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# HEAT KERNELS, OLD AND NEW

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**Abstract**

This article is a résumé of ongoing investigations into the nature and form of heat kernels of second order partial differential operators. Our operators are given as a sum of squares of bracket generating vector fields; thus they are (sub)elliptic and induce a (sub)Riemannian geometry.

The principal part of a heat kernel of an elliptic operator is an exponential whose exponent is a solution of the associated Hamilton-Jacobi equation. Genuinely subelliptic heat kernels are given by integrals, where the integrands are similar in form to elliptic heat kernels. There are differences. In particular, some of the exponents in the known subelliptic integrands are solutions of a modified Hamilton-Jacobi equation. To clarify this difference we propose a calculation which may lead to an invariant interpretation of the modification.

## 1. Introduction

Given a negative operator $A$ and time $t > 0$, the exponential $e^{tA}$ is the heat operator associated to $A$. When $A = \Delta$, the Laplace-Beltrami operator on a manifold $M$, then, physically, $e^{t\Delta}$ represents the time evolution of the temperature of $M$:

"If $M$ has temperature $u(x)$ at time $t = 0$, then its temperature $u_t(x)$ at time $t$ is given by

$$u_t(x) = e^{t\Delta}u(x)." \tag{1.1}$$

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Mathematically, the knowledge of $e^{tA}$ yields all powers of the operator $A$, namely,

$$(-A)^{-z} = \frac{1}{\Gamma(z)} \int_0^\infty e^{tA} t^{z-1}\, dt, \qquad z \neq 0, -1, -2, \ldots, \tag{1.2}$$

a simple consequence of Euler's integral formula for the gamma function; (1.2) is a useful tool when working with analytic functions of $A$. Note that (1.1) is a solution of the heat equation

$$\frac{\partial u_t}{\partial t} - A u_t = 0. \tag{1.3}$$

Furthermore, if $u(t)$ is a function-valued function of $t$, then

$$\int_0^t e^{(t-s)A} u(s) ds \tag{1.4}$$

inverts the heat operator:

$$\frac{\partial}{\partial t} \int_0^t e^{(t-s)A} u(s) ds \;=\; u(t) + A \int_0^t e^{(t-s)A} u(s) ds,$$

or,

$$\left( \frac{\partial}{\partial t} - A \right) \int_0^t e^{(t-s)A} u(s) ds \;=\; u(t). \tag{1.5}$$

This result has been used to construct the heat operator $e^{tA}$. Finally, if $e^{tA}$ is an integral operator with kernel $p(t, x, y)$, then $p$ is its heat kernel. Note that $p$ is characterized by

$$\frac{\partial p}{\partial t} - Ap = 0, \qquad \text{and} \qquad \lim_{t \to 0} p(t, x, y) = \delta(x - y). \tag{1.6}$$

In this paper $A$ is a second order (partial) differential operator. “Old” refers to heat kernels of elliptic operators and “New” to subelliptic heat kernels.

## 2. Elliptic operators

We start with examples.

**2.1.** $M = \mathbb{R}$ and $\Delta = \frac{1}{2}\frac{d^2}{dx^2}$:

$$p(t,x,y) = \frac{1}{\sqrt{2\pi t}} e^{-\frac{|x-y|^2}{2t}}. \tag{2.1}$$

**2.2.** $M = \mathbb{R}^n$ and $\Delta = \frac{1}{2}\sum_{j=1}^n \frac{\partial^2}{\partial x_j^2}$:

$$p(t,x,y) = \frac{1}{(2\pi t)^{n/2}} e^{-\frac{|x-y|^2}{2t}}, \qquad x, y \in \mathbb{R}^n. \tag{2.2}$$

One should note that the exponent is

$$-\frac{[\text{distance}(x,y)]^2}{2t}, \tag{2.3}$$

and $|x|^2/(2t)$ is a solution of the Hamilton-Jacobi equation

$$\frac{\partial}{\partial t}\left(\frac{|x|^2}{2t}\right) + \frac{1}{2}\sum_{j=1}^n \left(\frac{\partial}{\partial x_j}\frac{|x|^2}{2t}\right)^2 = 0. \tag{2.4}$$

To find $z = z(x,t)$, the solution of (2.4), we calculate as follows. Set $\gamma = \partial z/\partial t$, $\xi_j = \partial z/\partial x_j$, $j = 1, \dots, n$, and

$$F = \gamma + H(\nabla_x z) = \gamma + \frac{1}{2}\sum_{j=1}^n \xi_j^2 \,. \tag{2.5}$$

Then the bicharacteristic curve $\big(x(s), t(s), \xi(s), \gamma(s)\big)$, $0 \le s \le t$, between $(0,0)$ and $(x,t)$ is a solution of

$$\begin{aligned} &\dot{x}_j = F_{\xi_j} = \xi_j, \quad \dot{\xi}_j = -F_{x_j} = 0, \qquad j = 1, \dots, n, \\ &\dot{t} = F_\gamma = 1, \quad \dot{\gamma} = -F_t = 0, \end{aligned} \tag{2.6}$$

so $\xi_j(s) = \xi_j(0) = \xi_j$, $j = 1, \dots, n$, $\gamma(s) = \gamma(0) = \gamma$, $t(s) = s$, $0 \le s \le t$, and

$$x_j(s) = \frac{x_j}{t}s, \qquad j = 1, \dots, n, \tag{2.7}$$

since $x_j(t) = x_j$ and one starts from the origin. Also,

$$\dot{z}(s) = \sum_{j=1}^{n} \xi_j F_{\xi_j} + \gamma F_\gamma = |\xi|^2 + \gamma = \frac{1}{2}|\xi|^2, \tag{2.8}$$

since $\gamma + \frac{1}{2}|\xi|^2 = 0$ by hypothesis. Consequently,

$$z(x,t) = \frac{1}{2}\int_0^t |\xi(s)|^2 ds = \frac{|x|^2}{2t}\,, \tag{2.9}$$

as expected.

**2.3.** $M = S^1$ and $\Delta = \frac{1}{2}\frac{d^2}{d\theta^2}$, $S^1$ is parameterized by $\theta$. $p(t,\theta,\gamma)$ is obtained by summing over an orthonormal basis of $L^2(S^1)$:

$$p = \sum_{k=-\infty}^{\infty} e^{-\frac{1}{2}k^2 t} \frac{e^{ik\theta}}{\sqrt{2\pi}} \frac{e^{-ik\gamma}}{\sqrt{2\pi}} = \frac{1}{2\pi}\Theta\left(\frac{1}{2}(\theta-\gamma), \frac{i}{2}\frac{t}{\pi}\right) \tag{2.10}$$

is Jacobi's theta function. The Poisson summation formula yields the needed geometric version:

$$p(t,\theta) = \frac{1}{\sqrt{2\pi t}} \sum_{k=-\infty}^{\infty} e^{-\frac{(\theta+2k\pi)^2}{2t}}. \tag{2.11}$$

Note that

$$\frac{1}{\sqrt{2\pi t}} e^{-\frac{\theta^2}{2t}} \tag{2.12}$$

is a solution of the heat equation on $(0, 2\pi]$ and

$$\lim_{t\to 0} \frac{1}{\sqrt{2\pi t}} e^{-\frac{\theta^2}{2t}} = \delta(\theta),$$

but (2.12) is not continuous at $\theta = 0$. This can be corrected if we recall that $\frac{1}{2}\frac{d^2}{d\theta^2}$ is a periodic operator and the periodic extension (2.11) of (2.12) is continuous in $\theta$. In particular,

$$p(0,\theta) = \sum_{k=-\infty}^{\infty} \delta(\theta + 2k\pi). \tag{2.13}$$

When $k = 0$, $\theta^2 =$ (distance from 0 to $\theta)^2$. When $k \neq 0$, one gets $\theta +$

the length of additional great circles. In geometric terms, they represent the lengths of all the geodesics connecting 0 and $\theta$. For us a geodesic is the projection of a bicharacteristic onto the base manifold. The Hamiltonian is $H = \frac{1}{2}\xi^2$ and the bicharacteristic curve in cotangent space $(\theta(s), \xi(s))$ is a solution of

$$\dot{\theta}(s) = H_\xi = \xi, \quad \dot{\xi}(s) = -H_\theta = 0, \quad \Longrightarrow \quad \xi(s) = \text{constant},$$

so $\theta(s) = \xi s + c$,

$$\theta(0) = 0 = c, \quad \theta(\theta) = \theta \quad \Longrightarrow \quad \xi = 1, \quad \theta(s) = s,$$

and the point $\theta$ is reached at $s = \theta + 2k\pi$, $k = 0, \pm 1, \pm 2, \ldots$.

In particular, this teaches us that all the geodesic lengths contribute to the heat kernel.

**2.4.** The final elliptic example is the extension of **2.3** to $S^{2n+1} \subset \mathbb{C}^{n+1}$; this will be useful in the study of subelliptic operators expressed in terms of Heisenberg vector fields with variable coefficients. The Laplacian $\Delta$ in $\mathbb{C}^{n+1}$ is

$$\Delta = 2\sum_{j=1}^{n+1} \frac{\partial}{\partial z_j}\frac{\partial}{\partial \overline{z_j}} = -\sum_{j=1}^{n+1}\left(Z_j^* Z_j + \overline{Z_j^*}\,\overline{Z_j}\right), \tag{2.14}$$

where $z = (z_1, \ldots, z_{n+1})$, $z_j = x_j + ix_{j+n+1}$, $j = 1, \ldots, n+1$, are coordinates in $\mathbb{C}^{n+1}$ and $\sqrt{2}Z_1, \ldots, \sqrt{2}Z_{n+1}$ denote an orthonormal basis of holomorphic vector fields on $\mathbb{C}^{n+1}$ with respect to the Euclidean metric, $Z_j = \sum_{k=1}^{n+1} a_{jk}\frac{\partial}{\partial z_k}$, $j = 1, \ldots, n+1$, and $Z_j^*$ denotes the adjoint of $Z_j$ with respect to the Euclidean volume $dx = dx_1 \wedge \cdots \wedge dx_{2n+2}$. We let $\Delta_S$ denote the restriction of the Laplacian $\Delta$ to $S^{2n+1}$. To find the heat kernel for $\Delta_S$ one introduces spherical coordinates:

$$\begin{aligned} z_1 &= r\cos\theta_1 e^{i\varphi_1}, \\ &\vdots \\ z_k &= r\sin\theta_1\cdots\sin\theta_{k-1}\cos\theta_k e^{i\varphi_k}, \qquad k = 2, \ldots, n, \\ &\vdots \\ z_{n+1} &= r\sin\theta_1\cdots\sin\theta_{n-1}\sin\theta_n e^{i\varphi_{n+1}}, \end{aligned} \tag{2.15}$$

$0 \le \theta_j \le \pi/2$, $j = 1, \dots n$, $-\pi < \varphi_j \le \pi$, $j = 1, \dots, n+1$, and $0 \le r < \infty$. Then

$$\Delta = \frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{2n+1}{r}\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\Delta_S. \tag{2.16}$$

On $S^{2n+1}$ the heat kernel for $\Delta_S$ only depends on the angle $\gamma$ between the origin, which we may choose to denote by $(1, 0, \dots, 0)$, and the point $z = (z_1, \dots, z_{n+1}) \in S^{2n+1}$. In the above coordinate system $\cos\gamma = \cos\theta_1 \cos\varphi_1$. On functions of $\theta_1$ and $\varphi_1$ only $\Delta_S$ is reduced to $\mathcal{L}_S$,

$$\mathcal{L}_S = \frac{1}{2}\frac{\partial^2}{\partial\theta_1^2} + \big((n-1)\cot\theta_1 + \cot(2\theta_1)\big)\frac{\partial}{\partial\theta_1} + \frac{1}{2}\frac{1}{\cos^2\theta_1}\frac{\partial^2}{\partial\varphi_1^2}. \tag{2.17}$$

In particular, the heat kernel for $\mathcal{L}_S$ is also the heat kernel for $\Delta_S$ after normalization on $S^{2n+1}$. Setting $x_1 = \cos\theta_1\cos\varphi_1$, one has

$$\mathcal{L}_S = \frac{1}{2}(1 - x_1^2)\frac{d^2}{dx_1^2} - \left(n + \frac{1}{2}\right)x_1\frac{d}{dx_1}, \tag{2.18}$$

or

$$\mathcal{L}_S = \frac{1}{2}\frac{d^2}{d\gamma^2} + n(\cot\gamma)\frac{d}{d\gamma}, \qquad x_1 = \cos\gamma. \tag{2.19}$$

To find the heat kernel for $\mathcal{L}_S$ we shall work with the formula (2.17). With $(\theta_1, \varphi_1)$ and the dual variables $(\omega_1, \tau_1)$ the Hamiltonian is

$$H = \frac{1}{2}\left(\omega_1^2 + \frac{\tau_1^2}{\cos^2\theta_1}\right), \tag{2.20}$$

and the bicharacteristic curve is a solution of

$$\dot\theta_1(s) = H_{\omega_1} = \omega_1 = \pm\sqrt{2H - \frac{\tau_1^2}{\cos^2\theta_1}}, \tag{2.21}$$

$$\dot\varphi_1(s) = H_{\tau_1} = \frac{\tau_1}{\cos^2\theta_1}, \qquad \dot\tau_1 = -H_{\varphi_1} = 0. \tag{2.22}$$

Hence, $\tau_1 =$ constant and so is $H$ along the bicharacteristic.

**Lemma 1.** *Let $E^2 = 2H$. Assuming $\theta_1(0) = 0$, $\varphi_1(0) = 0$, one has*

$$\sin^2\theta_1(s) = \left(1 - \frac{\tau_1^2}{E^2}\right)\sin^2(Es), \tag{2.23}$$

$$\varphi_1(s) = \tan^{-1}\left(\frac{\tau_1}{E}\tan(Es)\right), \tag{2.24}$$

*which can be continued for all $s > 0$.*

We have two arbitrary constants $\tau_1$ and $H$ which can be used to fix $\theta_1(t) = \theta_1$, $\varphi_1(t) = \varphi_1$. The solution $S$ of the Hamilton-Jacobi equation

$$0 = \frac{\partial S}{\partial t} + \frac{1}{2}\left(\frac{\partial S}{\partial \theta_1}\right)^2 + \frac{1}{2}\frac{1}{\cos^2\theta_1}\left(\frac{\partial S}{\partial \varphi_1}\right)^2 = \frac{\partial S}{\partial t} + H\left(\nabla_{\theta_1,\varphi_1} S\right) \qquad (2.25)$$

can be found from

$$\dot{S}(s) \;=\; \omega_1\dot{\theta}_1 + \tau_1\dot{\varphi}_1 - H = H, \qquad (2.26)$$

so

$$S \;=\; Ht = \frac{1}{2}E^2 t,$$

and a bit of work with (2.23) and (2.24) yields

$$S = Ht = \frac{\left(\cos^{-1}(\cos\theta_1\cos\varphi_1) + 2k\pi\right)^2}{2t} = \frac{(\gamma + 2k\pi)^2}{2t}, \qquad (2.27)$$

$k \in \mathbb{Z}$. A consequence of these calculations is the following result.

**Theorem 2.** *Given $z, w \in S^{2n+1}$, let $\gamma$ denote the angle subtended by the arc that joins $z$ and $w$ on a great circle, $0 \le \gamma \le \pi$. Then the heat kernel $p_S$ of $\Delta_S$ on $S^{2n+1}$ is given by*

$$p_S \;=\; \frac{e^{\frac{n^2}{2}t}}{(2\pi t)^{n+1/2}} \sum_{k=-\infty}^{\infty} e^{-\frac{(\gamma+2k\pi)^2}{2t}} v_n(\gamma + 2k\pi, t), \qquad (2.28)$$

*where*

$$v_n(\gamma, t) \;=\; v^n w_n = \left(\frac{\gamma}{\sin\gamma}\right)^n \left(\sum_{l=0}^{n-1} w_{n,l}(\gamma) t^l\right), \qquad (2.29)$$

*with $w_{n,0} = 1$ and $w_{n,l}$, $l = 1, 2, \ldots, n-1$ are found by iteration,*

$$w_{n,l}(\gamma) = \frac{1}{\gamma^l}\int_0^\gamma v^{-n}\sigma^{l-1}\left(\mathcal{L}_S - \frac{n^2}{2}\right) v_{n,l-1} d\sigma, \qquad (2.30)$$

*$v_{n,l}(\gamma) = v(\gamma)^n w_{n,l}(\gamma)$.*

**Remark 3.** Let $\mathcal{L}_S^{(n)}$ denote the reduced operator of $\Delta_S^{(n)}$, i.e. of $\Delta_S$ on

$S^{2n+1}$, and let $u_n$ denote a solution of $\partial u/\partial t = \mathcal{L}_S^{(n)} u$. Then,

$$u_{n+1} = e^{\frac{2n+1}{2}t} \frac{\partial u_n}{2\pi \partial x_1} = e^{\frac{2n+1}{2}t} \frac{\partial u_n}{2\pi \partial(\cos\gamma)} \tag{2.31}$$

is a solution of $\partial u/\partial t = \mathcal{L}_S^{(n+1)} u$. In particular, one has

**Lemma 4.** *Let $p_S^{(n)}$ stand for $p_S$ on $S^{2n+1}$. Then,*

$$p_S^{(n)} = e^{\frac{n^2-1}{2}t} \left( \frac{\partial}{2\pi \partial(\cos\gamma)} \right)^{n-1} p_S^{(1)}, \qquad n > 1, \tag{2.32}$$

*which yields an easy derivation of $p_S^{(n)}$ from $p_S^{(1)}$.*

We look at $p_S^{(1)}$ more carefully. One has

$$p_S^{(1)} = \frac{e^{\frac{1}{2}t}}{(2\pi t)^{3/2}} \sum_{k=-\infty}^{\infty} e^{-\frac{(\gamma+2k\pi)^2}{2t}} \frac{\gamma + 2k\pi}{\sin\gamma}. \tag{2.33}$$

First note that the $k = 0$ term is well defined on $0 \le |\gamma| < \pi$, but not at $\gamma = \pi$. All other terms are defined on $0 < |\gamma| < \pi$ only. This is just a problem of summation. The sum of the $k$-th and $(-k)$-th terms is well defined at $\gamma = 0$, and then summing $k$ from 0 to $\infty$ yields the extension of $p_S^{(1)}$ from $0 < |\gamma| < \pi$ to $0 \le |\gamma| < \pi$. Next write

$$p_S^{(1)} = \sum_{k=-\infty}^{\infty} p_{S,k}^{(1)}, \tag{2.34}$$

and note that $p_{S,k}^{(1)} + p_{S,-k-1}^{(1)}$ is well defined at $\gamma = \pi$, hence

$$\sum_{k=0}^{\infty} \left( p_{S,k}^{(1)} + p_{S,-k-1}^{(1)} \right) \tag{2.35}$$

extends $p_S^{(1)}$ from $0 < |\gamma| < \pi$ to $0 < |\gamma| \le \pi$, and we have defined $p_S^{(1)}$ on all of $S^3$. Similar construction yields $p_S^{(n)}$ on all of $S^{2n+1}$.

The following formula is useful in the quantitative study of $p_S^{(n)}$.

**Lemma 5.** *Given $\varepsilon > 0$, one has*

$$p_S^{(n)} = \frac{\Gamma(n)e^{\frac{n^2}{2}t}}{(2\pi)^{n-1}(2\pi t)^{3/2}} \frac{1}{2\pi i} \int_{\varepsilon - i\infty}^{\varepsilon + i\infty} \frac{e^{\lambda/t} d\lambda}{(\cosh\sqrt{2\lambda} - \cos\gamma)^n}; \tag{2.36}$$

*we note that* (2.28) *is the residue expansion of* (2.36).

Finally, one may use

$$\cos\gamma = x_1 y_1 + \cdots + x_{2n+2} y_{2n+2} = x \cdot y \tag{2.37}$$

to return to the original coordinates, where we set $z_j = x_j + i x_{n+1+j}$ and $w_j = y_j + i y_{n+1+j}$, $j = 1, \dots, n+1$.

We are ready to construct local heat kernels for general second order elliptic differential operators.

**2.5.** A second order partial differential operator $\Delta$ is elliptic if one can write it in the following form

$$\Delta = \frac{1}{2} \sum_{j=1}^{n} X_j^2 + \cdots, \tag{2.38}$$

where $X_1, \dots, X_n$ are linearly independent vector fields on an $n$-dimensional manifold $M_n$ and $\cdots$ stands for lower order terms. Letting $X_1, \dots, X_n$ represent an orthonormal basis of $TM_n$ one obtains a Riemannian metric. With such a metric $M_n$ is a Riemannian manifold. Given an arbitrary point $Q \in M_n$, which we may call the origin, one can always find a sufficiently small neighbourhood of $Q$ in which every point has a unique geodesic connection to the origin. $p(t, x, y)$ is a local heat kernel for $\Delta$ if in a small neighbourhood $U$ of the origin one has

$$\frac{\partial p}{\partial t} - \Delta p = 0, \quad \text{and} \quad \lim_{t \to 0} p(t, x, y) = \delta(x - y), \quad x, y \in U. \tag{2.39}$$

**2.4** suggests the following:

"One should look for a heat kernel $p$ in the form

$$p(t, x, y) = \frac{C}{t^{n/2}} e^{-\frac{f(x,y)}{t}} \big(a_0(x, y) + a_1(x, y)t + \cdots\big), \tag{2.40}$$

where $C$ is a constant and $a_j(x,y)$, $j=1,2,\ldots$, are smooth functions near the diagonal."

With (2.40) one has

$$\begin{aligned}&\frac{\partial p}{\partial t}-\Delta p\\ &=\frac{C}{t^{n/2}}e^{-\frac{f}{t}}\Big\{\Big[\frac{\partial}{\partial t}\Big(-\frac{f}{t}\Big)-\frac{1}{2}\sum_{j=1}^{n}\Big(X_j\Big(-\frac{f}{t}\Big)\Big)^2\Big]a_0(x,y)+O\Big(\frac{1}{t}\Big)\Big\},\end{aligned}\tag{2.41}$$

where the square bracket is of the order of $1/t^2$. Hence the necessary vanishing of (2.41) implies that

$$\frac{\partial}{\partial t}\left(-\frac{f}{t}\right)-\frac{1}{2}\sum_{j=1}^{n}\left(X_j\Big(-\frac{f}{t}\Big)\right)^2=0,\tag{2.42}$$

*i.e.* $f/t$ is the solution of a Hamilton-Jacobi equation. A simple consequence is that $f$ is a solution of the eiconal equation

$$\frac{1}{2}\sum_{j=1}^{n}\big(X_j\,f\big)^2=f,\tag{2.43}$$

and thus represents the local Riemannian distance. Again, the $a_j$'s are obtained by iteration.

## 3. Subelliptic Operators

Consider

$$\Delta=\frac{1}{2}\sum_{j=1}^{m}X_j^2+\cdots,\tag{3.1}$$

on an $n$-dimensional manifold $M_n$, where $X_1,\ldots,X_m$ are linearly independent vector fields and $m<n$. $\Delta$ is not elliptic, but if we assume that $X_1,\ldots,X_m$, the horizontal vector fields, are bracket generating then one has the following a-priori estimate on $\Delta$,

$$\|u\|_\varepsilon\le C\|\Delta u\|_0\,,\qquad 0<\varepsilon<2,\tag{3.2}$$

locally, see Hörmander [7]; note that $\varepsilon=2$ when $m=n$ and $\Delta$ is elliptic, and when $\varepsilon < 2$, $\Delta$ of (3.2) is subelliptic. Bracket generating means that the horizontal vector fields and their Lie brackets, $X_1, \ldots, X_m, \ldots, [X_i, X_j], \ldots,$ $\big[X_j, [X_k, X_l]\big], \ldots$ generate $TM_n$.

In 1939 Chow [4] showed that given bracket generating vector fields $X_1, \ldots, X_m$, $m \leq n$, two points can always be joined by a horizontal curve, that is, a curve, all of whose tangents are linear combinations of the horizontal vector fields $X_1, \ldots, X_m$. This yields a geometry. Assume that $X_1, \ldots, X_m$ are orthogonal and have length one. If $m = n$ one obtains a Riemannian metric, but if $m < n$ one has a subRiemannian, not Riemannian, metric. In particular, given a subRiemannian metric we can calculate the lengths of horizontal curves, and by minimizing these lengths between two given points we obtain a subRiemannian distance, often referred to as the Carnot-Carathéodory distance. This yields a subRiemannian geometry. The Hamiltonian attached to (3.1) is still

$$H = \frac{1}{2} \sum_{j=1}^{m} X_j(x, \xi)^2, \tag{3.3}$$

which yields bicharacteristic curves whose projections onto $M_n$ are geodesics. The principal difference between Riemannian and subRiemannian geometry which effects us is that in a Riemannian geometry sufficiently near points are joined by a unique geodesic connection, while in a subRiemannian geometry arbitrarily near points may have multiple geodesic connections. Consequently, in subRiemannian geometry one cannot fix the bicharacteristic curve by giving the endpoints of its projection onto the base, instead one must make use of the dual variables. Since heat kernels should not contain dual variables we shall sum over them. A few examples are in order.

### 3.1. The subLaplacian on the Heisenberg group

The $(2n+1)$-dimensional Heisenberg group $H_n$ is $\mathbb{C}^n \times \mathbb{R} = \mathbb{R}^{2n} \times \mathbb{R}$ equipped with the group law

$$(x, y) \circ (x', y') = \Big(x + x', y + y' + 2 \sum_{j=1}^{n} a_j (x_{2j} x'_{2j-1} - x_{2j-1} x'_{2j})\Big), \tag{3.4}$$

with $a = (a_1, \ldots, a_n)$ ordered as

$$0 < a_1 \le a_2 \le \cdots \le a_p \le \cdots \le a_n, \tag{3.5}$$

see [1]. The horizontal vector fields

$$X_{2j-1} = \frac{\partial}{\partial x_{2j-1}} + 2a_j x_{2j} \frac{\partial}{\partial y}, \qquad X_{2j} = \frac{\partial}{\partial x_{2j}} - 2a_j x_{2j-1} \frac{\partial}{\partial y}, \tag{3.6}$$

$j = 1, \ldots, n$, are left-invariant with respect to the above Heisenberg translation and are bracket generating, since

$$[X_{2j-1}, X_{2j}] = X_{2j-1}X_{2j} - X_{2j}X_{2j-1} = -4a_j \frac{\partial}{\partial y}. \tag{3.7}$$

As the first bracket suffices we refer to $X_1, \ldots, X_{2n}$ as step 2. The subLaplacian is

$$\Delta_H = \frac{1}{2} \sum_{j=1}^{2n} X_j^2. \tag{3.8}$$

We shall work with $H_1$ only and set $a_1 = 1$; the general $H_n$ is similar. For the Heisenberg subLaplacian

$$\Delta_H = \frac{1}{2}\left(\frac{\partial}{\partial x_1} + 2x_2 \frac{\partial}{\partial y}\right)^2 + \frac{1}{2}\left(\frac{\partial}{\partial x_2} - 2x_1 \frac{\partial}{\partial y}\right)^2 \tag{3.9}$$

on $H_1$ we again try for a heat kernel in the form

$$\frac{1}{t^\alpha} e^{-f/t} \ldots \tag{3.10}$$

where $h = f/t$ is a solution of

$$\frac{\partial h}{\partial t} + \frac{1}{2}\left(\frac{\partial h}{\partial x_1} + 2x_2 \frac{\partial h}{\partial y}\right)^2 + \frac{1}{2}\left(\frac{\partial h}{\partial x_2} - 2x_1 \frac{\partial h}{\partial y}\right)^2 = 0. \tag{3.11}$$

Thus we start with

$$\frac{\partial z}{\partial t} + H(\nabla z) = 0, \tag{3.12}$$

where $\nabla$ is the gradient in the base variables only, and

$$H = \frac{1}{2}(\xi_1 + 2x_2\eta)^2 + \frac{1}{2}(\xi_2 - 2x_1\eta)^2 = \frac{1}{2}\zeta_1^2 + \frac{1}{2}\zeta_2^2, \tag{3.13}$$

and $\eta$ is dual to $y$. As usual, one reduces this question to finding a solution of a system of ordinary differential equations as follows. Set

$$F(x, y, t, z, \xi, \eta, \gamma) = \gamma + H(x, y, \xi, \eta) = 0, \tag{3.14}$$

where $\xi = \nabla_x z$, $\eta = \partial z/\partial y$ and $\gamma = \partial z/\partial t$. We shall find the bicharacteristic curves, solutions to

$$\begin{aligned}
\dot{x}_1 &= F_{\xi_1} = \xi_1 + 2x_2\eta = \zeta_1, \quad \dot{x}_1 = \frac{dx_1}{ds}, \\
\dot{x}_2 &= F_{\xi_2} = \xi_2 - 2x_1\eta = \zeta_2, \\
\dot{y} &= F_\eta = 2x_2\dot{x}_1 - 2x_1\dot{x}_2, \\
\dot{t} &= F_\gamma = 1, \\
\dot{\xi}_1 &= -F_{x_1} - \xi_1 F_z = 2\eta\dot{x}_2, \\
\dot{\xi}_2 &= -F_{x_2} - \xi_2 F_z = -2\eta\dot{x}_1, \\
\dot{\eta} &= -F_y - \eta F_z = 0, \\
\dot{\gamma} &= -F_t - \gamma F_z = 0, \\
\dot{z} &= \xi \cdot \nabla_\xi F + \eta F_\eta + \gamma F_\gamma = \xi \cdot \dot{x} + \eta\dot{y} - H,
\end{aligned} \tag{3.15}$$

since $\dot{t} = 1$ and $\gamma = -H$. With $0 \le s \le t$,

$$\begin{aligned}
\gamma(s) = \gamma = -H = \text{constant}, \\
\eta(s) = \eta = \text{constant}, \\
t(s) = s,
\end{aligned} \tag{3.16}$$

constant meaning “constant along the bicharacteristic curve”. Another way to see that $H$ is constant along the bicharacteristic, note that

$$\begin{aligned}
\ddot{x}_1 &= \dot{\xi}_1 + 2\eta\dot{x}_2 = 4\eta\dot{x}_2, \\
\ddot{x}_2 &= \dot{\xi}_2 - 2\eta\dot{x}_1 = -4\eta\dot{x}_1,
\end{aligned} \tag{3.17}$$

therefore

$$\ddot{x}_1\dot{x}_1 + \ddot{x}_2\dot{x}_2 = 0,$$

and

$$H = \frac{1}{2}\dot{x}_1^2 + \frac{1}{2}\dot{x}_2^2 = \text{constant}. \tag{3.18}$$

A bit of calculation yields the classical action,

$$\begin{aligned} S(t) &= \int_0^t (\xi\cdot\dot{x}+\eta\dot{y}-H)ds \\ &= \eta[y-y(0)+2(x_1(0)x_2-x_1x_2(0))+|x-x(0)|^2\cot(2\eta t)], \end{aligned} \tag{3.19}$$

and then

$$\begin{aligned} h &= \eta(0)y(0)+S(t) \\ &= \eta y+2\eta(x_1(0)x_2-x_1x_2(0))+\eta|x-x(0)|^2\cot(2\eta t) \end{aligned} \tag{3.20}$$

is a solution of the Hamilton-Jacobi equation (3.12). Since $x(0)=0$, one has

$$h(x,y,\eta,t)=\eta y+\eta|x|^2\cot(2\eta t). \tag{3.21}$$

Recall that we may have multiple geodesic connections between $(0,0)$ and $(x,y)$, so one cannot choose $y(0)=0$ and $y(0)$ is replaced by the free parameter $\eta$. To recapitulate, the principal part of the heat kernel is

$$\cdots e^{-h}\cdots, \tag{3.22}$$

and $h$ contains the dual variable $\eta$. Since the heat kernel is not supposed to have dual variables we shall sum over $\eta$ or, for the sake of convenience, over $-i\tau=2\eta t$. Setting

$$h = \frac{f}{t}, \tag{3.23}$$

one has

$$\begin{aligned} f &= \frac{1}{2}(2\eta t)\big(y+|x|^2\cot(2\eta t)\big) \\ &= -\frac{1}{2}i\tau y+\frac{1}{2}\tau|x|^2\coth\tau, \end{aligned} \tag{3.24}$$

and we look for $p$ in the form

$$p(t,x,y)=\frac{1}{(2\pi t)^\alpha}\int_{-\infty}^{\infty}e^{-\frac{f(x,y,\tau)}{t}}V(\tau)\,d\tau. \tag{3.25}$$

Applying the heat operator to $p$ one has

$$\begin{aligned} 0 &= \left(\Delta_H-\frac{\partial}{\partial t}\right)\frac{1}{(2\pi t)^\alpha}\int_{-\infty}^{\infty}e^{-\frac{f}{t}}V\,d\tau \\ &= -\frac{2\pi}{(2\pi t)^{\alpha+1}}\int_{-\infty}^{\infty}e^{-\frac{f}{t}}\left\{\tau\frac{dV}{d\tau}+(\Delta_H f-\alpha+1)V\right\}, \end{aligned}$$

so we set

$$\tau\frac{dV}{d\tau}+(\tau\coth\tau+1-\alpha)V=0,$$

which gives

$$V(\tau)=\frac{(C\tau)^{\alpha-1}}{\sinh\tau}, \tag{3.26}$$

and with $\alpha=2$ we have

**Theorem 6.** *The heat kernel of $\Delta_H$ is*

$$p(t,x,y)=\frac{1}{(2\pi t)^2}\int_{-\infty}^{\infty}e^{-\frac{f}{t}}\frac{\tau}{\sinh\tau}\,d\tau. \tag{3.27}$$

From $f=f(x,y,\gamma)$, $\gamma=2\eta t$, and

$$\frac{\partial(f/t)}{\partial t}+H\big(\nabla(f/t)\big)\;=\;0,$$

one has

$$-\frac{f}{t^2}+\frac{2\eta}{t}\frac{\partial f}{\partial\gamma}+\frac{1}{t^2}H(\nabla f)\;=\;0,$$

or,

$$\gamma\frac{\partial f}{\partial\gamma}+H(\nabla f)\;=\;f,$$

and with $\gamma=-i\tau$, one has the modified eiconal equation,

$$\tau\frac{\partial f}{\partial\tau}+H(\nabla f)=f. \tag{3.28}$$

(1.62) and (1.69) of [1] imply

$$\frac{\partial f}{\partial(-i\tau)}=y(0;x,y,-i\tau), \tag{3.29}$$

so at the critical points of $f$ with respect to $\tau$ one has $y(0)=0$. In particular, the critical points of $f$ are in 1-1 correspondence with the geodesics between the origin and $(x,y)$, and, in view of (3.28), at the critical point $\tau=\tau_c$ one has

$$f(x,y,\tau_c)=\frac{1}{2}\ell_{\tau_c}(x,y;0,0)^2, \tag{3.30}$$

where $\ell_{\tau_c}$ is the length of the geodesic associated to $\tau_c$. Note that all critical points of $f$ are on the imaginary $\tau$-axis.

### 3.2. Grushin operator

Consider the following vector fields on $\mathbb{R}^2$

$$X = \frac{\partial}{\partial x}, \qquad Y = x\frac{\partial}{\partial y}. \tag{3.31}$$

$X$ and $Y$ always yield two directions on $\mathbb{R}^2$ except on the $y$-axis, where their bracket $[X, Y] = \frac{\partial}{\partial y}$ yields the missing direction. The step two Grushin operator

$$\Delta_G = \frac{1}{2}(X^2 + Y^2) = \frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2\frac{\partial^2}{\partial y^2} \tag{3.32}$$

is therefore subelliptic. Using the same approach as in **3.1**, one can show that the heat kernel of $\Delta_G$ is given by

$$p(t, x_0, y_0, x, y) = \frac{1}{(2\pi t)^{3/2}}\int_{-\infty}^{\infty} e^{-f(\tau)/t}V(\tau)\,d\tau, \tag{3.33}$$

where $(x_0, y_0)$ and $(x, y)$ are two points on $\mathbb{R}^2$, the modified complex action function is

$$f(\tau) = -i(y - y_0) + \frac{\tau}{2\sinh\tau}\left[(x^2 + x_0^2)\cosh\tau - 2xx_0\right], \tag{3.34}$$

and the volume element is

$$V(\tau) = \left(\frac{\tau}{\sinh\tau}\right)^{\frac{1}{2}}. \tag{3.35}$$

**3.3.** On $\mathbb{C}^2$ we introduce the vector fields $Z$,

$$Z = \frac{\overline{z_2}}{r}\frac{\partial}{\partial z_1} - \frac{\overline{z_1}}{r}\frac{\partial}{\partial z_2}, \qquad \|\sqrt{2}Z\| = 1, \tag{3.36}$$

which is tangent to $S^3$ since $Zr = 0$. Setting $r = 1$,

$$\begin{aligned} \Delta_C &= 2\mathrm{Re}Z\overline{Z} = Z\overline{Z} + \overline{Z}Z \\ &= \frac{1}{2}\frac{\partial^2}{\partial\theta^2} + (\cot 2\theta)\frac{\partial}{\partial\theta} + \frac{1}{2}\left((\tan\theta)\frac{\partial}{\partial\varphi_1} + (\cot\theta)\frac{\partial}{\partial\varphi_2}\right)^2 \end{aligned} \tag{3.37}$$

is the subelliptic Laplacian on $S^3$, *i.e.* the $S^3$-subLaplacian. A Hamiltonian formalism shows that the heat kernel for the reduced operator $\mathcal{L}_C$,

$$\mathcal{L}_C = \frac{1}{2}\frac{\partial^2}{\partial\theta^2} + (\cot 2\theta)\frac{\partial}{\partial\theta} + \frac{1}{2}(\tan^2\theta)\frac{\partial^2}{\partial\varphi_1^2}, \tag{3.38}$$

is also the heat kernel for $\Delta_C$ when normalized. $\mathcal{L}_C$ is not elliptic since $\tan\theta = 0$ at $\theta = 0$, but

$$\left[\frac{\partial}{\partial\theta}, (\tan\theta)\frac{\partial}{\partial\varphi_1}\right] = \frac{1}{\cos^2\theta}\frac{\partial}{\partial\varphi_1} \neq 0 \tag{3.39}$$

at $\theta = 0$, hence $\mathcal{L}_C$ is subelliptic.

**Theorem 7.** *One has*

$$p_C = \frac{e^{\frac{1}{2}t}}{(2\pi t)^2}\sum_{k\in\mathbb{Z}}\int_{-\infty}^{\infty} e^{-\frac{f(\sigma - i\varphi_1, \kappa + i2k\pi)}{t}}\frac{\kappa + i2k\pi}{\sinh\kappa}d\sigma, \tag{3.40}$$

$$f(\sigma,\kappa) = \frac{1}{2}\sigma^2 - \frac{1}{2}\kappa^2, \qquad \kappa = \cosh^{-1}(\cos\theta\cosh\sigma). \tag{3.41}$$

The heat kernel for $\Delta_C$ on $S^{2n+1}$ is analogous. Note the similarity of (3.40) and (3.27). Everything we said about $f$ and $y(0)$ for $\Delta_H$ holds for $f$ and $\varphi_1(0)$ for $\Delta_C$, except that equation (3.28) must be replaced by

$$\frac{\sigma}{\cos^2\theta}\frac{\partial f}{\partial\sigma} + H(\nabla f) = f + \frac{\varphi_1(0)}{\cos^2\theta}\left[\varphi_1 - \frac{1}{2}\varphi_1(0)\right]. \tag{3.42}$$

In particular, $f/t$ is not a solution of the Hamilton-Jacobi equation of $\Delta_C$. We do not need this, so we do not get it. What we need is that

$$\frac{\partial(f/t)}{\partial t} + H\left(\nabla\Big(\frac{f}{t}\Big)\right) = \frac{d}{d\tau}g(\tau) \tag{3.43}$$

for some $g$, so its integral vanishes. This happens for $f/t$ of $\Delta_C$.

One may try to understand this difference between (3.42) and (3.28) by representing $\Delta_C$ in terms of the Heisenberg vector fields and then compare the associated heat kernels.

## 4. On the Cayley transform of $\Delta_C$

To compare the subelliptic heat kernels on $S^{2n+1}$ and on $H_n$ we shall send $\Delta_C$ from $S^{2n+1}$ to $H_n$ via the Cayley transform. $\Delta_C$ on $H_n$ will be represented by the Heisenberg vector fields, but with variable coefficients; we shall continue to refer it as $\Delta_C$. Not to complicate matters we shall work with $\Delta_C$ on $S^3 \subset \mathbb{C}^2$.

Assuming our origin is $(z_1, z_2) = (1, 0) \in S^3$, we shall leave out the antipodal point $(-1, 0)$. Then the Cayley transform $\zeta = (\zeta_1, \zeta_2) = C(z_1, z_2)$ is given by

$$\zeta = C(z_1, z_2) = \left( i\frac{1 - z_1}{1 + z_1}, \frac{z_2}{1 + z_1} \right) = (\zeta_1, \zeta_2). \tag{4.1}$$

Note that $(\zeta_1, \zeta_2) = (0, 0)$ if and only if $(z_1, z_2) = (1, 0)$. In particular, one has

$$\begin{aligned} \zeta_1 &= u_1 + iv_1 = \frac{2y_1}{(1 + x_1)^2 + y_1^2} + i\frac{1 - |z_1|^2}{(1 + x_1)^2 + y_1^2}, \\ |\zeta_2|^2 &= \frac{|z_2|^2}{(1 + x_1)^2 + y_1^2}, \end{aligned} \tag{4.2}$$

hence

$$v_1 - |\zeta_2|^2 = \frac{1 - |z|^2}{|1 + z_1|^2} > 0 \qquad \text{iff} \qquad |z|^2 < 1. \tag{4.3}$$

We set

$$\mathscr{D}_2 = \left\{ \text{Im}\zeta_1 > |\zeta_2|^2 \right\}, \qquad b\mathscr{D}_2 = \left\{ \text{Im}\zeta_1 = |\zeta_2|^2 \right\}. \tag{4.4}$$

Note that

$$(z_1, z_2) = C^{-1}(\zeta_1, \zeta_2) = \left( \frac{1 + i\zeta_1}{1 - i\zeta_1}, \frac{2\zeta_2}{1 - i\zeta_1} \right). \tag{4.5}$$

Recall the tangential holomorphic vector field $Z$,

$$Z = \frac{\overline{z_2}}{r}\frac{\partial}{\partial z_1} - \frac{\overline{z_1}}{r}\frac{\partial}{\partial z_2}, \tag{4.6}$$

$Zr = 0$ and $\|\sqrt{2}\, Z\| = 1$ in Euclidean metric. In $(\zeta_1, \zeta_2)$ coordinates one has

$$\frac{\partial}{\partial z_1} = -\frac{1}{2}(1 - i\zeta_1)\left( i(1 - i\zeta_1)\frac{\partial}{\partial \zeta_1} + \zeta_2\frac{\partial}{\partial \zeta_2} \right), \tag{4.7}$$

$$\frac{\partial}{\partial z_2} = \frac{1}{2}(1 - i\zeta_1)\frac{\partial}{\partial \zeta_2}\,, \tag{4.8}$$

and then

$$rZ = -\frac{1}{2}\frac{1 - i\zeta_1}{1 + i\overline{\zeta_1}}\left\{2i\overline{\zeta_2}(1 - i\zeta_1)\frac{\partial}{\partial \zeta_1} + \left(2|\zeta_2|^2 + 1 - i\overline{\zeta_1}\,\right)\frac{\partial}{\partial \zeta_2}\right\} \tag{4.9}$$

on $\mathbb{C}^2 \setminus \{\zeta_1 = -i\}$. Restricting $Z$ to $b\mathscr{D}_2 = C\left\{S^3 \setminus (-1, 0)\right\}$ one obtains

$$Z = -\frac{1}{2}\frac{(1 + |\zeta_2|^2 - iu_1)^2}{1 + |\zeta_2|^2 + iu_1}\left(\frac{\partial}{\partial \zeta_2} + 2i\overline{\zeta_2}\frac{\partial}{\partial \zeta_1}\right). \tag{4.10}$$

The following formula

$$1 - r^2 = \chi = \frac{4}{|1 - i\zeta_1|^2}\left(\mathrm{Im}\zeta_1 - |\zeta_2|^2\right) > 0 \tag{4.11}$$

defines $\mathscr{D}_2$; it is easy to see that $Z(\chi) = 0$ on $\mathscr{D}_2$, so $Z$ is tangent to the surfaces $\sigma = r^2 = \text{const}$. Next we find $Z$ in tangential coordinates $\left(u, \sigma, \zeta_2', \overline{\zeta_2'}\right)$ on $\mathscr{D}_2$, where

$$\begin{cases} u = u_1 = \dfrac{1}{2}(\zeta_1 + \overline{\zeta_1}), \\ \sigma = r^2 = \dfrac{|1 + i\zeta_1|^2 + 4|\zeta_2|^2}{|1 - i\zeta_1|^2}, \\ \zeta_2' = \zeta_2, \qquad \overline{\zeta_2'} = \overline{\zeta_2}. \end{cases} \tag{4.12}$$

Using formulas (5.30) and (5.31) a bit of work yields

$$Z = -\frac{1}{2}\frac{(1 - i\zeta_1)^2}{1 + i\overline{\zeta_1}}\left(\frac{1 - \frac{v_1 - |\zeta_2|^2}{1 + |\zeta_2|^2 - iu}}{1 + \frac{v_1 - |\zeta_2|^2}{1 + |\zeta_2|^2 - iu}}\frac{\partial}{\partial \zeta_2'} + i\overline{\zeta_2'}\frac{\partial}{\partial u}\right) \tag{4.13}$$

on $\mathscr{D}_2$; again note that $Z\sigma = 0$ hence $Z$ is tangent to $\sigma = \text{const}$. Writing $\zeta_2' = \zeta$, one finally has $Z$ on $b\mathscr{D}_2$,

$$Z = -\frac{1}{2}\frac{(1 + |\zeta|^2 - iu)^2}{1 + |\zeta|^2 + iu}\left(\frac{\partial}{\partial \zeta} + i\overline{\zeta}\frac{\partial}{\partial u}\right), \tag{4.14}$$

which is the Heisenberg vector field on $H_1$ modulo a nonconstant factor.

Also,

$$\overline{Z} = -\frac{1}{2}\frac{(1+|\zeta|^2+iu)^2}{1+|\zeta|^2-iu}\left(\frac{\partial}{\partial\overline{\zeta}} - i\zeta\frac{\partial}{\partial u}\right), \tag{4.15}$$

so,

$$\begin{aligned} Z\overline{Z} =& \frac{1}{4}\left|1+|\zeta|^2+iu\right|^2\left(\frac{\partial}{\partial\zeta} + i\overline{\zeta}\frac{\partial}{\partial u}\right)\left(\frac{\partial}{\partial\overline{\zeta}} - i\zeta\frac{\partial}{\partial u}\right) \\ &- \frac{1}{2}\overline{\zeta}\left(1+|\zeta|^2+iu\right)\left(\frac{\partial}{\partial\overline{\zeta}} - i\zeta\frac{\partial}{\partial u}\right), \end{aligned} \tag{4.16}$$

which yields

$$\begin{aligned} \Delta_C &= Z\overline{Z} + \overline{Z}Z \\ &= \frac{1}{2}\left|1+|\zeta|^2+iu\right|^2\left\{\left(\frac{\partial}{\partial\zeta} + i\overline{\zeta}\frac{\partial}{\partial u}\right)\left(\frac{\partial}{\partial\overline{\zeta}} - i\zeta\frac{\partial}{\partial u}\right) + i\frac{\partial}{\partial u}\right\} \\ &\quad -\frac{1}{2}\overline{\zeta}\left(1+|\zeta|^2+iu\right)\left(\frac{\partial}{\partial\overline{\zeta}} - i\zeta\frac{\partial}{\partial u}\right) \\ &\quad -\frac{1}{2}\zeta\left(1+|\zeta|^2-iu\right)\left(\frac{\partial}{\partial\zeta} + i\overline{\zeta}\frac{\partial}{\partial u}\right). \end{aligned} \tag{4.17}$$

Thus $\Delta_C$ is given in terms of the Heisenberg vector fields with variable coefficients. According to (3.42) the exponent in the Cayley transform of (3.40) will not be a solution of the Hamilton-Jacobi equation and the question is what are the geometric differences between $\Delta_C$ and $\Delta_H$ which produce this state of affairs. To help us better understand what goes on in $b\mathscr{D}_2$, we shall study the Cayley transform of $\Delta_S$ more closely.

## 5. The Cayley transform of $\Delta_S$

We shall use both $\partial_x$ and $\partial/\partial x$ for the same derivative. Also,

$$\partial_z = \frac{\partial}{\partial z} = \frac{1}{2}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right). \tag{5.1}$$

Not to complicate the notation we work with $\mathbb{C}^2$ only, so $z = (z_1, z_2)$, $z_j = x_j + iy_j$, $j = 1, 2$. Set

$$Z = \frac{\overline{z_2}}{r}\frac{\partial}{\partial z_1} - \frac{\overline{z_1}}{r}\frac{\partial}{\partial z_2}, \tag{5.2}$$

$$N = \frac{z_1}{r}\frac{\partial}{\partial z_1} + \frac{z_2}{r}\frac{\partial}{\partial z_2}\,; \tag{5.3}$$

again note that $Zr = 0$, so $Z$ is tangent to spheres $r^2 = \|z\|^2 = |z_1|^2 + |z_2|^2 =$ const. In Euclidean metric both $(\sqrt{2}\partial_{z_1}, \sqrt{2}\partial_{z_2})$ and $(\sqrt{2}Z, \sqrt{2}N)$ represent an orthonormal basis of the holomorphic tangent space of $\mathbb{C}^2$. Consequently,

$$\Delta = 2\frac{\partial^2}{\partial z_1 \partial \overline{z_1}} + 2\frac{\partial^2}{\partial z_2 \partial \overline{z_2}} = -(Z^* Z + \overline{Z^*}\,\overline{Z}) - (N^* N + \overline{N^*}\,\overline{N}) \tag{5.4}$$

with

$$-Z^* = \overline{Z}, \qquad \text{and} \qquad -N^* = \overline{N} + \frac{3}{2r}; \tag{5.5}$$

$Z^*$ and $N^*$ represent the adjoint operators of $Z$ and $N$ with respect to Euclidean metric. All these calculations can be found in §2 of [2], where they are worked out in $\mathbb{C}^{n+1}$. One sets

$$\Delta_S = \Delta\big|_{S^3}. \tag{5.6}$$

The following complex spherical coordinates are convenient:

$$z_1 = r\cos\theta e^{i\varphi_1}, \qquad z_2 = r\sin\theta e^{i\varphi_2}, \tag{5.7}$$

$0 \le \theta \le \pi/2$, $-\pi < \varphi_j \le \pi$, $j = 1, 2$; for $\mathbb{C}^{n+1}$ see (2.15). Then

$$N = \frac{1}{2}\frac{\partial}{\partial r} - \frac{i}{2r}\left(\frac{\partial}{\partial \varphi_1} + \frac{\partial}{\partial \varphi_2}\right) = \frac{1}{2}\partial_r - \frac{i}{2r}\partial_\varphi\,, \tag{5.8}$$

see (2.28) of [2], where we set

$$\partial_\varphi = \partial_{\varphi_1} + \partial_{\varphi_2}\,, \tag{5.9}$$

for convenience. Also,

$$-(N^* N + \overline{N^*}\,\overline{N}) = -2\mathrm{Re}(N^* N) = \frac{1}{2}\left(\partial_r^2 + \frac{3}{r}\partial_r\right) + \frac{1}{2r^2}\partial_\varphi^2\,, \tag{5.10}$$

and one has

$$\Delta = 2\mathrm{Re}\overline{Z}Z + \frac{1}{2}\left(\partial_r^2 + \frac{3}{r}\partial_r\right) + \frac{1}{2r^2}\partial_\varphi^2$$

$$= \frac{1}{2}\left(\partial_r^2 + \frac{3}{r}\partial_r\right) + \frac{1}{r^2}\Delta_S\,, \tag{5.11}$$

where

$$\frac{1}{r^2}\Delta_S \;=\; 2\mathrm{Re}Z\overline{Z} + \frac{1}{2r^2}\partial_\varphi^2 = \Delta - \frac{1}{2}\left(\partial_r^2 + \frac{3}{r}\partial_r\right). \tag{5.12}$$

We also set

$$\Delta_C \;=\; 2\mathrm{Re}Z\overline{Z} = \frac{1}{2}(2X)^2 + \frac{1}{2}(2Y)^2; \tag{5.13}$$

in particular, $2\Delta_C$ is the sum of squares of unit vector fields which are orthonormal to each other. We used $Z = X + iY$. Now (5.8) implies that

$$\partial_\varphi = -2r\mathrm{Im}N = ir\left(N - \overline{N}\right). \tag{5.14}$$

Since $N \perp Z$, we have $\partial_\varphi \perp Z$, and since $\partial_\varphi$ is real, $\partial_\varphi \perp X$ and $\partial_\varphi \perp Y$. An easy calculation yields $\|\partial_\varphi\| = r$, hence $\|\partial_\varphi\| = 1$ on $S^3$. Consequently, (5.12) gives

$$\Delta_S = \Delta_C + \frac{1}{2}\partial_\varphi^2 = \frac{1}{2}(2X)^2 + \frac{1}{2}(2Y)^2 + \frac{1}{2}\partial_\varphi^2 \tag{5.15}$$

on $S^3$, *i.e.* $\Delta_S$ is $\frac{1}{2}$ times the sum of squares of three orthonormal vector fields on $S^3$, hence elliptic.

Let us recapitulate what we are trying to do. Our long term aim is to find heat kernels for subelliptic operators. The formulas we are looking for should be given in geometric terms and be as precise as are the well known formulas for heat kernels of elliptic operators, which should be special cases of subelliptic heat kernels, of course. To achieve this objective we work with a Hamiltonian formalism. So far very few subelliptic heat kernels have been found. Most of the work has gone into the study of the heat kernels of $\Delta_H$, the Heisenberg subLaplacian, and of $\Delta_G$, the step 2 Grushin operator; lately the heat kernel of $\Delta_C$ on $S^{2n+1}$ has been worked out. They are all given as integrals of exponentials, where the exponent is the solution of a Hamilton-Jacobi equation, a kind of distance function, at least in the case of $\Delta_H$ and $\Delta_G$; one may call these flat. The formula for the heat kernel for $\Delta_C$ on $S^{2n+1}$ is very similar, but the exponent in the integrand is not a solution of the associated Hamilton-Jacobi equation. It is a solution of a modified Hamilton-Jacobi equation; this may be true in general. Consequently it is essential to find this modification in geometrically invariant terms. The first step is to compare the heat kernel of the Cayley transform of $\Delta_C$ on $b\mathscr{D}_2$

with the heat kernel of $\Delta_H$; they both make sense on the Heisenberg group if we look on the Cayley transform of $\Delta_C$ as a Heisenberg subLaplacian with variable coefficients.

So our first job is to understand how to work with the Cayley transform of $S^{2n+1}$. To this end, we shall devote the rest of §5 to the explicit derivation of the heat kernel of $\Delta_S$ on $b\mathscr{D}_2$. In particular we need to show that the heat kernel is a function of one variable only. The calculations are elementary but complicated, so we shall include enough detail, not all, to convince the reader. To obtain $\Delta_S$ on $b\mathscr{D}_2$ one uses (5.12) in the form

$$\frac{1}{r^2}\Delta_S = \Delta - \frac{1}{2}\left(\partial_r^2 + \frac{3}{r}\partial_r\right), \tag{5.16}$$

and note that (5.8) implies

$$\partial_r = N + \overline{N}, \tag{5.17}$$

so one has

$$\frac{1}{r^2}\Delta_S = \Delta - \frac{1}{2}\left[\left(N + \overline{N}\right)^2 + \frac{3}{r}\left(N + \overline{N}\right)\right]. \tag{5.18}$$

We start with calculating the variable $x = \cos\theta\cos\varphi_1$ in $b\mathscr{D}_2$ coordinates. (4.5) yields

$$z_1 = r\cos\theta e^{i\varphi_1} = \frac{1 + i\zeta_1}{1 - i\zeta_1}, \quad \text{so} \quad \cos\theta = \frac{|1 + i\zeta_1|}{|1 - i\zeta_1|} \tag{5.19}$$

on $b\mathscr{D}_2$, *i.e.* when $r = 1$. Also, on $b\mathscr{D}_2$, $1 + i\zeta_1 = 1 + iu_1 - v_1 = 1 - |\zeta_2|^2 + iu$, so

$$\cos^2\theta = \frac{\left|1 - |\zeta|^2 + iu\right|^2}{\left|1 + |\zeta|^2 - iu\right|^2} = \frac{(1-\rho)^2 + u^2}{(1+\rho)^2 + u^2}\,, \tag{5.20}$$

where we set $\rho = |\zeta|^2$. Also

$$\begin{aligned} z_1 =& r\cos\theta\cos\varphi_1 + ir\cos\theta\sin\varphi_1 \\ =& \frac{1 + i\zeta_1}{1 - i\zeta_1} = \frac{1 - |\zeta_1|^2 + i(\zeta_1 + \overline{\zeta_1})}{|1 - i\zeta_1|^2}, \end{aligned} \tag{5.21}$$

and then

$$\tan\varphi_1 = \frac{\zeta_1+\overline{\zeta_1}}{1-|\zeta_1|^2}\,, \tag{5.22}$$

so one has

$$\cos^2\varphi_1 = \frac{1}{1+\tan^2\varphi_1} = \frac{\big(1-|\zeta_1|^2\big)^2}{1+\zeta_1^2+\overline{\zeta_1}^2+|\zeta_1|^4}\,. \tag{5.23}$$

Now,

$$\begin{aligned} 1+\zeta_1^2+\overline{\zeta_1}^2+|\zeta_1|^4 &= 1+2(u_1^2-v_1^2)+(u_1^2+v_1^2)^2 \\ &= 1+2u^2-2|v_1|^2+u^4+2u^2|v_1|^2+|v_1|^4 \\ &= (1+|v_1|^2)^2-4|v_1|^2+u^4+2u^2(1+|v_1|^2) \\ &= \big((1+|v_1|^2)+u^2\big)^2-4|v_1|^2 \\ &= \big((1-|v_1|)^2+u^2\big)\big((1+|v_1|)^2+u^2\big), \end{aligned}$$

since $v_1=|\zeta_2|^2\geq 0$ on $b\mathscr{D}_2$. Thus

$$\begin{aligned} \cos^2\varphi_1 &= \frac{\big(1-|\zeta_1|^2\big)^2}{\big((1-|v_1|)^2+u^2\big)\big((1+|v_1|)^2+u^2\big)} \\ &= \frac{\big(1-|\zeta_1|^2\big)^2}{|1+i\zeta_1|^2|1-i\zeta_1|^2}\,, \end{aligned} \tag{5.24}$$

or

$$\cos\varphi_1 = \frac{1-|\zeta_1|^2}{|1+i\zeta_1|\,|1-i\zeta_1|}\,, \tag{5.25}$$

and in view of (5.19) we have derived

**Lemma 8.** *The Cayley transform of $x=\cos\theta\cos\varphi_1$ on $S^3$ is*

$$x=\frac{1-|\zeta_1|^2}{|1-i\zeta_1|^2}=\frac{1-\rho^2-u^2}{(1+\rho)^2+u^2}\,, \tag{5.26}$$

*where we let $x$ also represent the Cayley transform of $\cos\theta\cos\varphi_1$ on $b\mathscr{D}_2$.*

**Lemma 9.** *Let $\Delta_S$ also denote the Cayley transform of $\Delta_S$ acting on $b\mathscr{D}_2$. With $x$ given by (5.26) one has*

$$\Delta_S f(x)=\frac{1}{2}(1-x^2)\frac{d^2f}{dx^2}-\frac{3}{2}x\frac{df}{dx}. \tag{5.27}$$

***Proof.*** We use (5.18); the calculation is elementary but somewhat lengthy. Starting with

$$\Delta = 2\frac{\partial}{\partial z_1}\frac{\partial}{\partial \overline{z_1}} + 2\frac{\partial}{\partial z_2}\frac{\partial}{\partial \overline{z_2}}\,, \tag{5.28}$$

(4.7) and (4.8) yield

$$\begin{aligned}\frac{\partial}{\partial z_1}\frac{\partial}{\partial \overline{z_1}} &= \frac{1}{4}|1-i\zeta_1|^2\left(i(1-i\zeta_1)\frac{\partial}{\partial\zeta_1}+\zeta_2\frac{\partial}{\partial\zeta_2}\right)\left(-i(1+i\overline{\zeta_1})\frac{\partial}{\partial\overline{\zeta_1}}+\overline{\zeta_2}\frac{\partial}{\partial\overline{\zeta_2}}\right),\\ \frac{\partial}{\partial z_2}\frac{\partial}{\partial \overline{z_2}} &= \frac{1}{4}|1-i\zeta_1|^2\frac{\partial}{\partial\zeta_2}\frac{\partial}{\partial\overline{\zeta_2}}\,,\end{aligned}$$

so in $(\zeta_1,\zeta_2)$-coordinates one has

$$\begin{aligned}\Delta &= \frac{1}{2}|1-i\zeta_1|^2\left\{|1-i\zeta_1|^2\frac{\partial}{\partial\zeta_1}\frac{\partial}{\partial\overline{\zeta_1}}+i(1-i\zeta_1)\overline{\zeta_2}\frac{\partial}{\partial\zeta_1}\frac{\partial}{\partial\overline{\zeta_2}}\right.\\ &\qquad\left.-i(1+i\overline{\zeta_1})\zeta_2\frac{\partial}{\partial\overline{\zeta_1}}\frac{\partial}{\partial\zeta_2}+(1+|\zeta_2|^2)\frac{\partial}{\partial\zeta_2}\frac{\partial}{\partial\overline{\zeta_2}}\right\}.\end{aligned} \tag{5.29}$$

We need to write $\Delta$ in tangential coordinates. In view of (4.12), one has

$$\frac{\partial}{\partial\zeta_1} = \frac{1}{2}\frac{\partial}{\partial u} + \frac{2i\big(1-i\overline{\zeta_1}+2|\zeta_2|^2\big)}{(1-i\zeta_1)^2(1+i\overline{\zeta_1})}\frac{\partial}{\partial\sigma}\,, \tag{5.30}$$

$$\frac{\partial}{\partial\zeta_2} = \frac{4\overline{\zeta_2}}{|1-i\zeta_1|^2}\frac{\partial}{\partial\sigma} + \frac{\partial}{\partial\zeta_2'}\,, \tag{5.31}$$

and

$$\begin{aligned}\frac{\partial}{\partial\zeta_1}\frac{\partial}{\partial\overline{\zeta_1}} &= \frac{\partial}{\partial\zeta_1}\left\{\frac{1}{2}\frac{\partial}{\partial u}-\frac{2i\big(1+i\zeta_1+2|\zeta_2|^2\big)}{(1+i\overline{\zeta_1})^2(1-i\zeta_1)}\frac{\partial}{\partial\sigma}\right\}\\ &= \left(\frac{1}{2}\frac{\partial}{\partial u}+\frac{2i\big(1-i\overline{\zeta_1}+2|\zeta_2|^2\big)}{(1-i\zeta_1)^2(1+i\overline{\zeta_1})}\frac{\partial}{\partial\sigma}\right)\frac{1}{2}\frac{\partial}{\partial u}\\ &\quad-\frac{\partial}{\partial\zeta_1}\left(\frac{2i\big(1+i\zeta_1+2|\zeta_2|^2\big)}{(1+i\overline{\zeta_1})^2(1-i\zeta_1)}\right)\frac{\partial}{\partial\sigma}\\ &\quad-\frac{2i\big(1+i\zeta_1+2|\zeta_2|^2\big)}{(1+i\overline{\zeta_1})^2(1-i\zeta_1)}\left(\frac{1}{2}\frac{\partial}{\partial u}+\frac{2i\big(1-i\overline{\zeta_1}+2|\zeta_2|^2\big)}{(1-i\zeta_1)^2(1+i\overline{\zeta_1})}\frac{\partial}{\partial\sigma}\right)\frac{\partial}{\partial\sigma}.\end{aligned}$$

Similarly,

$$\frac{\partial}{\partial\zeta_1}\frac{\partial}{\partial\overline{\zeta_2}} = \left(\frac{\partial}{\partial\zeta_1}\frac{4\zeta_2}{|1-i\zeta_1|^2}+\frac{4\zeta_2}{|1-i\zeta_1|^2}\frac{\partial}{\partial\zeta_1}\right)\frac{\partial}{\partial\sigma}$$

$$+\left(\frac{1}{2}\frac{\partial}{\partial u}+\frac{2i\left(1-i\overline{\zeta_1}+2|\zeta_2|^2\right)}{(1-i\zeta_1)^2(1+i\overline{\zeta_1})}\frac{\partial}{\partial\sigma}\right)\frac{\partial}{\partial\overline{\zeta_2'}},$$

$$\frac{\partial}{\partial\zeta_2}\frac{\partial}{\partial\overline{\zeta_2}} = \left(\frac{\partial}{\partial\zeta_2}\frac{4\zeta_2}{|1-i\zeta_1|^2}+\frac{4\zeta_2}{|1-i\zeta_1|^2}\left\{\frac{4\overline{\zeta_2}}{|1-i\zeta_1|^2}+\frac{\partial}{\partial\zeta_2'}\right\}\right)\frac{\partial}{\partial\sigma}$$
$$+\frac{4\overline{\zeta_2}}{|1-i\zeta_1|^2}\frac{\partial}{\partial\sigma}\frac{\partial}{\partial\overline{\zeta_2'}}+\frac{\partial}{\partial\zeta_2'}\frac{\partial}{\partial\overline{\zeta_2'}}.$$

Note that (5.15) is

$$\Delta_S=\frac{1}{2}(2\mathrm{Re}Z)^2+\frac{1}{2}(2\mathrm{Im}Z)^2+\frac{1}{2}\partial_\varphi^2\,, \tag{5.32}$$

and each vector field vanishes on $\sigma=r^2$, hence none of them has $\partial/\partial\sigma$ terms and neither does $\Delta_S$. Consequently, dropping the $\partial/\partial\sigma$ terms from (5.29) when written in tangential coordinates, the above calculations yield

$$\begin{aligned}\Delta_\sigma=\frac{1}{2}|1-i\zeta_1|^2\Big\{&\left(1+|\zeta|^2\right)\frac{\partial}{\partial\zeta}\frac{\partial}{\partial\overline{\zeta}}\\&+\frac{1}{2}i\left(\left(1+|\zeta|^2-iu\right)\overline{\zeta}\frac{\partial}{\partial\overline{\zeta}}-\left(1+|\zeta|^2+iu\right)\zeta\frac{\partial}{\partial\zeta}\right)\frac{\partial}{\partial u}\\&+\frac{1}{4}\left|1+|\zeta|^2-iu\right|^2\frac{\partial^2}{\partial u^2}\Big\},\end{aligned} \tag{5.33}$$

where we set $\zeta_2'=\zeta$, $\overline{\zeta_2'}=\overline{\zeta}$. Note that $\Delta_\sigma\neq\Delta_S$, since the second term on the right side of (5.18) does not vanish after dropping all $\sigma$-derivatives; see (5.44) for 2nd derivatives when applied to $f(\rho,u)$. We need the behavior of $\Delta_\sigma$ on

$$f(\rho,u)=g(x)=g\left(\frac{1-\rho^2-u^2}{(1+\rho)^2+u^2}\right), \tag{5.34}$$

so we look at $\Delta_\sigma f(\rho,u)=\Delta f(\rho,u)$.

(i) $$\frac{\partial f}{\partial\overline{\zeta}}=\zeta\frac{\partial f}{\partial\rho},\qquad \frac{\partial}{\partial\zeta}\frac{\partial f}{\partial\overline{\zeta}}=\rho\frac{\partial^2 f}{\partial\rho^2}+\frac{\partial f}{\partial\rho}\,,$$

(ii) $$\left(\overline{\zeta}\frac{\partial}{\partial\overline{\zeta}}-\zeta\frac{\partial}{\partial\zeta}\right)\frac{\partial f}{\partial u}=\frac{\partial}{\partial u}\left(|\zeta|^2-|\zeta|^2\right)\frac{\partial f}{\partial\rho}=0,$$

(iii) $$\left(\overline{\zeta}\frac{\partial}{\partial\overline{\zeta}}+\zeta\frac{\partial}{\partial\zeta}\right)\frac{\partial f}{\partial u}=2|\zeta|^2\frac{\partial^2 f}{\partial\rho\partial u}=2\rho\frac{\partial^2 f}{\partial\rho\partial u}\,,$$

so one has

$$\begin{aligned}\Delta f(|\zeta|^2,u) \;=\; & \frac{1}{2}\big((1+\rho)^2+u^2\big)\left\{\rho(1+\rho)\frac{\partial^2 f}{\partial\rho^2}+(1+\rho)\frac{\partial f}{\partial\rho}+\rho u\frac{\partial^2 f}{\partial\rho\partial u}\right.\\ & \left.+\frac{1}{4}\big((1+\rho)^2+u^2\big)\frac{\partial^2 f}{\partial u^2}\right\}. \qquad (5.35)\end{aligned}$$

Let $f(|\zeta|^2,u)=g(x)$. With

$$x+1=\frac{2(1+\rho)}{(1+\rho)^2+u^2}\,, \qquad (5.36)$$

one has

$$\begin{aligned}\frac{\partial x}{\partial\rho} &= \frac{2}{(1+\rho)^2+u^2}-(x+1)^2,\\ \frac{\partial^2 x}{\partial\rho^2} &= 2(x+1)^3-\frac{6(x+1)}{(1+\rho)^2+u^2},\\ \frac{\partial x}{\partial u} &= -\frac{2(x+1)u}{(1+\rho)^2+u^2}\,,\\ \frac{\partial^2 x}{\partial u^2} &= \frac{6(x+1)}{(1+\rho)^2+u^2}-2(x+1)^3=-\frac{\partial^2 x}{\partial\rho^2}\,,\\ \frac{\partial^2 x}{\partial\rho\partial u} &= \frac{4(x+1)^2u}{(1+\rho)^2+u^2}-\frac{4u}{\big((1+\rho)^2+u^2\big)^2}\,.\end{aligned}$$

This leads to

$$\begin{aligned}\frac{\partial g}{\partial\rho} &= \left(\frac{2}{(1+\rho)^2+u^2}-(x+1)^2\right)\frac{dg}{dx},\\ \frac{\partial^2 g}{\partial\rho^2} &= \left(\frac{2}{(1+\rho)^2+u^2}-(x+1)^2\right)^2\frac{d^2g}{dx^2}+\left(2(x+1)^3-\frac{6(x+1)}{(1+\rho)^2+u^2}\right)\frac{dg}{dx},\\ \frac{\partial g}{\partial u} &= -\frac{2(x+1)u}{(1+\rho)^2+u^2}\frac{dg}{dx}\,,\\ \frac{\partial^2 g}{\partial u^2} &= \frac{4(x+1)^2u^2}{\big((1+\rho)^2+u^2\big)^2}\frac{d^2g}{dx^2}+\left(\frac{6(x+1)}{(1+\rho)^2+u^2}-2(x+1)^3\right)\frac{dg}{dx}\,,\\ \frac{\partial^2 g}{\partial\rho\partial u} &= -\left(\frac{2}{(1+\rho)^2+u^2}-(x+1)^2\right)\frac{2(x+1)u}{(1+\rho)^2+u^2}\frac{d^2g}{dx^2}\end{aligned}$$

$$+\left(\frac{4(x+1)^2u}{(1+\rho)^2+u^2}-\frac{4u}{\big((1+\rho)^2+u^2\big)^2}\right)\frac{dg}{dx}\,.$$

Substituting into (5.35) one finds

$$\begin{aligned}\Delta g \;=\; & \frac{1}{2}\left((1+\rho)^2+u^2\right)\\ & \cdot\Bigg\{\rho(1+\rho)\left(\frac{2}{(1+\rho)^2+u^2}-(x+1)^2\right)^2\frac{d^2g}{dx^2}\\ & \quad +\rho(1+\rho)\left(2(x+1)^3-\frac{6(x+1)}{(1+\rho)^2+u^2}\right)\frac{dg}{dx}\\ & \quad +(1+\rho)\left(\frac{2}{(1+\rho)^2+u^2}-(x+1)^2\right)\frac{dg}{dx}\\ & \quad -\rho\left(\frac{2}{(1+\rho)^2+u^2}-(x+1)^2\right)\frac{2(x+1)u^2}{(1+\rho)^2+u^2}\frac{d^2g}{dx^2}\\ & \quad +\rho\left(\frac{4(x+1)^2u^2}{(1+\rho)^2+u^2}-\frac{4u^2}{\big((1+\rho)^2+u^2\big)^2}\right)\frac{dg}{dx}\\ & \quad +\frac{(x+1)^2u^2}{(1+\rho)^2+u^2}\frac{d^2g}{dx^2}+(x+1)\left(\frac{3}{2}-(x+1)(1+\rho)\right)\frac{dg}{dx}\Bigg\}. \end{aligned} \tag{5.37}$$

First we collect the coefficients of $d^2g/dx^2$:

$$\begin{aligned} & \frac{2\rho(1+\rho)}{(1+\rho)^2+u^2}\left(1-(x+1)(1+\rho)\right)^2-\frac{2\rho(x+1)u^2}{(1+\rho)^2+u^2}\\ & \quad +\rho(x+1)^3u^2+\frac{1}{2}(x+1)^2u^2\\ =\;& (x+1)\Bigg\{\rho-2\rho(x+1)(1+\rho)+\rho(x+1)^2(1+\rho)^2-\frac{2\rho u^2}{(1+\rho)^2+u^2}\\ & \qquad +\rho(x+1)^2u^2+\frac{1}{2}(x+1)u^2\Bigg\}\\ =\;& (x+1)\left\{\rho-\frac{2\rho u^2}{(1+\rho)^2+u^2}+\frac{1}{2}(x+1)u^2\right\}\\ =\;& \frac{x+1}{(1+\rho)^2+u^2}\left(\rho(1+\rho)^2-\rho u^2+(1+\rho)u^2\right)\\ =\;& \frac{2[\rho(1+\rho)^3+(1+\rho)u^2]}{\big((1+\rho)^2+u^2\big)^2}\,. \end{aligned}$$

Continuing, the coefficient of $dg/dx$ is

$$\begin{aligned}
&2\rho(1+\rho)^2(x+1)^2 - 3\rho(1+\rho)(x+1) + 1 + \rho - (1+\rho)^2(x+1)\\
&\qquad +2\rho u^2(x+1)^2 - \frac{2\rho u^2}{(1+\rho)^2+u^2} + \frac{3}{2}(1+\rho) - (1+\rho)^2(x+1)\\
&= \rho(1+\rho)(x+1) + \frac{5}{2}(1+\rho) - 2(1+\rho)^2(x+1) - \frac{2\rho u^2}{(1+\rho)^2+u^2}\\
&= \frac{1}{(1+\rho)^2+u^2}\left\{2\rho(1+\rho)^2 - 4(1+\rho)^3 - 2\rho u^2\right\} + \frac{5}{2}(1+\rho)\\
&= \frac{1}{(1+\rho)^2+u^2}\left\{-2\rho((1+\rho)^2+u^2) - 4(1+\rho)^2\right\} + \frac{5}{2}(1+\rho)\\
&= \frac{5}{2} + \frac{1}{2}\rho - \frac{4(1+\rho)^2}{(1+\rho)^2+u^2}\,.
\end{aligned}$$

Consequently, one has

$$\Delta g = \frac{2[\rho(1+\rho)^3 + (1+\rho)u^2]}{\big((1+\rho)^2+u^2\big)^2}\frac{d^2 g}{dx^2} + \left(\frac{5}{2} + \frac{1}{2}\rho - \frac{4(1+\rho)^2}{(1+\rho)^2+u^2}\right)\frac{dg}{dx}\,. \quad (5.38)$$

We are using (5.18) to find $\Delta_S\, g$. So far we obtained $\Delta g$ and we still need $\frac{1}{2}(N+\overline{N})^2 g + \frac{3}{2r}(N+\overline{N})g$. A simple calculation yields

$$N = -\frac{1}{2r}(1-i\zeta_1)\left\{i(1+i\zeta_1)\frac{\partial}{\partial\zeta_1} - \zeta_2\frac{\partial}{\partial\zeta_2}\right\}. \quad (5.39)$$

1) We start by finding the coefficient of $d^2g/dx^2$ in

$$\frac{1}{2}(N+\overline{N})^2 g = \mathrm{Re}(N^2 + N\overline{N})g. \quad (5.40)$$

Let $[N^2]_{,2}$ denote the second order $(\zeta_1,\zeta_2)$-derivatives in $N^2$. Then on $b\mathscr{D}_2$, *i.e.* when $r=1$, one has

$$\begin{aligned}
4\left[N^2\right]_{,2} &= (1-i\zeta_1)\zeta_2(2N)\frac{\partial}{\partial\zeta_2} - i(1+\zeta_1^2)(2N)\frac{\partial}{\partial\zeta_1}\\
&= (1-i\zeta_1)^2\zeta_2^2\frac{\partial^2}{\partial\zeta_2^2} - i(1-i\zeta_1)\zeta_2(1+\zeta_1^2)\frac{\partial}{\partial\zeta_1}\frac{\partial}{\partial\zeta_2}\\
&\qquad -i(1-i\zeta_1)\zeta_2(1+\zeta_1^2)\frac{\partial}{\partial\zeta_2}\frac{\partial}{\partial\zeta_1} - (1+\zeta_1^2)^2\frac{\partial^2}{\partial\zeta_1^2}\,. \quad (5.41)
\end{aligned}$$

We replace the derivatives by (5.30) and (5.31) and set $\zeta_2' = \zeta$. Then,

$$
\begin{aligned}
4\left[N^2\right]_{,2} f &= (1-i\zeta_1)^2|\zeta|^4\frac{\partial^2 f}{\partial\rho^2} \\
&\quad -i(1-i\zeta_1)(1+\zeta_1^2)|\zeta|^2\frac{\partial^2 f}{\partial\rho\partial u} - \frac{1}{4}(1+\zeta_1^2)^2\frac{\partial^2 f}{\partial u^2}. \qquad (5.42)
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
4\left[N\overline{N}\right]_{,2} f &= |1-i\zeta_1|^2|\zeta|^2\left(\frac{\partial f}{\partial\rho} + |\zeta|^2\frac{\partial^2 f}{\partial\rho^2}\right) \\
&\quad -\frac{1}{2}i|\zeta|^2\left\{(1+\zeta_1^2)(1+i\overline{\zeta_1}) - (1+\overline{\zeta_1}^2)(1-i\zeta_1)\right\}\frac{\partial^2 f}{\partial\rho\partial u} \\
&\quad +\frac{1}{4}(1+\zeta_1^2)(1+\overline{\zeta_1}^2)\frac{\partial^2 f}{\partial u^2}, \qquad (5.43)
\end{aligned}
$$

and then

$$
\begin{aligned}
&4\left[N^2 + N\overline{N}\right]_{,2} f \\
&= \left\{(1-i\zeta_1)^2 + |1-i\zeta_1|^2\right\}|\zeta|^4\frac{\partial^2 f}{\partial\rho^2} \\
&\quad -\frac{1}{2}i|\zeta|^2\left\{(1+\zeta_1^2)(1+i\overline{\zeta_1}) - (1+\overline{\zeta_1}^2)(1-i\zeta_1) + 2(1-i\zeta_1)(1+\zeta_1^2)\right\}\frac{\partial^2 f}{\partial\rho\partial u} \\
&\quad -\frac{1}{4}\left\{(1+\zeta_1^2)^2 - (1+\zeta_1^2)(1+\overline{\zeta_1}^2)\right\}\frac{\partial^2 f}{\partial u^2} + |1-i\zeta_1|^2|\zeta|^2\frac{\partial f}{\partial\rho}.
\end{aligned}
$$

To this we add its complex conjugate which yields

$$
\begin{aligned}
8\mathrm{Re}\left[N^2+N\overline{N}\right]_{,2} f &= \left[(1-i\zeta_1) + (1+i\overline{\zeta_1})\right]^2|\zeta|^4\frac{\partial^2 f}{\partial\rho^2} \\
&\quad -i|\zeta|^2\left[(1+\zeta_1^2) - (1+\overline{\zeta_1}^2)\right]\left[1 - i\zeta_1 + 1 + i\overline{\zeta_1}\right]\frac{\partial^2 f}{\partial\rho\partial u} \\
&\quad -\frac{1}{4}\left[(1+\zeta_1^2) - (1+\overline{\zeta_1}^2)\right]^2\frac{\partial^2 f}{\partial u^2} + 2|1-i\zeta_1|^2|\zeta|^2\frac{\partial f}{\partial\rho} \\
&= 4\rho^2(1+\rho)^2\frac{\partial^2 f}{\partial\rho^2} + 8\rho^2(1+\rho)u\frac{\partial^2 f}{\partial\rho\partial u} + 4\rho^2u^2\frac{\partial^2 f}{\partial u^2} \\
&\quad +2\rho\left((1+\rho)^2 + u^2\right)\frac{\partial f}{\partial\rho}. \qquad (5.44)
\end{aligned}
$$

From (5.40),

$$\operatorname{Re}\left(N^2+N\overline{N}\right) = \frac{1}{2}\left(N+\overline{N}\right)^2, \tag{5.45}$$

so

$$\frac{1}{2}\left[\left(N+\overline{N}\right)^2\right]_{,2} f = \frac{1}{2}\rho^2(1+\rho)^2\frac{\partial^2 f}{\partial\rho^2}+\rho^2(1+\rho)u\frac{\partial^2 f}{\partial\rho\partial u} + \frac{1}{2}\rho^2u^2\frac{\partial^2 f}{\partial u^2}+\frac{1}{4}\rho\left((1+\rho)^2+u^2\right)\frac{\partial f}{\partial\rho}. \tag{5.46}$$

We might as well find the coefficients of $g''(x)$ just to make sure that we are on the right track. Set $f(\rho,u)=g(x)$ and replace the $(\rho,u)$-derivatives with the $x$-derivatives using the formulas between (5.36) and (5.37):

$$\begin{aligned}\frac{1}{2}\left[\left(N+\overline{N}\right)^2\right]_{,2} g = \rho^2\Bigg\{ & 2(1+\rho)^2\left(\frac{1-(x+1)(1+\rho)}{(1+\rho)^2+u^2}\right)^2\frac{d^2g}{dx^2} \\ & +(1+\rho)^2\left((x+1)^3-\frac{3(x+1)}{(1+\rho)^2+u^2}\right)\frac{dg}{dx} \\ & -2(1+\rho)\frac{1-(x+1)(1+\rho)}{(1+\rho)^2+u^2}\frac{2(x+1)u^2}{(1+\rho)^2+u^2}\frac{d^2g}{dx^2} \\ & +4(1+\rho)\left(\frac{(x+1)^2u^2}{(1+\rho)^2+u^2}-\frac{u^2}{\left((1+\rho)^2+u^2\right)^2}\right)\frac{dg}{dx} \\ & +\frac{2(x+1)^2u^4}{\left((1+\rho)^2+u^2\right)^2}\frac{d^2g}{dx^2} \\ & +u^2\left(\frac{3(x+1)}{(1+\rho)^2+u^2}-(x+1)^3\right)\frac{dg}{dx}\Bigg\} \\ & +\frac{1}{2}\rho\big(1-(x+1)(1+\rho)\big)\frac{dg}{dx}. \end{aligned} \tag{5.47}$$

We collect the coefficients of $d^2g/dx^2$:

$$\begin{aligned}&\frac{1}{2}\left[\left(N+\overline{N}\right)^2\right]_{,2} g \\ &= \frac{2\rho^2}{\left((1+\rho)^2+u^2\right)^2} \\ &\quad\cdot\Big\{(1+\rho)^2\big(1-(x+1)(1+\rho)\big)^2 \\ &\qquad -2(1+\rho)\big(1-(x+1)(1+\rho)\big)(x+1)u^2+(x+1)^2u^4\Big\}\frac{d^2g}{dx^2}+\cdots\end{aligned}$$

$$
\begin{aligned}
&= \frac{2\rho^2}{\big((1+\rho)^2+u^2\big)^2}\left[(1+\rho)\big(1-(x+1)(1+\rho)\big)-(x+1)u^2\right]^2\frac{d^2g}{dx^2}+\cdots \\
&= \frac{2\rho^2}{\big((1+\rho)^2+u^2\big)^2}\left[(1+\rho)-(x+1)\big((1+\rho)^2+u^2\big)\right]^2\frac{d^2g}{dx^2}+\cdots \\
&= \frac{2\rho^2(1+\rho)^2}{\big((1+\rho)^2+u^2\big)^2}\frac{d^2g}{dx^2}+\cdots\,, \qquad (5.48)
\end{aligned}
$$

where $\cdots$ denotes $dg/dx$ terms. Consequently, (5.37), (5.48) and (5.18) yield

$$
\begin{aligned}
\Delta_S\, g &= \Delta g-\frac{1}{2}\left(N+\overline{N}\right)^2 g-\frac{3}{2}\left(N+\overline{N}\right) g \\
&= \frac{2[\rho(1+\rho)^3+(1+\rho)u^2]-2\rho^2(1+\rho)^2}{\big((1+\rho)^2+u^2\big)^2}\frac{d^2g}{dx^2}+\cdots \\
&= \frac{2[\rho(1+\rho)^2+(1+\rho)u^2]}{\big((1+\rho)^2+u^2\big)^2}\frac{d^2g}{dx^2}+\cdots\,, \qquad (5.49)
\end{aligned}
$$

where we set $r=1$. Now

$$
\begin{aligned}
&4\rho(1+\rho)^2+4(1+\rho)u^2 \\
&= \left[(1+\rho)^4-(1-\rho^2)^2\right]+2u^2\left[(1+\rho)^2+(1-\rho^2)\right] \\
&= \left[\big((1+\rho)^2+u^2\big)-\big(1-\rho^2-u^2\big)\right]\left[\big((1+\rho)^2+u^2\big)+\big(1-\rho^2-u^2\big)\right] \\
&= \big((1+\rho)^2+u^2\big)^2-\big(1-\rho^2-u^2\big)^2, \qquad (5.50)
\end{aligned}
$$

so,

$$
\Delta_S\, g=\frac{1}{2}(1-x^2)\frac{d^2g}{dx^2}+\cdots\,, \qquad (5.51)
$$

as expected.

2) To find the coefficient of $dg/dx$ start with

$$
\frac{1}{2}\left[\left(N+\overline{N}\right)^2\right]_{,1}=\mathrm{Re}\left[N^2+N\overline{N}\right]_{,1}\,. \qquad (5.52)
$$

We use (5.39) in the form

$$
N=\frac{(1-i\zeta_1)\zeta_2}{2r}\frac{\partial}{\partial\zeta_2}-i\frac{1+\zeta_1^2}{2r}\frac{\partial}{\partial\zeta_1}\,, \qquad (5.53)
$$

and note that $Nr = \overline{N}r = 1/2$. Then

$$\begin{aligned}\left[N^2\right]_{,1} &= N\left(\frac{(1-i\zeta_1)\zeta_2}{2r}\right)\frac{\partial}{\partial\zeta_2} - iN\left(\frac{1+\zeta_1^2}{2r}\right)\frac{\partial}{\partial\zeta_1} \\ &= -\frac{(1-i\zeta_1)(1+2i\zeta_1)}{4r^2}\left\{\zeta_2\frac{\partial}{\partial\zeta_2} - i(1+i\zeta_1)\frac{\partial}{\partial\zeta_1}\right\}. \qquad (5.54)\end{aligned}$$

Similarly,

$$\left[N\overline{N}\right]_{,1} = -\frac{1+i\overline{\zeta_1}}{4r^2}\left\{\overline{\zeta_2}\frac{\partial}{\partial\overline{\zeta_2}} + i(1-i\overline{\zeta_1})\frac{\partial}{\partial\overline{\zeta_1}}\right\}. \qquad (5.55)$$

In tangential coordinates, (5.30), (5.31), one has

$$4\left[N^2\right]_{,1} = -(1-i\zeta_1)(1+2i\zeta_1)\left\{\zeta\frac{\partial}{\partial\zeta} - i(1+i\zeta_1)\frac{1}{2}\frac{\partial}{\partial u}\right\}; \qquad (5.56)$$

after dropping $\partial/\partial\sigma$ and setting $r = 1$. Also

$$4\left[N\overline{N}\right]_{,1} = -(1+i\overline{\zeta_1})\left\{\overline{\zeta}\frac{\partial}{\partial\overline{\zeta}} + i\left(1-i\overline{\zeta_1}\right)\frac{1}{2}\frac{\partial}{\partial u}\right\}, \qquad (5.57)$$

and

$$\begin{aligned}&4\left[N^2+N\overline{N}\right]_{,1} \\ &= -(1-i\zeta_1)(1+2i\zeta_1)\zeta\frac{\partial}{\partial\zeta} - (1+i\overline{\zeta_1})\overline{\zeta}\frac{\partial}{\partial\overline{\zeta}} \\ &\quad + \frac{1}{2}i\{(1-i\zeta_1)(1+i\zeta_1)(1+2i\zeta_1) - (1+i\overline{\zeta_1})(1-i\overline{\zeta_1})\}\frac{\partial}{\partial u}. \qquad (5.58)\end{aligned}$$

Working with (5.58),

$$\begin{aligned}\{\cdots\} &= (1+\rho-iu)(1-\rho+iu)(1-2\rho+2iu) - (1+\rho+iu)(1-\rho-iu) \\ &= 2\rho(\rho^2-1-3u^2) + i2u(1+2\rho-3\rho^2+u^2), \qquad (5.59)\end{aligned}$$

and the rest of (5.58) applied to $f(|\zeta|^2, u)$ yields

$$\begin{aligned}&-(1-i\zeta_1)(1+2i\zeta_1)\zeta\frac{\partial f}{\partial\zeta} - \left(1+i\overline{\zeta_1}\right)\overline{\zeta}\frac{\partial f}{\partial\overline{\zeta}} \\ &= -\rho\left\{(1+\rho-iu)(1-2\rho+2iu) + (1+\rho+iu)\right\}\frac{\partial f}{\partial\rho} \\ &= \left\{2\rho(\rho^2-1-u^2) - i2\rho u(1+2\rho)\right\}\frac{\partial f}{\partial\rho}. \qquad (5.60)\end{aligned}$$

Hence, (5.58), (5.59) and (5.60) give

$$\begin{aligned}\frac{1}{2}\left[\left(N+\overline{N}\right)^2\right]_{,1} f &= \mathrm{Re}\left[N^2+N\overline{N}\,\right]_{,1} f \\ &= \frac{1}{2}\rho(\rho^2-1-u^2)\frac{\partial f}{\partial\rho}+\frac{1}{4}u(3\rho^2-2\rho-1-u^2)\frac{\partial f}{\partial u}. \quad (5.61)\end{aligned}$$

To find $\left(N+\overline{N}\right) f$ we introduce tangential coordinates in (5.53), drop $\partial/\partial\sigma$ and set $r=1$. Then

$$\begin{aligned}&\left(N+\overline{N}\right) f \\ &= \frac{1}{2}\left\{(1-i\zeta_1)\zeta\frac{\partial f}{\partial\zeta}+(1+i\overline{\zeta_1})\overline{\zeta}\frac{\partial f}{\partial\overline{\zeta}}-i(1+\zeta_1^2)\frac{1}{2}\frac{\partial f}{\partial u}+i(1+\overline{\zeta_1}^2)\frac{1}{2}\frac{\partial f}{\partial u}\right\} \\ &= \rho(1+\rho)\frac{\partial f}{\partial\rho}+\rho u\frac{\partial f}{\partial u}\,. \quad (5.62)\end{aligned}$$

Collecting all the first order $(\rho,u)$-derivatives, including the one in (5.46), one has

$$\begin{aligned}c_1 &= \frac{1}{2}\left[\left(N+\overline{N}\right)^2\right]_{,1} f+\frac{3}{2}\left(N+\overline{N}\right) f+\frac{1}{4}\rho\left((1+\rho)^2+u^2\right)\frac{\partial f}{\partial\rho} \\ &= \frac{1}{4}\rho\left(3(1+\rho)^2+2(1+\rho)-u^2\right)\frac{\partial f}{\partial\rho}+\frac{1}{4}u(3\rho^2+4\rho-1-u^2)\frac{\partial f}{\partial u}, \quad (5.63)\end{aligned}$$

and setting $f(\rho,u)=g(x)$ one finds

$$\begin{aligned}c_1 = \frac{1}{2\left((1+\rho)^2+u^2\right)}&\left\{\left(3\rho(1+\rho)^2+2\rho(1+\rho)-\rho u^2\right)\left(1-(1+\rho)(x+1)\right)\right. \\ &\left.-(3\rho^2+4\rho-1-u^2)(x+1)u^2\right\}\frac{dg}{dx}\,. \quad (5.64)\end{aligned}$$

We simplify this:

$$\begin{aligned}\{\cdots\} &= 3\rho(1+\rho)^2-2\rho(1+\rho)-\rho u^2 \\ &\quad +\left(-3\rho(1+\rho)^3-2\rho^2u^2-\rho u^2+u^2+u^4\right)(x+1) \\ &= 3\rho(1+\rho)^2-2\rho(1+\rho)-\rho u^2+(x+1)\big[-2\rho(1+\rho)^2 \\ &\quad -(\rho+2\rho^2)\left((1+\rho)^2+u^2\right)-\rho^2(1+\rho)^2+u^2+u^4\big] \\ &= 3\rho(1+\rho)^2-4\rho(1+\rho)-\rho u^2-4\rho^2(1+\rho) \\ &\quad +(x+1)\big[u^2+u^4-(2\rho+\rho^2)(1+\rho)^2\big] \\ &= -\rho\left((1+\rho)^2+u^2\right)+2(1+\rho)-(x+1)\left((1+\rho)^4-u^4\right)\end{aligned}$$

$$= -\rho\left((1+\rho)^2+u^2\right)+2(1+\rho)-2(1+\rho)\left((1+\rho)^2-u^2\right),$$

so,

$$c_1 = \left(\frac{(1+\rho)(1+u^2-(1+\rho)^2)}{(1+\rho)^2+u^2}-\frac{1}{2}\rho\right)\frac{dg}{dx}. \tag{5.65}$$

$c_1$ does not include all the first order $x$-derivatives of $g$ in

$$\Delta g-\frac{1}{r^2}\Delta_S\, g=\frac{1}{2}\left[(N+\overline{N})^2+\frac{3}{r}(N+\overline{N})\right]g,$$

see (5.18). There are 3 more such terms which come from the second order $(\rho, u)$-derivatives of $g$ in (5.47). We collect these in

$$\frac{\rho^2}{(1+\rho)^2+u^2}\{2(1+\rho)(x+1)^2((1+\rho)^2+u^2)-3(x+1)(1+\rho)^2+(x+1)u^2\}$$
$$=\frac{2\rho^2(1+\rho)}{(1+\rho)^2+u^2}.$$

Adding this to $c_1$ yields

$$\left(\frac{(1+\rho)(\rho^2+u^2-2\rho)}{(1+\rho)^2+u^2}-\frac{1}{2}\rho\right)\frac{dg}{dx}. \tag{5.66}$$

To find the coefficient of $dg/dx$ in $\Delta_S$ we subtract the coefficient in (5.66) from the coefficient of $dg/dx$ in (5.38), as in (5.18), and find

$$\begin{aligned}
&\frac{5}{2}+\rho-\frac{(1+\rho)(4+4\rho+\rho^2+u^2-2\rho)}{(1+\rho)^2+u^2}\\
&= \frac{5}{2}+\rho-\frac{(1+\rho)\big((1+\rho)^2+u^2+3\big)}{(1+\rho)^2+u^2}\\
&= \frac{3}{2}\left[1-\frac{2(1+\rho)}{(1+\rho)^2+u^2}\right]\\
&= -\frac{3}{2}x,
\end{aligned} \tag{5.67}$$

and we have completed the derivation of Lemma 9. □

Finally, the combination of Lemma 9 and the Cayley transform implies

**Theorem 10.** *The heat kernel $p_S$ of $\Delta_S$ on $b\mathscr{D}_2$ is given by*

$$p_S = \frac{e^{\frac{1}{2}t}}{(2\pi t)^{3/2}} e^{-\frac{\gamma^2}{2t}} \frac{\gamma}{\sin\gamma}, \tag{5.68}$$

*where*

$$\gamma = \cos^{-1} x = \cos^{-1} \frac{1-\rho^2-u^2}{(1+\rho)^2+u^2}, \tag{5.69}$$

*and*

$$\sin\gamma = \frac{2\sqrt{(1+\rho)\,(\rho(1+\rho)+u^2)}}{(1+\rho)^2+u^2}. \tag{5.70}$$

One notes that the higher dimensional heat kernels can be obtained by differentiating (5.68). Also, (5.68) is the heat kernel from the origin. Given two arbitrary points, $p_S$ has the form (5.68) after moving the origin to one of the given points by the Cayley transform of the appropriate element of the Euclidean rotation group.


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