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The subelliptic heat kernel on SU(2): representations, asymptotics and gradient bounds

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Abstract The Lie group $\mathbf{SU}(2)$ endowed with its canonical subriemannian structure appears as a three-dimensional model of a *positively curved* subelliptic space. The goal of this work is to study the subelliptic heat kernel on it and some related functional inequalities.

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1 Introduction

The goal of this work is to study in details the heat kernel and some related functional inequalities in one of the simplest sub-elliptic models after the Heisenberg group: the Lie group **SU**(2) endowed with its canonical subriemannian structure (coming from the Hopf fibration $\mathbb{S}^2 \to \mathbb{S}^3$, see [25]). In the classification of three-dimensional homogeneous subriemannian structures (see page 22 in [15]) the role played by this group could be compared to the role played by the sphere in Riemannian geometry: It should be a three-dimensional model of a compact positively curved subriemannian space.

In the flat three-dimensional subelliptic model, that is the Heisenberg group, the subelliptic heat kernel is quite well understood. In his celebrated paper [14], Gaveau gave a useful integral representation and deduced from it small times asymptotics. Since, numerous papers have been devoted to the study of this kernel (see for instance [9,22] and the references therein). In the case of **SU**(2), we will see that a quite similar study can be made: we will obtain an integral representation of the heat kernel and will deduce from it the small times asymptotics. These asymptotics give, in particular, a way to compute explicitly the Carnot–Carathéodory distance associated to the subriemannian structure of **SU**(2).

On the other hand, recent works have started to study gradient estimates for subelliptic semigroups (see for instance [5,13,22,24]). From the point of view of partial differential equations (see [4,21]), gradient estimates had proved to be a very efficient tool for the control of the rate of convergence to equilibrium, quantitative estimates on the regularization properties of heat kernels, functional inequalities such as Poincaré, logarithmic Sobolev, Gaussian isoperimetric inequalities for heat kernel measures, etc. When dealing with linear heat equations, those gradient estimates often rely on the control of the intrinsic Ricci curvature associated to the generator of the heat equation (Bakry–Emery criterion, see [2]). Those methods basically require some form of ellipticity of the generator and fail in typical subelliptic situations, like for instance in the Heisenberg group (see [5]). From the point of view of geometry, these gradient estimates are interesting, because they should contain information on the curvature of the space. For instance, in Riemannian geometry (see [3,31]), the functional inequality $\|\nabla e^{t\Delta} f\|^2 \leq e^{-2\rho t} e^{t\Delta}(\|\nabla f\|^2)$ is equivalent to the lower bound **Ricc** $\geq \rho$, where **Ricc** denotes the Ricci curvature. In subriemannian geometry there is no real analogue of Ricci curvature; for instance, in Lott–Villani–Sturm sense (see [23,28,29]), the Ricci curvature of the simplest subelliptic model, the Heisenberg group, is $-\infty$ (see [17]). However, we will show in this paper that we obtain exponential decays for the long-time behaviour of gradient estimates of the subelliptic semigroup on the model space **SU**(2) and controls on the small-time behaviour. Nevertheless, as it appears from our methods, the exponential decays we obtain are optimal but are mainly consequences of spectral properties, so that we do not really rely on any notion of *intrinsic Ricci curvature* except in the Li-Yau type estimate that we obtain. In the future, we hope to extend those methods to cover more general situations and to make the link with more geometrically oriented works like for instance [27], where a Bonnet-Myers type theorem is obtained in a hypoelliptic situation.

So, finally, this work is mainly divided into two parts. In a first part (Sect. 3), we will study the subelliptic heat kernel on **SU**(2). We provide its spectral decomposition, prove an integral representation of it and compute its small times asymptotics. In the second part (Sect. 4) we will focus on gradient estimates, using the previous results.

2 Preliminaries on SU(2)

In what follows, we consider the Lie group **SU**(2), i.e., the group of 2×2, complex, unitary matrices of determinant 1. Its Lie algebra $\mathfrak{su}(2)$ consists of 2×2, complex, skew-adjoint matrices of trace 0. A basis of $\mathfrak{su}(2)$ is formed by the Pauli matrices:

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

for which the following relationships hold

$$[Z, X] = 2Y, \quad [X, Y] = 2Z, \quad [Y, Z] = 2X. \tag{2.1}$$

We denote X, Y, Z the left invariant vector fields on **SU**(2) corresponding to the Pauli matrices. The Laplace–Beltrami operator for the bi-invariant Riemannian structure of $\mathbf{SU}(2) \simeq \mathbb{S}^3$ is

$$\Delta = X^2 + Y^2 + Z^2.$$

It is in the center of the universal enveloping algebra of the vector fields X, Y, Z. In the sequel, we shall mainly be interested in the operator

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

According to the relations (2.1) and due to Hörmander's theorem, $\mathcal{L}$ is subelliptic but not elliptic so that the associated geometry is not Riemannian but only subriemannian.

Associated to $\mathcal{L}$, there is a notion of distance given

$$\delta(g_1, g_2) = \sup_{f \in \mathcal{C}} \{| \, f(g_1) - f(g_2) \, |\}$$

where $\mathcal{C}$ is the set of smooth maps $\mathbf{SU}(2) \to \mathbb{R}$ that satisfy $(Xf)^2 + (Yf)^2 \leq 1$. This distance is the Carnot-Carathéodory distance. Via Chow's theorem, it can also be defined as the minimal length of horizontal curves joining two given points (see Chapter 3 of [7]).

To study $\mathcal{L}$, we will use the cylindric coordinates introduced in [11]:

$$(r, \theta, z) \to \exp{(r \cos \theta X + r \sin \theta Y)} \exp(zZ) = \begin{pmatrix} \cos(r)e^{iz} & \sin(r)e^{i(\theta - z)} \\ -\sin(r)e^{-i(\theta - z)} & \cos(r)e^{-iz} \end{pmatrix},$$

with

$$0 \leq r < \frac{\pi}{2}, \quad \theta \in [0, 2\pi], \quad z \in [-\pi, \pi].$$

Simple but tedious computations show that in these coordinates, the left-regular representation sends the matrices X, Y and Z to the left-invariant vector fields:

$$X = \cos(-\theta + 2z)\frac{\partial}{\partial r} + \sin(-\theta + 2z)\left(\tan r \frac{\partial}{\partial z} + \left(\tan r + \frac{1}{\tan r}\right)\frac{\partial}{\partial \theta}\right),$$

$$Y = -\sin(2z - \theta)\frac{\partial}{\partial r} + \cos(2z - \theta)\left(\tan r \frac{\partial}{\partial z} + \left(\tan r + \frac{1}{\tan r}\right)\frac{\partial}{\partial \theta}\right),$$

$$Z = \frac{\partial}{\partial z},$$

and that the bi-invariant normalized Haar measure reads:

$$d\mu = \frac{1}{4\pi^2} \sin 2r \, dr \, d\theta \, dz$$

Remark 2.1 The right regular representation sends the matrices X, Y and Z to the right-invariant vector fields

$$\hat{X} = \cos\theta \frac{\partial}{\partial r} + \sin\theta \left(\tan r \frac{\partial}{\partial z} + \left(\tan r - \frac{1}{\tan r} \right) \frac{\partial}{\partial \theta} \right)$$

$$\hat{Y} = \sin\theta \frac{\partial}{\partial r} - \cos\theta \left(\tan r \frac{\partial}{\partial z} + \left(\tan r - \frac{1}{\tan r} \right) \frac{\partial}{\partial \theta} \right).$$

$$\hat{Z} = \frac{\partial}{\partial z} + 2 \frac{\partial}{\partial \theta}$$

We therefore obtain

$$\mathcal{L} = X^2 + Y^2$$
$$= \frac{\partial^2}{\partial r^2} + 2 \cotan 2r \frac{\partial}{\partial r} + \left(2 + \frac{1}{\tan^2 r} + \tan^2 r \right) \frac{\partial^2}{\partial \theta^2} + \tan^2 r \frac{\partial^2}{\partial z^2} + 2(1 + \tan^2 r) \frac{\partial^2}{\partial z \partial \theta}$$

and

$$\Delta = X^2 + Y^2 + Z^2$$
$$= \frac{\partial^2}{\partial z^2} + \mathcal{L}$$

Note that $\mathcal{L}$ commutes with $\frac{\partial}{\partial \theta}$ and with $\frac{\partial}{\partial z}$.

3 The subelliptic heat kernel on SU(2)

By hypoellipticity, the heat semigroup $P_t = e^{t\mathcal{L}}$ admits a smooth kernel with respect to the Haar measure μ of **SU**(2). Our goal in this section will be to derive various representations of this kernel and to get precise asymptotics in small times.

3.1 Spectral decomposition of the heat kernel

Since $\mathcal{L}$ commutes with $\frac{\partial}{\partial \theta}$ that vanishes at 0, we deduce that the heat kernel (issued from the identity) of $P_t = e^{t\mathcal{L}}$, only depends on (r, z). It will be denoted by $p_t(r, z)$.

We first obtain the spectral decomposition of $p_t(r, z)$:

Proposition 3.1 *For $t > 0$, $0 \le r < \frac{\pi}{2}$, $z \in [-\pi, \pi]$.*

$$p_t(r, z) = \sum_{n=-\infty}^{+\infty} \sum_{k=0}^{+\infty} (2k + |n| + 1) e^{-(4k(k+|n|+1)+2|n|)t} e^{inz} (\cos r)^{|n|} P_k^{0,|n|}(\cos 2r),$$

where

$$P_k^{0,|n|}(x) = \frac{(-1)^k}{2^k k! (1+x)^{|n|}} \frac{d^k}{dx^k} \left((1+x)^{|n|} (1-x^2)^k \right)$$

is a Jacobi polynomial.

Proof Since the points (r, θ, z) and $(r, \theta, z + 2\pi)$ are the same, we can define $p_t(r, z)$ for all $z \in \mathbb{R}$ and it is 2π-periodic. The idea is then to expand $p_t(r, z)$ as a Fourier series in z:

$$p_t(r, z) = \sum_{n=-\infty}^{+\infty} e^{inz} \Phi_n(t, r)$$

Since $p_t(r, z)$ satisfies the partial differential equation,

$$\frac{\partial p_t}{\partial t} = \mathcal{L} p_t,$$

we obtain for Φ_n the following equation

$$\frac{\partial \Phi_n}{\partial t} = \frac{\partial^2 \Phi_n}{\partial r^2} + 2 \cot an 2r \frac{\partial \Phi_n}{\partial r} - n^2 \tan^2 r \Phi_n$$

and look for a solution under the form

$$\Phi_n(t, r) = e^{-2nt} (\cos r)^{|n|} g_n(t, \cos 2r).$$

We get:

$$\frac{\partial g_n}{\partial t} = 4\mathcal{G}_n(g_n)$$

where

$$\mathcal{G}_n = (1 - x^2) \frac{\partial^2}{\partial x^2} + (|n| - (2 + |n|)x) \frac{\partial}{\partial x}$$

It is well-known that eigenvectors of $\mathcal{G}_n$ are the Jacobi polynomials:

$$P_k^{0,|n|}(x) = \frac{(-1)^k}{2^k k! (1 + x)^{|n|}} \frac{d^k}{dx^k} \left((1 + x)^{|n|} (1 - x^2)^k \right)$$

In fact we have

$$\mathcal{G}_n(P_k^{0,|n|})(x) = -k(k + n + 1) P_k^{0,|n|}(x)$$

So we are finally led to put

$$p_t(r, z) = \sum_{n=-\infty}^{+\infty} \sum_{k=0}^{+\infty} \alpha_{k,n} e^{-(4k(k+|n|+1)+2|n|)t} e^{inz} (\cos r)^{|n|} P_k^{0,|n|}(\cos 2r)$$

for some $\alpha_{k,n}$, where the $\alpha_{k,n}$ will be determined by the initial condition at time 0.

Clearly p_t satisfies the equation $\frac{\partial p_t}{\partial t} = \mathcal{L} p_t$ and, by using the fact that $(P_k^{0,|n|})_{k \geq 0}$ is an orthogonal basis of $L^2([-1, 1], (1 + x)^{|n|} du)$ with $||P_k^{0,|n|}||^2 = \frac{2^{|n|+1}}{2k+|n|+1}$ we easily check that for a smooth f

$$\frac{1}{2\pi} \int_0^{\frac{\pi}{2}} \int_0^{2\pi} p_t(r, z) f(r, z) \sin(2r) dr dz \rightarrow_{t \to 0} f(0, 0)$$

as soon as $\alpha_{k,n} = 2k + |n| + 1$. $\qquad\square$

Remark 3.2 By using the representation theory of **SU**(2), a similar spectral decomposition is given in [8]. Nevertheless, for the sake of completeness, we included this elementary proof.

3.2 Integral representation of the heat kernel

We now provide an integral representation of p_t based on the following formula:

$$e^{t\mathcal{L}} = e^{-t\frac{\partial^2}{\partial z^2}} e^{t\Delta}$$

that stems from the commutation between Δ and $\frac{\partial}{\partial z}$. Since Δ is the Laplace–Beltrami operator on the three-dimensional sphere which has a well-known heat kernel, it will lead to an expression of p_t.

Let us consider on the interval $[-1, 1]$ the second order differential operator

$$\mathcal{J} = (1 - x^2)\frac{d^2}{dx^2} - 3x\frac{d}{dx}.$$

For $m \geq 0$, let U_m denotes the Chebyshev polynomial of the second kind:

$$U_m(\cos x) = \frac{\sin(m + 1)x}{\sin x},$$

and

$$q_t(x) = \sum_{m=0}^{+\infty}(m + 1)e^{-m(m+2)t}U_m(x), \quad x \in [-1, 1]. \tag{3.2}$$

It is known that if f is a smooth function $[-1, 1] \to \mathbb{R}$, then

$$(e^{t\mathcal{J}}f)(1) = \frac{2}{\pi}\int_{-1}^{1} q_t(x)f(x)(1 - x^2)^{1/2}dx,$$

Lemma 3.3 *If f is a smooth function* $\mathbf{SU}(2) \to \mathbb{R}$*, then for* $t \geq 0$*,*

$$(e^{t\Delta}f)(0) = \frac{1}{4\pi^2}\int_0^{\frac{\pi}{2}}\int_0^{2\pi}\int_{-\pi}^{\pi} q_t(\cos r \cos z)f(r, \theta, z)\sin 2r\, dr\, d\theta\, dz$$

Proof An easy calculation shows that the function $q_t(\cos r \cos z)$ solves the heat equation

$$\frac{\partial}{\partial t}(q_t(\cos r \cos z)) = \Delta(q_t(\cos r \cos z)).$$

Now we have to check the initial condition. We must show

$$\frac{1}{2\pi}\int_0^{\pi/2}\int_0^{2\pi} q_t(\cos r \cos z)f(r, z)\sin 2r\, dr\, dz \longrightarrow_{t\to 0} f(0, 0)$$

Since we will make the following change of variables:

$$\begin{cases} u = \cos r \cos z \\ v = \cos r \sin z \end{cases}$$

we take the function f of the form $f(r, z) = g(\cos r \cos z)h(\cos r \sin z)$. The new domain is $D = \{(x, y), x^2 + y^2 \leq 1\}$ and the Jacobian determinant is $\frac{1}{2}\sin 2r$. So

$$\frac{1}{2\pi} \int\limits_{r=0}^{\pi/2} \int\limits_{z=0}^{2\pi} q_t(\cos r \cos z) g(\cos r \cos z) h(\cos r \sin z) \sin 2r \, dr \, dz$$

$$= \frac{1}{\pi} \int\limits_{D} \int q_t(u) g(u) h(v) \, du \, dv$$

$$= \frac{1}{\pi} \int\limits_{-1}^{1} \left(\int\limits_{-(1-u^2)^{1/2}}^{(1-u^2)^{1/2}} h(v) \, dv \right) q_t(u) g(u) \, du$$

We may rewrite it as

$$\frac{2}{\pi} \int\limits_{-1}^{1} q_t(u) l(u) (1 - u^2)^{1/2} \, du$$

where l is the continuous function

$$l(u) = g(u) \left(\frac{\int_{-(1-u^2)^{1/2}}^{(1-u^2)^{1/2}} h(v) \, dv}{2(1 - u^2)^{1/2}} \right)$$

Now, since q_t is the heat kernel of a diffusion issued of 1 with respect to the measure $\frac{2}{\pi}(1-u^2)^{1/2} du$ and l is continuous, the last quantity is converging towards $l(1) = g(1)h(0) = f(0,0)$ and the lemma is proved. $\square$

Remark 3.4 The previous lemma shows that if ρ is the Riemannian distance from 0, then in our cylindric coordinates, we have

$$\cos \rho = \cos r \cos z.$$

From the previous proposition, we can now derive an expression for p_t in terms of q_t.

Let us first describe some properties of q_t that will be useful in the sequel. From the Poisson summation formula, we obtain that for $\theta \in \mathbb{R}$:

$$q_t(\cos \theta) = \frac{\sqrt{\pi} e^t}{4t^{\frac{3}{2}}} \frac{1}{\sin \theta} \sum_{k \in \mathbb{Z}} (\theta + 2k\pi) e^{-\frac{(\theta + 2k\pi)^2}{4t}}$$

$$= \frac{\sqrt{\pi} e^t}{4t^{\frac{3}{2}}} \frac{\theta}{\sin \theta} e^{-\frac{\theta^2}{4t}} \left(1 + 2 \sum_{k=1}^{+\infty} e^{-\frac{k^2 \pi^2}{t}} \left(\cosh \frac{k\pi\theta}{t} + 2k\pi \frac{\sinh \frac{k\pi\theta}{t}}{\theta} \right) \right)$$

These expressions show that $q_t(\cos \theta)$ admits an analytic extension for $\theta \in \mathbb{C}$. We moreover obtain precise estimates:

- Let $\varepsilon > 0$, for $x \in (-1+\varepsilon, 1]$ and $t > 0$:

$$q_t(x) = \frac{\sqrt{\pi} e^t}{4t^{\frac{3}{2}}} \frac{\arccos x}{\sqrt{1-x^2}} e^{-\frac{(\arccos x)^2}{4t}} (1 + R_1(t, x)), \tag{3.3}$$

where for some positive constants C_1 and C_2 depending only in ε, $|R_1(t, x)| \leq C_1 e^{-\frac{C_2}{t}}$.

- For $x \in [1, +\infty)$ and $t > 0$:

$$q_t(x) = \frac{\sqrt{\pi}e^t}{4t^{\frac{3}{2}}} \frac{\text{arcosh}x}{\sqrt{x^2-1}} e^{-\frac{(\text{arcosh}x)^2}{4t}} (1 + R_2(t, x)),$$ (3.4)

where for some positive constants C_3 and C_4, $\mid R_2(t, x) \mid \leq C_3 e^{-\frac{C_4}{t}}$.

Proposition 3.5 *We have for* $t > 0$, $r \in [0, \pi/2)$, $z \in [-\pi, \pi]$,

$$p_t(r, z) = \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{+\infty} e^{-\frac{(y+iz)^2}{4t}} q_t(\cos r \cosh y) dy$$

Proof Let

$$h_t(r, z) = \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{+\infty} e^{-\frac{(y+iz)^2}{4t}} q_t(\cos r \cosh y) dy;$$

the integral being well defined thanks to the estimates on q_t. By using the fact that

$$\frac{\partial}{\partial t}\left(\frac{e^{-\frac{y^2}{4t}}}{\sqrt{4\pi t}}\right) = \frac{\partial^2}{\partial y^2}\left(\frac{e^{-\frac{y^2}{4t}}}{\sqrt{4\pi t}}\right)$$

and

$$\frac{\partial}{\partial t}(q_t(\cos r \cos z)) = \Delta(q_t(\cos r \cos z)),$$

a double integration by parts with respect to the variable y shows that

$$\frac{\partial h_t}{\partial t} = \mathcal{L}h_t.$$

Let us now check the initial condition. Let $f(r, z) = e^{i\lambda z} g(r)$ where $\lambda \in \mathbb{R}$ and g is a smooth function. We have

$$\frac{1}{4\pi^2} \int_0^{\frac{\pi}{2}} \int_0^{2\pi} \int_{-\pi}^{\pi} h_t(r, z) f(r, z) \sin 2r dr d\theta dz = e^{t\lambda^2} \left(e^{t\Delta} g\right)(0),$$

so that we obtain the required result. □

We are now in position to collect some properties of p_t.

Proposition 3.6 *For* $\lambda \in \mathbb{C}$, **Re**$\lambda > 0$, $r \in [0, \pi/2)$, $z \in [-\pi, \pi]$,

$$\int_0^{+\infty} p_t(r, z) e^{-t-\frac{\lambda}{t}} dt = \int_{-\infty}^{+\infty} \frac{dy}{8\pi^2 \left(\cosh\sqrt{y^2+4\lambda} - \cos r \cos(z+iy)\right)}$$

Proof We have

$$\int_0^{+\infty} e^{-\frac{\lambda}{t}} p_t(r, z) e^{-t} dt = \frac{1}{\sqrt{4\pi}} \int_{-\infty}^{+\infty} \int_0^{+\infty} e^{-t-\frac{y^2+4\lambda}{4t}} q_t(\cos r \cos(z+iy)) \frac{dt}{\sqrt{t}} dy$$

We now compute

$$\int\limits_0^{+\infty} e^{-t-\frac{y^2+4\lambda}{4t}} q_t(\cos r \cos(z+iy)) \frac{dt}{\sqrt{t}}$$

by using the symbolic calculus on differential operators (it can be made rigorous with 3.2).

$$\int\limits_0^{+\infty} e^{-t-\frac{y^2+4\lambda}{4t}} e^{t\Delta} \frac{dt}{\sqrt{t}} dt = \int\limits_0^{+\infty} e^{-\frac{y^2+4\lambda}{4t}} e^{-t(-\Delta+1)} \frac{dt}{\sqrt{t}} dt$$

$$= \frac{\sqrt{\pi}}{\sqrt{-\Delta+1}} e^{-\sqrt{y^2+4\lambda}\sqrt{-\Delta+1}}$$

But from Taylor [30, pp. 95],

$$\frac{1}{\sqrt{-\Delta+1}} e^{-\sqrt{y^2+4\lambda}\sqrt{-\Delta+1}} = \frac{1}{4\pi^2 \left(\cosh\sqrt{y^2+4\lambda} - \cos r \cos z\right)},$$

which implies the result. $\qquad\square$

If we fix, $r \in [0, \pi/2)$, $z \in [-\pi, \pi]$, we observe that it possible to find $\theta(r, z) \in \mathbb{R}$, such that for $\lambda \in \mathbb{C}$, **Re**$\lambda > 0$ and $y \in \mathbb{R}$,

$$\cosh\sqrt{y^2+4\lambda} = \cos r \cos(z+iy) \Rightarrow \textbf{Re}\lambda \leq \theta(r,z),$$

where we use the principal branch of the square root. By inverting the last Laplace transform of the previous proposition, we therefore get:

Corollary 3.7 *We have for $t > 0$, $r \in [0, \pi/2)$, $z \in [-\pi, \pi]$, and $\gamma > \theta(r, z)$,*

$$p_t(r, z) = \frac{e^t}{16i\pi^3 t^2} \int\limits_{\lambda=\gamma-i\infty}^{\gamma+i\infty} \int\limits_{y=-\infty}^{+\infty} \frac{e^{\frac{\lambda}{t}} dy d\lambda}{\cosh\sqrt{y^2+4\lambda} - \cos r \cos(z+iy)}$$

From Proposition 3.6, we also deduce:

Proposition 3.8 *The Green function of the operator $-\mathcal{L} + 1$ is given by*

$$G(r, z) = \frac{1}{8\pi} \frac{1}{\sqrt{1 - 2\cos r \cos z + \cos^2 r}}.$$

Proof Let us assume $r \neq 0$, $z \neq 0$. In that case the Laplace transform of Proposition 3.6 can be extended to $\lambda = 0$ and we have:

$$G(r, z) = \int_{-\infty}^{+\infty} \frac{dy}{8\pi^2 \left(\cosh y - \cos r \cos(z + iy)\right)}$$

$$= \int_{-\infty}^{+\infty} \frac{dy}{8\pi^2 \left((1 - \cos r \cos z) \cosh y - i \cos r \sin z \sinh y\right)}$$

$$= \frac{1}{8\pi^2} \frac{1}{\sqrt{1 - 2 \cos r \cos z + \cos^2 r}} \int_{-\infty}^{+\infty} \frac{dy}{\cosh y}$$

$$= \frac{1}{8\pi} \frac{1}{\sqrt{1 - 2 \cos r \cos z + \cos^2 r}}$$

□

3.3 Asymptotics of the heat kernel in small times

The goal of this section is to obtain the precise asymptotics of the heat kernel when $t \to 0$. We start with the points of the form $(0, z)$ that lie on the cut-locus of 0.

Proposition 3.9 *For $t > 0$ and $z \in [0, \pi)$,*

$$p_t(0, z) = \frac{\pi^2 e^t}{4t^2} e^{-\frac{2\pi z - z^2}{4t}} \sum_{k \in \mathbb{Z}} e^{-\frac{k(k+1)\pi^2}{t}} \frac{(2k + 1) + 2k e^{-\frac{\pi}{2t}(z + 2k\pi)}}{\left(1 + e^{-\frac{\pi}{2t}(z + 2k\pi)}\right)^2}$$

therefore, when $t \to 0$,

$$p_t(0, z) = \frac{\pi^2 e^t}{4t^2} e^{-\frac{2\pi z - z^2}{4t}} \left(1 + O(e^{-\frac{C}{t}})\right)$$

Proof Let $z \in (0, \pi]$. We have

$$p_t(0, z) = \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{+\infty} e^{-\frac{y^2}{4t}} q_t(\cosh(y - iz))) dy,$$

But

$$q_t(\cosh(y - iz)) = \frac{\sqrt{\pi} e^t}{4t^{\frac{3}{2}}} \frac{1}{\sinh(y - iz)} \sum_{k \in \mathbb{Z}} (y - iz - 2ik\pi) e^{\frac{(y - iz - 2ik\pi)^2}{4t}}$$

and for $k \in \mathbb{Z}$, from the residue theorem,

$$\int_{-\infty}^{+\infty} \frac{y - iz - 2ik\pi}{\sinh(y - iz)} e^{-\frac{iy}{2t}(z + 2k\pi)} dy = 2\pi^2 e^{\frac{(z + 2k\pi)^2 - (2k+1)\pi(z + 2k\pi)}{2t}} \frac{(2k + 1) + 2k e^{-\frac{\pi}{2t}(z + 2k\pi)}}{\left(1 + e^{-\frac{\pi}{2t}(z + 2k\pi)}\right)^2}.$$

The result easily follows.   □

We now come to points (r, z) that do not lie on the cut-locus, that is $r \neq 0$.

Proposition 3.10 *For $r \in \left(0, \frac{\pi}{2}\right)$, when $t \to 0$,*

$$p_t(r, 0) \sim \frac{r}{\sin r} \sqrt{\frac{1}{1 - r \cot\! n r}} \frac{\sqrt{\pi} e^{-\frac{r^2}{4t}}}{4t^{\frac{3}{2}}}.$$

Proof We fix $r \in \left(0, \frac{\pi}{2}\right)$. From the proposition 3.5 and due to the estimates on q_t we get:

$$p_t(r, 0) \sim_{t \to 0} \frac{1}{8t^2} (J_1(t) + J_2(t)),$$

where

$$J_1(t) = \int_{\cosh y \le \frac{1}{\cos r}} e^{-\frac{y^2 + (\arccos(\cos r \cosh y))^2}{4t}} \frac{\arccos(\cos r \cosh y)}{\sqrt{1 - \cos^2 r \cosh^2 y}} dy$$

and

$$J_2(t) = \int_{\cosh y \ge \frac{1}{\cos r}} e^{-\frac{y^2 - (\operatorname{arcosh}(\cos r \cosh y))^2}{4t}} \frac{\operatorname{arcosh}(\cos r \cosh y)}{\sqrt{\cos^2 r \cosh^2 y - 1}} dy.$$

We now analyze the two above integrals in small times thanks to the Laplace method and show that $J_2(t)$ can be omitted.

On the interval $\left[-\operatorname{arcosh}\frac{1}{\cos r}, \operatorname{arcosh}\frac{1}{\cos r}\right]$, the function

$$f(y) = y^2 + (\arccos(\cos r \cosh y))^2$$

has a unique minimum which is attained at $y = 0$ and, at this point:

$$f''(0) = 2(1 - r \cot\! n r).$$

Therefore, thanks to the Laplace method

$$J_1(t) \sim_{t \to 0} e^{-\frac{r^2}{4t}} \frac{r}{\sin r} \sqrt{\frac{4\pi t}{1 - r \cot\! n r}}.$$

We now analyze the second integral. On $\left(-\infty, -\operatorname{arcosh}\frac{1}{\cos r}\right) \cup \left(\operatorname{arcosh}\frac{1}{\cos r}, +\infty\right)$, the function

$$g(y) = y^2 - (\operatorname{arcosh}(\cos r \cosh y))^2,$$

has no minimum. Therefore, from the Laplace method $J_2(t)$ is negligible with respect to $J_1(t)$ when $t \to 0$. $\square$

The previous proposition can be extended by the same method when $z \ne 0$. If we fix $r \in \left(0, \frac{\pi}{2}\right), z \in [-\pi, \pi]$, then the function

$$f(y) = (y - iz)^2 + (\arccos(\cos r \cosh y))^2,$$

defined on the strip $|\operatorname{Re}(y)| < \operatorname{arcosh}\frac{1}{\cos r}$ has a critical point at $i\theta(r, z)$ where $\theta(r, z)$ is the unique solution in $[-\pi, \pi]$ to the equation:

$$\theta(r, z) - z = \cos r \sin \theta(r, z) \frac{\arccos(\cos \theta(r, z) \cos r)}{\sqrt{1 - \cos^2 r \cos^2 \theta(r, z)}}.$$

Indeed, with $u = \cos r \cos \theta$

$$\frac{\partial}{\partial \theta}\left(\theta - \cos r \sin \theta \frac{\arccos(\cos \theta \cos r)}{\sqrt{1 - \cos^2 r \cos^2 \theta}}\right) = \frac{\sin^2 r}{1 - u(r,z)^2}\left(1 - \frac{u(r,z)\arccos u(r,z)}{\sqrt{1 - u^2(r,z)}}\right)$$

which is positive. So this last function is bijective from $[-\pi, \pi]$ on itself.

We observe that at the point $\theta(r, z)$, $f''(i\theta(r, z))$ is a positive real number:

$$f''(i\theta(r, z)) = 2\frac{\sin^2 r}{1 - u(r,z)^2}\left(1 - \frac{u(r,z)\arccos u(r,z)}{\sqrt{1 - u^2(r,z)}}\right)$$

where $u(r, z) = \cos r \cos \theta(r, z)$. By the same method than in the previous proposition, we obtain:

Proposition 3.11 *Let* $r \in \left(0, \frac{\pi}{2}\right)$, $z \in [-\pi, \pi]$. *When* $t \to 0$,

$$p_t(r, z) \sim \frac{1}{\sin r}\frac{\arccos u(r, z)}{\sqrt{1 - \frac{u(r,z)\arccos u(r,z)}{\sqrt{1 - u^2(r,z)}}}}\frac{\sqrt{\pi}e^{-\frac{(\theta(r,z)-z)^2 \tan^2 r}{4t \sin^2 \theta(r,z)}}}{4t^{\frac{3}{2}}}.$$

Remark 3.12 According to Léandre results [19] and [20] (see also [18]), the previous asymptotics give a way to compute the sub-Riemannian distance from 0 to the point $(r, \theta, z) \in \mathbf{SU}(2)$ by computing $\lim_{t\to 0} -4t \ln p_t(r, z)$. This distance does not depend on the variable θ and shall be denoted by $d(r, z)$.

- For $z \in [-\pi, \pi]$,

$$d^2(0, z) = 2\pi \mid z \mid -z^2.$$

- For $z \in [-\pi, \pi]$, $r \in \left(0, \frac{\pi}{2}\right)$,

$$d^2(r, z) = \frac{(\theta(r, z) - z)^2 \tan^2 r}{\sin^2 \theta(r, z)}.$$

In particular, $d^2(r, 0) = r^2$.

We can observe that the subriemannian diameter of $\mathbf{SU}(2)$ is thus π^2.

To conclude this section on the asymptotics in small times, we show that after a convenient scaling, the heat kernel of $\mathbf{SU}(2)$ uniformly (on compact sets) converges to the heat kernel of the Heisenberg group. This scaling is related to the fact that dilation of $\mathbf{SU}(2)$ leads to the Heisenberg group (see for instance [26] and its extension [12]).

Let us first recall some basic properties of the three-dimensional Heisenberg group (see by, e.g., [5,7] and the references therein): $\mathbb{H}$ can be represented as $\mathbb{R}^3$ endowed with the polynomial group law:

$$(x_1, y_1, z_1)(x_2, y_2, z_2) = (x_1 + x_2, y_1 + y_2, z_1 + z_2 + x_1 y_2 - x_2 y_1).$$

The left invariant vector fields read in cylindric coordinates ($x = r \cos \theta$, $y = r \sin \theta$):

$$\tilde{X} = \cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r}\frac{\partial}{\partial \theta} - r \sin \theta \frac{\partial}{\partial z} \tag{3.5}$$

$$\tilde{Y} = \sin \theta \frac{\partial}{\partial r} + \frac{\cos \theta}{r}\frac{\partial}{\partial \theta} + r \cos \theta \frac{\partial}{\partial z} \tag{3.6}$$

$$\tilde{Z} = \frac{\partial}{\partial z}. \tag{3.7}$$

And the following equalities hold

$$[\tilde{X}, \tilde{Y}] = 2\tilde{Z}, \quad [\tilde{X}, \tilde{Z}] = [\tilde{Y}, \tilde{Z}] = 0.$$

We denote

$$\tilde{\mathcal{L}} = \tilde{X}^2 + \tilde{Y}^2.$$

Due to Gaveau's formula (see [14,16]), with respect to the Lebesgue measure $r\,dr\,d\theta\,dz$ the heat kernel associated to the semigroup $(\tilde{P}_t)_{t\geq 0} = (e^{t\tilde{\mathcal{L}}})_{t\geq 0}$ writes

$$h_t(r, z) = \frac{1}{16\pi^2} \int_{-\infty}^{+\infty} e^{\frac{i\lambda z}{2}} \frac{\lambda}{\sinh \lambda t} e^{-\frac{r^2}{4}\lambda\coth\lambda t} d\lambda. \tag{3.8}$$

By using the explicit formula for p, we can prove:

Proposition 3.13 *Uniformly on compact sets of $\mathbb{R}_{\geq 0} \times \mathbb{R}$.*

$$\lim_{t\to 0} t^2 p_t(\sqrt{t}r, tz) = 2\pi^2 h_1(r, z)$$

Proof Let K be a compact of $\mathbb{R}_{\geq 0} \times \mathbb{R}$ and $t > 0$ sufficiently small so that $(\sqrt{t}r, tz) \in [0, \frac{\pi}{2}] \times [-\pi, \pi]$ for all $(r, z) \in K$.

According to Proposition 3.5 we have

$$t^2 p_t(\sqrt{t}r, tz) = \frac{t^{3/2}}{\sqrt{4\pi}} \int_{-\infty}^{\infty} e^{-\frac{(y+itz)^2}{4t}} q_t(\cos \sqrt{t}r \cosh y) dy.$$

The idea is now to use the estimates (3.3) and (3.4) and to study the two integrals:

$$J_1(t, r, z) = \int_{\cosh y \leq \frac{1}{\cos \sqrt{t}r}} e^{-\frac{(y+itz)^2 + \arccos^2(\cos \sqrt{t}r \cosh y)}{4t}} \frac{\arccos(\cos \sqrt{t}r \cosh y)}{\sqrt{1 - \cos^2 \sqrt{t}r \cosh^2 y}} dy$$

and

$$J_2(t, r, z) = \int_{\cosh y \geq \frac{1}{\cos \sqrt{t}r}} e^{-\frac{(y+itz)^2 - \text{arccosh}^2(\cos \sqrt{t}r \cosh y)}{4t}} \frac{\text{arccosh}(\cos \sqrt{t}r \cosh y)}{\sqrt{\cos^2 \sqrt{t}r \cosh^2 y - 1}} dy.$$

It is easily seen that for some constant $C > 0$, uniformly on K,

$$|J_1(t, r, z)| \leq Ce^{\frac{tz^2}{4}} \sqrt{t}r.$$

Therefore $J_1(t, r, z)$ goes uniformly to 0 on K.

Let us now turn to the integral $J_2(t, r, z)$ and let us show that, uniformly, $J_2(t, r, z)$ converges to $2\pi^2 h_1(r, z)$.

Let $\varepsilon > 0$. Let us observe that $\left| e^{\frac{iyz}{2}} e^{-\frac{r^2}{4}y\coth y} \frac{y}{\sinh y} \right|$ is less than ye^{-y} for big y and all r, z.

Note also that for all $1 < u \leq \cosh(y/2)$,

$$e^{-(\frac{y^2 - \text{arccosh}^2 u}{4t})} \frac{\text{arccosh} u}{\sqrt{u^2 - 1}} \leq e^{-\frac{y^2}{8t}}$$

and for all $\cosh(y/2) \le u \le \cosh(y)$

$$e^{-(\frac{y^2 - \text{arcosh}^2 u}{4t})} \frac{\text{arcosh}u}{\sqrt{u^2 - 1}} \le \frac{y/2}{\sinh y/2}.$$

The last three quantities are integrable and do not depend on r, z, so we can find $y_1 > 0$ so that

$$\int_{|y| \ge y_1} e^{\frac{iyz}{2}} e^{-\frac{r^2}{4} y \coth y} \frac{y}{\sinh y} dy \le \varepsilon.$$

and

$$\int_{|y| \ge y_1} e^{-\frac{(y+itz)^2 - \text{arccosh}^2(\cos \sqrt{tr} \cosh y)}{4t}} \frac{\text{arccosh}(\cos \sqrt{tr} \cosh y)}{\sqrt{\cos^2 \sqrt{tr} \cosh^2 y - 1}} dy \le \varepsilon.$$

Now we study the behavior of our integrals for small y. $|e^{\frac{iyz}{2}} e^{-\frac{r^2}{4} y \coth y} \frac{y}{\sinh y}|$ is less than 1 for small y and $e^{-\frac{(y+itz)^2 - \text{arccosh}^2(\cos \sqrt{tr} \cosh y)}{4t}} \frac{\text{arccosh}(\cos \sqrt{tr} \cosh y))}{\sqrt{\cos^2 \sqrt{tr} \cosh^2 y - 1}}$ is less than $e^{\frac{tz^2}{4}}$ for small y. Thus, as before there exists $0 < y_0$ such that

$$\int_{|y| \le y_0} e^{\frac{iyz}{2}} e^{-\frac{r^2}{4} y \coth y} \frac{y}{\sinh y} dy \le \varepsilon.$$

and

$$\int_{\text{arccosh}(\frac{1}{\cos \sqrt{tr}}) \le |y| \le y_0} e^{-\frac{(y+itz)^2 - \text{arccosh}^2(\cos \sqrt{tr} \cosh y)}{4t}} \frac{\text{arccosh}(\cos \sqrt{tr} \cosh y))}{\sqrt{\cos^2 \sqrt{tr} \cosh^2 y - 1}} dy \le \varepsilon.$$

Let $y_0 < y < y_1$ and $0 < u \le \cosh y - 1$ by the Taylor-Lagrange development formula we have the following equality

$$\text{arccosh}(\cosh y - u) = y - \frac{1}{\sinh y} u - \frac{\tilde{y}}{\sinh^{3/2} \tilde{y}} \frac{u^2}{2}.$$

for some $\tilde{y} \in]\text{arccosh}(\cosh y - u), y[$. By applying this to $\cos \sqrt{tr} \cosh y = \cosh y - tr^2 \cosh y + O(t^2 r^4) \cosh y$, we get

$$\text{arccosh}(\cos \sqrt{tr} \cosh y) = y - tr^2 \coth y + O(t^2 r^4) \left(\coth y + \cosh^2 y \frac{\tilde{y}}{\sinh^{3/2} \tilde{y}} \right)$$

for some $\tilde{y} \in]\text{arcosh}(\cos \sqrt{tr} \cosh y), y[$. So

$$\text{arccosh}^2(\cos \sqrt{tr} \cosh y) = y^2 - tr^2 y \coth y + O(t^2 r^4) \left(y \coth y + y \cosh^2 y \frac{\tilde{y}}{\sinh^{3/2} \tilde{y}} \right).$$

and

$$e^{-\frac{(y+itz)^2 - \text{arccosh}^2(\cos \sqrt{tr} \cosh y)}{4t}} = e^{\frac{-iyz}{2}} e^{-\frac{r^2}{4} y \coth y} e^{\frac{tz^2}{4}}$$

$$\times \left(1 + O(t^2 r^4) \left(y \coth y + y \cosh^2 y \frac{\tilde{y}}{\sinh^{3/2} \tilde{y}} \right) \right)$$

Finally, using also Taylor Lagrange development formula at order 1 we obtain

$$\frac{\operatorname{arccosh}(\cos\sqrt{t}r\cosh y)}{\sqrt{\cos^2\sqrt{t}r\cosh^2 y - 1}} = \frac{y}{\sinh y} - \frac{tr^2}{2}\cosh(y)\left(\frac{1}{\sinh^2\hat{y}} + 2\frac{\hat{y}\cosh\hat{y}}{\sinh^3\hat{y}}\right)$$

for some $\hat{y}\in{}]\operatorname{arcosh}(\cos\sqrt{t}r\cosh y),y[$.

So finally, we see we can pass uniformly to the limit under the integral for $y_0\le|y|\le y_1$ and obtain our proposition. □

4 Gradient bounds for the heat kernel measure

In this section, our main goal will be to quantify the regularization property of the semigroup $P_t = e^{t\mathcal{L}}$: We shall mainly be concerned with bounds for $(XP_t f)^2 + (YP_t f)^2$.

We shall often make use of the following notations (see [1,3]): We set for f, g smooth functions,

$$2\Gamma(f, g) = \mathcal{L}(fg) - f\mathcal{L}g - g\mathcal{L}f$$

and

$$2\Gamma_2(f, g) = \mathcal{L}\Gamma(f, g) - \Gamma(f, \mathcal{L}g) - \Gamma(g, \mathcal{L}f).$$

In the present setting,

$$\Gamma(f, f) = (Xf)^2 + (Yf)^2$$

and

$$\Gamma_2(f, f) = (X^2 f)^2 + (Y^2 f)^2 + \frac{1}{2}((XY + YX)f)^2 + 2(Zf)^2 + 4\Gamma(f, f)$$
$$-4(Xf)(YZf) + 4(Yf)(XZf). \tag{4.9}$$

In particular, if f is a smooth function that only depends on the variables r and z, we obtain

$$\Gamma(f, f) = \left(\frac{\partial f}{\partial r}\right)^2 + \tan^2 r\left(\frac{\partial f}{\partial z}\right)^2,$$

and

$$\Gamma_2(f, f) = \left(\frac{\partial^2 f}{\partial r^2}\right)^2 + 2\tan^2 r\left(\frac{\partial^2 f}{\partial r\partial z}\right)^2 + \tan^4 r\left(\frac{\partial^2 f}{\partial z^2}\right)^2 + \frac{2}{\cos^4 r}\left(\frac{\partial f}{\partial z}\right)^2$$
$$+\frac{4}{\sin^2 2r}\left(\frac{\partial f}{\partial r}\right)^2 + \frac{4\tan r}{\cos^2 r}\left(\frac{\partial f}{\partial z}\right)\left(\frac{\partial^2 f}{\partial r\partial z}\right) - \frac{2\tan r}{\cos^2 r}\left(\frac{\partial f}{\partial r}\right)\left(\frac{\partial^2 f}{\partial z^2}\right)$$
$$=\left(\frac{\partial^2 f}{\partial r^2}\right)^2 + \left(\tan^2 r\frac{\partial^2 f}{\partial z^2} - \frac{2}{\sin 2r}\frac{\partial f}{\partial r}\right)^2 + 2\left(\frac{1}{\cos^2 r}\frac{\partial f}{\partial z} + \tan r\frac{\partial^2 f}{\partial r\partial z}\right)^2.$$

Thus, as an interesting consequence, if f is a smooth function that only depends on the variables r and z, $\Gamma_2(f, f)\ge 0$.

4.1 A first gradient bound

Proposition 4.1 *Let $f : \mathbf{SU}(2) \to \mathbb{R}$ be a smooth function. For $t > 0$ and $g \in \mathbf{SU}(2)$,*

$$\Gamma(P_t f, P_t f)(g) \le A(t) \left(\int_{\mathbf{SU}(2)} f^2 d\mu - \left(\int_{\mathbf{SU}(2)} f d\mu \right)^2 \right)$$

where

$$A(t) = -\frac{1}{4} \frac{\partial}{\partial t} \int_{\mathbf{SU}(2)} p_t^2 d\mu.$$

Proof By left invariance, it is enough to prove this inequality at $g = 0$. We can moreover assume that $\int_{\mathbf{SU}(2)} f d\mu = 0$. If we denote by $\hat{X}$ and $\hat{Y}$ the right invariant vector fields, then we have:

$$\Gamma(P_t f, P_t f)(0) = (X P_t f)^2(0) + (Y P_t f)^2(0)$$

$$= (P_t \hat{X} f)^2(0) + (P_t \hat{Y} f)^2(0)$$

$$= \left(\int_{\mathbf{SU}(2)} p_t(r, z) \hat{X} f(r, \theta, z) d\mu \right)^2 + \left(\int_{\mathbf{SU}(2)} p_t(r, z) \hat{Y} f(r, \theta, z) d\mu \right)^2$$

$$= \left(\int_{\mathbf{SU}(2)} \hat{X} p_t(r, z) f(r, \theta, z) d\mu \right)^2 + \left(\int_{\mathbf{SU}(2)} \hat{Y} p_t(r, z) f(r, \theta, z) d\mu \right)^2$$

Now, let us observe that since p_t does not depend on θ, we have

$$\int_{\mathbf{SU}(2)} (\hat{X} p_t)^2 d\mu = \int_{\mathbf{SU}(2)} (\hat{Y} p_t)^2 d\mu = \frac{1}{2} \int_{\mathbf{SU}(2)} \Gamma(p_t, p_t) d\mu,$$

and

$$\int_{\mathbf{SU}(2)} \hat{X} p_t \hat{Y} p_t d\mu = 0.$$

Therefore, from Cauchy–Schwarz inequality, we conclude that:

$$\Gamma(P_t f, P_t f)(0) \le \frac{1}{2} \int_{\mathbf{SU}(2)} \Gamma(p_t, p_t) d\mu \int_{\mathbf{SU}(2)} f^2 d\mu,$$

which is the required inequality because:

$$\int_{\mathbf{SU}(2)} \Gamma(p_t, p_t) d\mu = - \int_{\mathbf{SU}(2)} p_t L p_t d\mu = -\frac{1}{2} \frac{\partial}{\partial t} \int_{\mathbf{SU}(2)} p_t^2 d\mu$$

$\square$

We now study the constant $A(t)$.

Proposition 4.2 *We have the following properties*:

- *A is decreasing*;
- $A(t) \sim_{t \to 0} \frac{\pi^2}{32t^3}$;
- $A(t) \sim_{t \to +\infty} 4e^{-4t}$.

Proof Let us first show that C is decreasing. We have:

$$A'(t) = - \int_{\mathbf{SU}(2)} \Gamma_2(p_t, p_t) d\mu.$$

Since p_t only depends on (r, z), $\Gamma_2(p_t, p_t) \geq 0$ and thus $A'(t) \leq 0$.

We can now observe that, due to the semigroup property,

$$\int_{\mathbf{SU}(2)} p_t^2 d\mu = p_{2t}(0)$$

But from Proposition 3.1 and 3.9,

$$p_t(0) = \sum_{n=-\infty}^{+\infty} \sum_{k=0}^{+\infty} (2k + |n| + 1) e^{-(4k(k+|n|+1)+2|n|)t}$$

$$= \frac{\pi^2 e^t}{4t^2} \sum_{k \in \mathbb{Z}} e^{-\frac{k(k+1)\pi^2}{t}} \frac{(2k+1) + 2ke^{-\frac{2k\pi^2}{t}}}{\left(1 + e^{-\frac{k\pi^2}{t}}\right)^2},$$

which implies the expected result. $\qquad\qquad\square$

4.2 Li-Yau type inequality

We now provide a Li-Yau type estimate for the heat semigroup. The inequality we obtain is an improvement in the specific case of $\mathbf{SU}(2)$ of the Cao-Yau gradient estimate for subelliptic operators that was obtained in [10]. The idea of the method that is used to prove Theorem 4.3 is due to Bakry and was given to the authors during personal discussions; It is close to [6]. We have the following inequality:

Theorem 4.3 *For all $\alpha > 2$, for every positive function f and $t > 0$,*

$$\Gamma(\ln P_t f) + \frac{t}{\alpha}(Z \ln P_t f)^2 \leq \left(\frac{3\alpha - 1}{\alpha - 1} - \frac{2t}{\alpha}\right)\frac{\mathcal{L}P_t f}{P_t f} + \frac{t}{\alpha} - \frac{3\alpha - 1}{\alpha - 1} + \frac{(3\alpha - 1)^2}{\alpha - 2}\frac{1}{t}$$

Proof We fix a positive function f and $t > 0$ and all the following computations are made at a given point $x \in \mathbf{SU}(2)$.

For $0 \leq s \leq t$, let

$$\Phi_1(s) = P_s((P_{t-s}f)\Gamma(\ln P_{t-s}f))$$

and

$$\Phi_2(s) = P_s((P_{t-s}f)(Z \ln P_{t-s}f)^2).$$

Straightforward, but heavy, computations show that

$$\Phi_1'(s) = 2P_s((P_{t-s}f)\Gamma_2(\ln P_{t-s}f))$$

and

$$\Phi_2'(s) = 2P_s((P_{t-s}f)\Gamma(Z\ln P_{t-s}f)).$$

Now, thanks to the Cauchy–Schwarz inequality, the expression 4.9, shows that for every $\lambda > 0$, and every smooth function g,

$$\Gamma_2(g) \geq \frac{1}{2}(\mathcal{L}g)^2 + 2(Zg)^2 + \left(4 - \frac{2}{\lambda}\right)\Gamma(g) - 2\lambda\Gamma(Zg).$$

We therefore obtain the following differential inequality

$$\Phi_1'(s) \geq P_s((P_{t-s}f)(\mathcal{L}\ln P_{t-s}f)^2) + 4\Phi_2(s) + \left(8 - \frac{4}{\lambda}\right)\Phi_1(s) - 2\lambda\Phi_2'(s).$$

We now have that for every $\gamma \in \mathbb{R}$,

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

and

$$\mathcal{L}\ln P_{t-s}f = \frac{\mathcal{L}P_{t-s}f}{P_{t-s}f} - \frac{\Gamma(P_{t-s}f)}{(P_{t-s}f)^2}.$$

Thus, for every $\lambda > 0$ and every $\gamma \in \mathbb{R}$,

$$\Phi_1'(s) \geq \left(8 - \frac{4}{\lambda} - 2\gamma\right)\Phi_1(s) + 4\Phi_2(s) - 2\lambda\Phi_2'(s) + 2\gamma\mathcal{L}P_tf - \gamma^2 P_tf.$$

Let now b a positive decreasing function on the time interval $[0, t)$. By choosing in the previous inequality

$$\lambda = -2\frac{b}{b'}$$

and

$$\gamma = \frac{1}{2}\left(8 + 2\frac{b'}{b} + \frac{b''}{b'}\right),$$

we get

$$\left(-\frac{1}{4}b'\Phi_1 + b\Phi_2\right)' \geq -\frac{1}{4}b'\left(\left(8 + 2\frac{b'}{b} + \frac{b''}{b'}\right)\mathcal{L}P_tf - \frac{1}{4}\left(8 + 2\frac{b'}{b} + \frac{b''}{b'}\right)^2 P_tf\right).$$

Integrating the previous inequality from 0 to t with the function $b(s) = (t-s)^\alpha$, $\alpha > 2$, gives the expected result. $\qquad\square$

Remark 4.4 Of course, by the same method, we obtain a Li-Yau type inequality for the heat kernel $p_t(r, z)$ itself.

Remark 4.5 Interestingly, we can obtain an exponential decay in the previous inequality. Indeed, if we use the function $b(s) = e^{-\frac{8s}{3}}\left(1 - e^{-\frac{8(t-s)}{3\alpha}}\right)^\alpha$, $\alpha > 2$, in the previous proof, then we obtain that for every $\alpha > 2, t > 0$,

$$\Gamma(\ln P_tf) + \frac{3}{2}\left(1 - e^{-\frac{8t}{3\alpha}}\right)(Z\ln P_tf)^2 \leq 6\left(-1 + \frac{1}{3\alpha}\right)^2\frac{\alpha}{\alpha - 2}\frac{e^{-\frac{16t}{3\alpha}}}{1 - e^{-\frac{8t}{3\alpha}}}$$

$$-3\left(-1 + \frac{1}{3\alpha}\right)\frac{\alpha}{\alpha - 1}e^{-\frac{8t}{3\alpha}}\frac{\mathcal{L}P_tf}{P_tf}.$$

As a direct corollary of the Li-Yau type inequality of Theorem 4.3, we classically deduce (by integrating along geodesics) the following Harnack type inequality: There exist positive constant A_1 and A_2 such that for $0 < t_1 < t_2 < 1$ and $g_1, g_2 \in \mathbf{SU}(2)$

$$\frac{p_{t_1}(g_1)}{p_{t_2}(g_2)} \leq \left(\frac{t_2}{t_1}\right)^{A_1} e^{A_2 \frac{\delta(g_1,g_2)^2}{t_2-t_1}} \tag{4.10}$$

where $\delta(g_1, g_2)$ denotes the Carnot-Caratheodory distance from g_1 to g_2.

As another corollary we can also prove the following global estimate:

Proposition 4.6 *There exists a constant $C > 0$ such that for $t \in (0, 1)$, $r \in [0, \pi/2]$, $z \in [-\pi, \pi]$,*

$$\sqrt{\Gamma(\ln p_t)(r, z)} \leq C\left(\frac{d(r, z)}{t} + \frac{1}{\sqrt{t}}\right),$$

where $d(r, z)$ denotes the Carnot Carathéodory distance from 0 to the point with cylindric coordinates (r, θ, z).

Proof In what follows, we fix $t \in (0, 1)$. Let

$$\phi(s) = P_s(p_{t-s} \ln p_{t-s})$$

so that

$$\phi'(s) = P_s(p_{t-s}\Gamma(\ln p_{t-s}))$$

and

$$\phi''(s) = P_s(p_{t-s}\Gamma_2(\ln p_{t-s})).$$

Since p_t only depends on (r, z) we have $\Gamma_2(\ln p_{t-s}) \geq 0$ and therefore $\phi''(s) \geq 0$. By integrating the last inequality from 0 to $t/2$, we obtain

$$\int_0^{\frac{t}{2}} \phi'(s)ds \geq \frac{t}{2}\phi'(0)$$

that is

$$p_t\Gamma(\ln p_t) \leq \frac{2}{t}\left(P_{t/2}\left(p_{t/2} \ln p_{t/2}\right) - p_t \ln p_t\right).$$

We finally estimate $P_{t/2}\left(p_{t/2} \ln p_{t/2}\right) - p_t \ln p_t$ by using first $\ln p_{t/2}(r, z) \leq \ln p_{t/4}(0)$ and then the Harnack inequality (4.10):

$$\ln \frac{p_{t/4}(0)}{p_t(r, z)} \leq C\left(\frac{d(r, z)^2}{t} + 1\right).$$

$\square$

4.3 The reverse spectral gap inequality

As in the Heisengroup case (see [5]), we can easily obtain a reverse Poincare inequality with a sharp constant for the subelliptic heat kernel measure on $\mathbf{SU}(2)$.

Proposition 4.7 *Let $f : \mathbf{SU}(2) \to \mathbb{R}$ be a smooth function. For $t > 0$ and $g \in \mathbf{SU}(2)$,*

$$\Gamma(P_t f, P_t f)(g) \le C(t) \left(P_t f^2(g) - (P_t f)^2(g) \right)$$

where

$$C(t) = -\frac{1}{2} \frac{\partial}{\partial t} \int\limits_{\mathbf{SU}(2)} p_t \ln p_t d\mu.$$

Proof By left invariance, it is enough to prove this inequality at $g = 0$. If $\hat{X}$ and $\hat{Y}$ are the right invariant vector fields (see Remark 2.1), then, as seen before, we have:

$$\Gamma(P_t f, P_t f)(0) = \left(\int\limits_{\mathbf{SU}(2)} \hat{X} p_t(r, z) f(r, z) d\mu \right)^2 + \left(\int\limits_{\mathbf{SU}(2)} \hat{Y} p_t(r, z) f(r, z) d\mu \right)^2$$

Since p_t does not depend on θ, we have

$$\int\limits_{\mathbf{SU}(2)} \frac{(\hat{X} p_t)^2}{p_t} d\mu = \int\limits_{\mathbf{SU}(2)} \frac{(\hat{Y} p_t)^2}{p_t} d\mu = \frac{1}{2} \int\limits_{\mathbf{SU}(2)} \frac{\Gamma(p_t, p_t)}{p_t} d\mu,$$

and

$$\int\limits_{\mathbf{SU}(2)} \frac{\hat{X} p_t \hat{Y} p_t}{p_t} d\mu = 0.$$

Therefore, from Cauchy–Schwarz inequality, we conclude that:

$$\Gamma(P_t f, P_t f)(0) \le \frac{1}{2} \int\limits_{\mathbf{SU}(2)} \frac{\Gamma(p_t, p_t)}{p_t} d\mu (P_t f^2)(0),$$

which is the required inequality because:

$$\int\limits_{\mathbf{SU}(2)} \frac{\Gamma(p_t, p_t)}{p_t} d\mu = \int\limits_{\mathbf{SU}(2)} \Gamma(\ln p_t, p_t) d\mu = -\int\limits_{\mathbf{SU}(2)} \ln p_t L p_t d\mu = -\frac{\partial}{\partial t} \int\limits_{\mathbf{SU}(2)} p_t \ln p_t d\mu$$

$\square$

Remark 4.8 Due to the use of the Cauchy–Schwarz inequality in the previous proof, we see that the previous inequality is sharp.

We now study the constant

$$C(t) = -\frac{1}{2} \frac{\partial}{\partial t} \int\limits_{\mathbf{SU}(2)} p_t \ln p_t d\mu.$$

Proposition 4.9 *We have the following properties*:

- *C is decreasing*;
- *$C(t) \sim_{t \to 0} \frac{1}{t}$*;
- *$C(t) \sim_{t \to +\infty} 4e^{-4t}$*.

Proof Let us first show that C is decreasing. After some computations, we obtain:

$$C'(t) = -\int_{\mathbf{SU}(2)} \Gamma_2(\ln p_t, \ln p_t) p_t d\mu.$$

But now, let us observe that p_t only depends on (r, z). Therefore $\Gamma_2(\ln p_t, \ln p_t) \geq 0$ and thus $C'(t) \leq 0$.

We now study $C(t)$ when $t \to 0$. The idea is that, asymptotically when $t \to 0$, the constant $C(t)$ has to behave like the best constant of the reverse spectral gap inequality on the Heisenberg group (see the Sect. 3.3.). From [5], this constant is known to be $1/t$.

We have:

$$tC(t) = \frac{t}{2} \int_{\mathbf{SU}(2)} p_t \Gamma(\ln p_t, \ln p_t) d\mu$$

$$= \int_{r=0}^{\frac{\pi}{2\sqrt{t}}} \int_{z=-\frac{\pi}{t}}^{\frac{\pi}{t}} t^{5/2} \frac{\sin 2\sqrt{t}r}{4\pi} p_t(\sqrt{t}r, tz)\Gamma(\ln p_t, \ln p_t)(\sqrt{t}r, tz)drdz$$

Now, by using the result of Section 3.3., we easily obtain that the following convergences hold

$$\lim_{t \to 0} t^{3/2} \frac{\sin 2\sqrt{t}r}{2\pi} p_t(\sqrt{t}r, tz) = 2\pi h_1(r, z)r$$

$$\lim_{t \to 0} t\Gamma(\ln p_t, \ln p_t)(\sqrt{t}r, tz) = (\tilde{X} \ln h_1)^2(r, z) + (\tilde{Y} \ln h_1)^2(r, z),$$

where $h_t(r, z)$, $\tilde{X}$ and $\tilde{Y}$ are defined in Sect. 3.3 (see 3.8, 3.5, 3.6). Moreover, thanks to Proposition 4.6, there exists a constant $C > 0$ such that

$$t\Gamma(\ln p_t, \ln p_t)(\sqrt{t}r, tz) \leq C, \quad t \in (0, 1).$$

We can therefore apply a dominated convergence to obtain:

$$\lim_{t \to 0} tC(t) = \frac{1}{2} \int_{\mathbb{R}^3} h_1(r, z) \left((\tilde{X} \ln h_1)^2(r, z) + (\tilde{Y} \ln h_1)^2(r, z) \right) rdrd\theta dz.$$

This last expression is equal to 1, according to [5].

We finally turn to the analysis of $C(t)$ when $t \to +\infty$. For that, we use the expression

$$C(t) = \frac{1}{2} \int_{\mathbf{SU}(2)} \frac{\Gamma(p_t, p_t)}{p_t} d\mu$$

and the spectral decomposition of Proposition 3.1 to get that uniformly on $\mathbf{SU}(2)$,

$$\Gamma(p_t, p_t) \sim_{t \to +\infty} 16e^{-4t} \Gamma(\cos r \cos z, \cos r \cos z)$$

Therefore,

$$C(t) \sim_{t \to \infty} 8e^{-4t} \int_{\mathbf{SU}(2)} \Gamma(\cos r \cos z, \cos r \cos z) d\mu,$$

and we compute

$$\int_{SU(2)} \Gamma(\cos r \cos z, \cos r \cos z)d\mu = \frac{1}{2},$$

to conclude. □

4.4 L^p gradient bounds

The goal of this section is to prove the following gradient bounds:

Theorem 4.10 *Let $p > 1$. There exists a constant $C_p > 1$ such that for any smooth f :* $SU(2) \to \mathbb{R}$ *and any $g \in SU(2)$*

$$\sqrt{\Gamma(P_t f, P_t f)(g)} \leq C_p e^{-2t} \left(P_t \Gamma(f, f)^{\frac{p}{2}}(g) \right)^{\frac{1}{p}}, \quad t \geq 0.$$

Remark 4.11 Let $f(r, \theta, z) = \cos r \cos z$. In that case, $\mathcal{L}f = -2f$ and $\Gamma(f, f) = \sin^2 r$. Therefore the exponential decay e^{-2t} is optimal and moreover:

$$\sin r \leq C_p P_t(\sin r)^p$$

which implies, by letting $t \to \infty$, $C_p \geq \left(1 + \frac{p}{2}\right)^{\frac{1}{p}}$.

Remark 4.12 We conjecture that the inequality still holds true for $p = 1$.

4.4.1 Long-time behavior

We first study the long-time behavior $\Gamma(P_t f, P_t f)$. For that we will rely on a commutation between the complex gradient and the semigroup P_t (such a type of commutation involving a Folland–Stein type operator has already been used in the Heisenberg group to study gradient estimates, see [5]).

The Lie algebra structure relations lead to:

$$(X + iY)L = (L - 4iZ + 4)(X + iY), \quad (4.11)$$

which leads to the *formal* commutation:

$$(X + iY)P_t = e^{t(L-4iZ+4)}(X + iY).$$

In what follows we give a precise analytical sense to the previous commutation.

Remark 4.13 We can observe that the constant that appears in the commutation is positive, which is quite striking because we expect an exponential decay. Nevertheless, as we will see below $e^{t(L-4iZ)}$ gives a decay e^{-6t} against complex gradients.

Lemma 4.14 *Let $t > 0$ and $r \geq 0$. The function*

$$z \to p_t(r, z) - \frac{1}{\left(1 - \cos r e^{iz-2t}\right)^2} - \frac{1}{\left(1 - \cos r e^{-iz-2t}\right)^2}$$

admits an analytic continuation on $\{z \in \mathbb{C}, | \mathbf{Im}z | < -\ln \cos r + 6t\}$. The function

$$z \to p_t(r, z)$$

is therefore meromorphic on $\{z \in \mathbb{C}, | \mathbf{Im}z | < -\ln \cos r + 6t\}$ with double poles at $-i(-\ln \cos r + 2t)$ and $i(-\ln \cos r + 2t)$.

Proof This is an easy consequence of the spectral decomposition of p_t:

$$p_t(r, z) = \sum_{n=-\infty}^{+\infty} \sum_{k=0}^{+\infty} (2k + |n| + 1) e^{-(4k(k+|n|+1)+2|n|)t} e^{inz} (\cos r)^{|n|} P_k^{0,|n|} (\cos 2r).$$

$\square$

Let us know observe that if $k = 0$ and $n \leq 0$,

$$(X + iY) e^{inz} (\cos r)^{|n|} P_k^{0,|n|} (\cos 2r) = 0.$$

If, for $t > 0$, $r \geq 0$, $z \in \mathbb{C} - \{-i(-\ln \cos r + 2t)\}$, $|\operatorname{Im} z| < -\ln \cos r + 6t$, we denote

$$p_t^*(r, z) = p_t(r, z) - \frac{1}{\left(1 - \cos r e^{-iz-2t}\right)^2},$$

we have therefore

$$(X + iY) p_t = (X + iY) p_t^*.$$

Combining this with (4.11) leads to:

Proposition 4.15 *If $f : \mathbf{SU}(2) \to \mathbb{R}$ is a smooth function, then*

$$(X + iY) P_t f(0) = e^{4t} \int_{\mathbb{H}} p_t^*(r, z + 4it)(X + iY) f(r, \theta, z) d\mu, \quad t > 0.$$

And, as a corollary:

Corollary 4.16 *There exists $t_0 > 0$ and $A > 0$ such that for any smooth $f : \mathbf{SU}(2) \to \mathbb{R}$,*

$$\sqrt{\Gamma(P_t f, P_t f)(0)} \leq A e^{-2t} P_t \sqrt{\Gamma(f, f)}(0), \quad t \geq t_0.$$

Proof We denote

$$\Phi(t) = \sup_{r \in [0, \frac{\pi}{2}]} \sup_{z \in [-\pi, \pi]} \frac{| p_t^*(r, z + 4it) |}{p_t(r, z)}.$$

Since,

$$p_t^*(r, z + 4it)$$
$$= \sum_{n=1}^{+\infty} (n + 1) e^{-6nt} e^{inz} (\cos r)^n$$
$$+ \sum_{n=-\infty}^{+\infty} \sum_{k=1}^{+\infty} (2k + |n| + 1) e^{-(4k(k+|n|+1)+2|n|)t} e^{inz} e^{-4nt} (\cos r)^{|n|} P_k^{0,|n|} (\cos 2r)$$

there exists $t_0 > 0$ and $A > 0$, such that for $t \geq t_0$,

$$\Phi(t) \leq \frac{| p_t^*(0) |}{1 - | 1 - p_t(0) |} \leq A e^{-6t},$$

and the proof is complete. $\square$

Remark 4.17 The above function $\Phi(t)$ explodes when $t \to 0$.

Remark 4.18 We conjecture that the ratio $\sup_{r, z \notin \Sigma_{R\sqrt{t}}} \frac{p_t(r, z+4it)}{p_t(r, z)}$ is bounded when $t \to 0$, where R is big enough and $\Sigma_{R\sqrt{t}}$ denotes the Carnot Carathéodory ball with radius $R\sqrt{t}$. By a partition of unity similar to [5], this would imply that Theorem 4.10 also holds for $p = 1$.

4.4.2 Short-time behavior

We now conclude the proof of Theorem 4.10, by showing that the inequality does not explode when $t \to 0$. We shall use here the commutation between left-invariant and right invariant vector fields. It relies on the following lemma:

Lemma 4.19 *Let $q > 1$. The limit*

$$\lim_{t \to 0} \int_{\mathbf{SU}(2)} (\sin 2r)^q \Gamma(\ln p_t, \ln p_t)^{\frac{q}{2}}(r, z) p_t(r, z) d\mu$$

is finite.

Proof The proof is similar to the proof of the second point of Proposition 4.9.: By scaling and a dominated convergence argument based on Proposition 4.6., we obtain:

$$\lim_{t \to 0} \int_{\mathbf{SU}(2)} (\sin 2r)^q \Gamma(\ln p_t, \ln p_t)^{\frac{q}{2}}(r, z) p_t(r, z) d\mu$$

$$= 2^q \int_{\mathbb{R}^3} r^q h_1(r, z) \left((\tilde{X} \ln h_1)^2(r, z) + (\tilde{Y} \ln h_1)^2(r, z) \right)^{q/2} r \, dr d\theta dz,$$

which is finite, due to known results on the Heisenberg group (see [5]). □

We can now deduce:

Proposition 4.20 *Let $p > 1$. There exists a constant $A_p > 0$ such that for any smooth $f : \mathbf{SU}(2) \to \mathbb{R}$ and any $g \in \mathbf{SU}(2)$*

$$\sqrt{\Gamma(P_t f, P_t f)(g)} \le A_p \left(P_t \Gamma(f, f)^{\frac{p}{2}}(g) \right)^{\frac{1}{p}}, t \in (0, 1).$$

Proof Due to the fact that the right-invariant vector fields $\hat{X}$, $\hat{Y}$ commute with $\mathcal{L}$, we get

$$(X P_t f)(0) = (P_t \hat{X} f)(0)$$

and

$$(Y P_t f)(0) = (P_t \hat{Y} f)(0).$$

Now, X, Y, Z form a basis at each point, there exist therefore smooth functions such that:

$$\hat{X} = \Omega_{1,1} X + \Omega_{1,2} Y + \Omega_{1,3} Z$$
$$\hat{Y} = \Omega_{2,1} X + \Omega_{2,2} Y + \Omega_{2,3} Z.$$

By using $[X, Y] = 2Z$ and integrating by parts, we obtain

$$(X P_t f)(0) = \int_{\mathbf{SU}(2)} \left(\Omega_{1,1} p_t + \frac{1}{2} Y(\Omega_{1,3} p_t) \right) (Xf) + \left(\Omega_{1,2} p_t - \frac{1}{2} X(\Omega_{1,3} p_t) \right) (Yf) d\mu$$

and

$$(Y P_t f)(0) = \int_{\mathbf{SU}(2)} \left(\Omega_{2,1} p_t + \frac{1}{2} Y(\Omega_{2,3} p_t) \right) (Xf) + \left(\Omega_{2,2} p_t - \frac{1}{2} X(\Omega_{2,3} p_t) \right) (Yf) d\mu.$$

We easily compute

$$\Omega_{1,3} = \sin\theta \sin 2r$$

and

$$\Omega_{2,3} = -\cos\theta \sin 2r.$$

By using Hölder's inequality the expected result follows from Lemma 4.19. $\qquad\square$

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