. J. Differential Geom. **39**, 281–330 (1994) Zbl 0973.53524 MR 1267892

[48] Strichartz, R.: Analysis of the Laplacian on the complete Riemannian manifold. J. Funct. Anal. **52**, 48–79 (1983) Zbl 0515.58037 MR 0705991

[49] Strichartz, R.: Sub-Riemannian geometry. J. Differential Geom. **24**, 221–263 (1986) Zbl 0609.53021 MR 0862049

[50] Strichartz, R.: Corrections to "Sub-Riemannian geometry". J. Differential Geom. **30**, 595–596 (1989) Zbl 0609.53021 MR 1010174

[51] Sturm, K. Th.: On the geometry of metric measure spaces I. Acta Math. **196**, 65–131 (2006) Zbl 1105.53035 MR 2237206

[52] Sturm, K. Th.: On the geometry of metric measure spaces II. Acta Math. **196**, 133–177 (2006) Zbl 1106.53032 MR 2237207

[53] Varopoulos, N., Saloff-Coste, L., Coulhon, T.: Analysis and Geometry on Groups. Cambridge Univ. Press (1992) Zbl 1179.22009 MR 1218884

[54] Yau, S. T.: Harmonic functions on complete Riemannian manifolds. Comm. Pure Appl. Math. **28**, 201–228 (1975) Zbl 0291.31002 MR 0431040

[55] Yau, S. T.: On the heat kernel of a complete Riemannian manifold. J. Math. Pures Appl. (9) **57**, 191–201 (1978) Zbl 0405.35025 MR 0505904