GENERALIZED HAMILTON-JACOBI EQUATION AND HEAT KERNEL ON STEP TWO NILPOTENT LIE GROUPS

OVIDIU CALIN, DER-CHEN CHANG, IRINA MARKINA

Abstract. We study geometrically invariant formulas for heat kernels of sub-elliptic differential operators on two step nilpotent Lie groups and for the Grusin operator in $\mathbb{R}^2$. We deduce a general form of the solution to the Hamilton-Jacobi equation and its generalized form in $\mathbb{R}^n \times \mathbb{R}^m$. Using our results, we obtain explicit formulas of the heat kernels for these differential operators.

1. Introduction

Let us start with the Laplace operator on $\mathbb{R}^n$,

$$\Delta = \frac{1}{2}\sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2}.$$

It is well-known that the heat kernel for Δ is the Gaussian:

$$P_t(\mathbf{x}, \mathbf{x}_0) = \frac{1}{(2\pi t)^{\frac{n}{2}}} e^{-\frac{|\mathbf{x}-\mathbf{x}_0|^2}{2t}}.$$

Given a general second order elliptic operator in n dimensional Euclidean space,

$$\Delta_X = \frac{1}{2}\sum_{j=1}^{n} X_j^2 + \text{lower order term},$$

where the $\{X_1, \dots, X_n\}$ is a linearly independent set of vector fields, the heat kernel takes the form

$$P_t(\mathbf{x}, \mathbf{x}_0) = \frac{1}{(2\pi t)^{\frac{n}{2}}} e^{-\frac{d^2(\mathbf{x},\mathbf{x}_0)}{2t}} \big(a_0 + a_1 t + a_2 t^2 + \cdots\big).$$

Here $d(\mathbf{x}, \mathbf{x}_0)$ stands for the Riemannian distance between $\mathbf{x}$ and $\mathbf{x}_0$ if the metric is induced by the orthonormal basis $\{X_1, \dots, X_n\}$. The a_j's are functions of $\mathbf{x}$ and $\mathbf{x}_0$. Note that

$$\frac{\partial}{\partial t}\Big(\frac{d^2}{2t}\Big) + \frac{1}{2}\sum_{j=1}^{n}\Big(X_j \frac{d^2}{2t}\Big)^2 = 0,$$

i.e., $\frac{d^2}{2t}$ is a solution of the Hamilton-Jacobi equation.

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Now let us move to subelliptic operators. We first consider the famous example: Heisenberg sub-Laplacian on $\mathbb{H}_1$

$$\Delta_X = \frac{1}{2}\Big(\frac{\partial}{\partial x_1} + 2x_2\frac{\partial}{\partial y}\Big)^2 + \frac{1}{2}\Big(\frac{\partial}{\partial x_2} - 2x_1\frac{\partial}{\partial y}\Big)^2. \tag{1.1}$$

We shall try for a heat kernel in the form

$$\frac{1}{t^q}e^{-\frac{f}{t}}\cdots$$

where $h = \frac{f}{t}$ is a solution of the Hamilton-Jacobi equation

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

In other words,

$$\frac{\partial h}{\partial t} + H(\mathbf{x}, \nabla h) = 0, \tag{1.2}$$

where

$$H = \frac{1}{2}\Big[\big(\xi_1 + 2x_2\eta\big)^2 + \big(\xi_2 - 2x_1\eta\big)^2\Big] = \frac{1}{2}\big[\zeta_1^2 + \zeta_2^2\big] \tag{1.3}$$

is the Hamilton function associated with the sub-elliptic operator (1.1) and ξ_1, ξ_2 and η are dual variable to x_1, x_2 and y respectively. Using the Lagrange-Chapit method, let us look at the following equation:

$$F(\mathbf{x}, y, t, h, \xi, \eta, \gamma) = \gamma + H(\mathbf{x}, y, \xi, \eta) = 0.$$

We shall find the bicharacteristic curves which are solutions to the following Hamilton system:

$$\begin{aligned}
\dot{x}_1 &= F_{\xi_1} = \xi_1 + 2x_2\eta = \zeta_1,\\
\dot{x}_2 &= F_{\xi_2} = \xi_2 - 2x_1\eta = \zeta_2,\\
\dot{y} &= F_\eta = 2\dot{x}_1x_2 - 2x_1\dot{x}_2,\\
\dot{t} &= F_\gamma = 1,\\
\dot{\xi}_1 &= -F_{x_1} - \xi_1F_h = 2\eta\dot{x}_2,\\
\dot{\xi}_2 &= -F_{x_2} - \xi_2F_h = -2\eta\dot{x}_1,\\
\dot{\eta} &= -F_y - \gamma F_h = 0,\\
\dot{\gamma} &= -F_t - \gamma F_h = 0,\\
\dot{h} &= \xi\cdot\nabla_\xi F + \eta F_\eta + \gamma F_\gamma = \xi\cdot\dot{x} + \eta\dot{y} - H
\end{aligned}$$

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

$$\begin{aligned}
\gamma(s) &= \gamma = \text{constant},\\
\eta(s) &= \eta = \text{constant},\\
t(s) &= s.
\end{aligned}$$

Here "constant" means "*constant along the bicharacteristic curve*". Furthermore,

$$H = \frac{1}{2}\dot{x}_1^2 + \frac{1}{2}\dot{x}_2^2 = E = \text{energy}.$$

Another way to see that E is constant along the bicharacteristic, note that

$$\begin{aligned}
\ddot{x}_1 &= \dot{\xi}_1 + 2\eta\dot{x}_2 = +4\eta\dot{x}_2,\\
\ddot{x}_2 &= \dot{\xi}_2 - 2\eta\dot{x}_1 = -4\eta\dot{x}_1.
\end{aligned} \tag{1.4}$$

Therefore, $\ddot{x}_1\dot{x}_1 + \ddot{x}_2\dot{x}_2 = 0$, and E =constant.

We need to find the classical action integral

$$S(t) = \int_0^t \big(\xi \cdot \dot{\mathbf{x}} + \eta\dot{y} - H\big)ds.$$

Let find ξ and $\mathbf{x}$ from the Hamilton system. We obtain

$$\dddot{x}_1 + 16\eta^2\dot{x}_1 = 0, \quad \dddot{x}_2 + 16\eta^2\dot{x}_2 = 0$$

from (1.4). Hence

$$\begin{aligned}\dot{x}_1(s) =& \dot{x}_1(0)\cos(4\eta s) + \frac{\ddot{x}_1(0)}{4\eta}\sin(4\eta s)\\ =& \dot{x}_1(0)\cos(4\eta s) + \dot{x}_2(0)\sin(4\eta s)\\ =& \zeta_1(0)\cos(4\eta s) + \zeta_2(0)\sin(4\eta s)\end{aligned} \tag{1.5}$$

and

$$\begin{aligned}\dot{x}_2(s) =& \dot{x}_2(0)\cos(4\eta s) + \frac{\ddot{x}_2(0)}{4\eta}\sin(4\eta s)\\ =& \dot{x}_2(0)\cos(4\eta s) - \dot{x}_1(0)\sin(4\eta s)\\ =& -\zeta_1(0)\sin(4\eta s) + \zeta_2(0)\cos(4\eta s),\end{aligned} \tag{1.6}$$

which yields

$$x_1(s) = x_1(0) + \zeta_1(0)\frac{\sin(4\eta s)}{4\eta} + \zeta_2(0)\frac{1-\cos(4\eta s)}{4\eta} \tag{1.7}$$

and

$$x_2(s) = x_2(0) - \zeta_1(0)\frac{1-\cos(4\eta s)}{4\eta} + \zeta_2(0)\frac{\sin(4\eta s)}{4\eta}. \tag{1.8}$$

At $s = t$ one has $x_1(t) = x_1$ and $x_2(t) = x_2$, so

$$\begin{aligned}\frac{1}{2}\zeta_1(0)\sin(4\eta t) + \frac{1}{2}\zeta_2(0)\big(1-\cos(4\eta t)\big) &= 2\eta\big(x_1 - x_1(0)\big),\\ -\frac{1}{2}\zeta_1(0)\big(1-\cos(4\eta t)\big) + \frac{1}{2}\zeta_2(0)\sin(4\eta t) &= 2\eta\big(x_2 - x_2(0)\big),\end{aligned}$$

or,

$$\begin{aligned}+\zeta_1(0)\cos(2\eta t) + \zeta_2(0)\sin(2\eta t) &= \frac{2\eta\big(x_1 - x_1(0)\big)}{\sin(2\eta t)},\\ -\zeta_1(0)\sin(2\eta t) + \zeta_2(0)\cos(2\eta t) &= \frac{2\eta\big(x_2 - x_2(0)\big)}{\sin(2\eta t)}.\end{aligned} \tag{1.9}$$

Hamilton's equations give

$$\begin{aligned}\xi_2(s) =& -2\eta x_1(s) + \big(\xi_2(0) + 2\eta x_1(0)\big)\\ =& -2\eta x_1(0) - \frac{1}{2}\zeta_1(0)\sin(4\eta s) - \frac{1}{2}\zeta_2(0)\big(1-\cos(4\eta s)\big) + \zeta_2(0) + 4\eta x_1(0)\\ =& 2\eta x_1(0) - \frac{1}{2}\Big[\zeta_1(0)\sin(4\eta s) - \zeta_2(0)\big(1+\cos(4\eta s)\big)\Big],\end{aligned}$$

and

$$\xi_1(s) = -2\eta x_2(0) + \frac{1}{2}\Big[\zeta_1(0)\big(1+\cos(4\eta s)\big) + \zeta_2(0)\sin(4\eta s)\Big].$$

The above calculations imply

$$\begin{aligned}\xi_1\dot{x}_1+\xi_2\dot{x}_2 =& -2\eta\dot{x}_1(s)x_2(0)+2\eta x_1(0)\dot{x}_2(s)+\frac{1}{2}\big(\zeta_1^2(0)+\zeta_2^2(0)\big)\big(1+\cos(4\eta s)\big)\\ =& -2\eta\big(\dot{x}_1(s)x_2(0)-x_1(0)\dot{x}_2(s)\big)+\big(1+\cos(4\eta s)\big)E,\end{aligned}$$

and

$$\int_0^t \big(\xi\cdot\dot{\mathbf{x}}+\eta\dot{y}-H\big)ds=\eta\Big[y-y(0)+2\big(x_1(0)x_2-x_1x_2(0)\big)+\frac{\sin(4\eta t)}{4\eta^2}E\Big].$$

To find E we square and add the two equations in (1.9),

$$E=\frac{1}{2}\zeta_1^2(0)+\frac{1}{2}\zeta_2^2(0)=2\eta^2\frac{|\mathbf{x}-\mathbf{x}_0|^2}{\sin^2(2\eta t)}.$$

Hence,

$$\begin{aligned}S(t)=&\int_0^t \big(\xi\cdot\dot{\mathbf{x}}+\eta\dot{y}-H\big)ds\\ =&\eta\Big[y-y(0)+2\big(x_1(0)x_2-x_1x_2(0)\big)+|\mathbf{x}-\mathbf{x}_0|^2\cot(2\eta t)\Big].\end{aligned}$$

We note that $\mathbf{x}$, y, t, $\mathbf{x}_0$ and $\eta=\eta(0)$ are free parameters while $y(0)=y(0;\mathbf{x},\mathbf{x}_0,y,\eta;t)$ is not. Therefore, we need to introduce one more free variable $h(0)$ such that $h(t)=h(0)+S(t)$ is a solution of the Hamilton-Jacobi equation (1.2).

It reduces to find $h(0)$. To find it we shall substitute S into (1.2). Straightforward computation shows that

$$\frac{\partial h}{\partial t}+H(\mathbf{x},y,\xi(t),\eta(t))=0$$

where

$$h(t)=\eta(0)y(0)+S(t),\quad \textit{i.e.},\quad h(0)=\eta(0)y(0). \tag{1.10}$$

This yields

$$\frac{\partial h}{\partial t}+H\Big(\mathbf{x},y,\nabla_{\mathbf{x}}h,\frac{\partial h}{\partial y}\Big)=0.$$

We have the following theorem.

Theorem 1.1. *We have shown that*

$$\begin{aligned}h=&\eta(0)y(0)+\int_0^t \big(\xi\cdot\dot{\mathbf{x}}+\eta\dot{y}-H\big)ds\\ =&\eta y+2\eta\big(x_1(0)x_2-x_1x_2(0)\big)+\eta|\mathbf{x}-\mathbf{x}_0|^2\cot(2\eta t)\end{aligned} \tag{1.11}$$

is a "complete integral" of (1.2) *and* (1.3)*, i.e., a solution of* (1.2) *and* (1.3) *which depends on* 3 *free parameters* $x_1(0)$, $x_2(0)$ *and* η.

Before we move further, let us consider a more general situation.

2. Generalized Hamilton-Jacobi equations

In this section we study the Hamilton-Jacobi equation which is crucial in the construction of the heat kernel associated with elliptic and sub-elliptic operators. We deduce a general form of the solution to the Hamilton-Jacobi equation and its generalized form. We consider an $(n+m)$-dimensional space $\mathbb{R}^n \times \mathbb{R}^m$. The coordinates are denoted $\mathbf{x} = (x_1, \dots, x_n) \in \mathbb{R}^n$ and $\mathbf{y} = (y_1, \dots, y_m) \in \mathbb{R}^m$ with dual variables $(\xi_1, \dots, \xi_n)$ and $(\eta_1, \dots, \eta_m)$ respectively. The roman indices $i, j, k, \dots$ will vary from 1 to n and the Greek indices $\alpha, \beta, \dots$ will vary from 1 to m. As usual, the Hamiltonian function $H(\mathbf{x}, \mathbf{y}, \xi, \eta)$ is a homogeneous polynomial of degree 2 in the variables (ξ, η) and has smooth coefficients in $(\mathbf{x}, \mathbf{y})$.

We have the following nice generalizaition of a result from [11].

Theorem 2.1. *Set*

$$h(t; \mathbf{x}, \mathbf{y}, \xi, \eta) = \sum_{\alpha=1}^{m} \eta_\alpha(0) y_\alpha(0) + S(t; \mathbf{x}, \mathbf{y}, \xi, \eta) \tag{2.1}$$

where

$$x_j = x_j(s; \mathbf{x}, \mathbf{y}, \xi, \eta; t), \quad j = 1, \dots, n; \qquad y_\alpha = y_\alpha(s; \mathbf{x}, \mathbf{y}, \xi, \eta; t), \quad \alpha = 1, \dots, m$$

and

$$S(t; \mathbf{x}, \mathbf{y}, \xi, \eta) = \int_0^t \Big(\xi(u) \cdot \dot{\mathbf{x}}(u) + \eta(u) \cdot \dot{\mathbf{y}}(u) - H(\mathbf{x}(u), \mathbf{y}(u), \xi(u), \eta(u)) \Big) du.$$

Then h satisfies the usual Hamilton-Jacobi equation:

$$\frac{\partial h}{\partial t} + H\Big(\mathbf{x}, \mathbf{y}, \nabla_{\mathbf{x}} h, \nabla_{\mathbf{y}} h\Big) = 0.$$

Proof. In order to prove the theorem, we first calculate the partial derivatives of the function S with respect to all variables explicitly. For $j = 1, \dots, n$,

$$\begin{aligned}
&\frac{\partial S}{\partial x_j}(t; \mathbf{x}, \mathbf{y}, \xi, \eta) \\
&= \int_0^t \Big[\sum_{k=1}^{n} \big(\frac{\partial \xi_k}{\partial x_j} \frac{dx_j}{ds} + \xi_k \frac{d}{ds} \frac{\partial x_k(s; \mathbf{x}, \mathbf{y}, \xi, \eta; t)}{\partial x_j} \big) + \sum_{\alpha=1}^{m} \big(\frac{\partial \eta_\alpha}{\partial x_j} \frac{dy_\alpha}{ds} + \eta_\alpha \frac{d}{ds} \frac{\partial y_\alpha(s; \mathbf{x}, \cdots; t)}{\partial x_j} \big) \\
&\quad - \sum_{k=1}^{n} \frac{\partial H}{\partial \xi_k} \frac{\partial \xi_k}{\partial x_j} - \sum_{\alpha=1}^{m} \frac{\partial H}{\partial \eta_\alpha} \frac{\partial \eta_\alpha}{\partial x_j} \\
&\quad - \sum_{k=1}^{n} \frac{\partial H}{\partial x_k} \frac{\partial x_k(s; \mathbf{x}, \mathbf{y}, \xi, \eta; t)}{\partial x_j} - \sum_{\alpha=1}^{m} \frac{\partial H}{\partial y_\alpha} \frac{\partial y_\alpha(s; \mathbf{x}, \mathbf{y}, \xi, \eta; t)}{\partial x_j} \Big] ds \\
&= \int_0^t \frac{d}{ds} \Big(\sum_{k=1}^{n} \xi_k \frac{\partial x_k(s; \mathbf{x}, \mathbf{y}, \xi, \eta; t)}{\partial x_j} + \sum_{\alpha=1}^{m} \eta_\alpha \frac{\partial y_\alpha(s; \mathbf{x}, \mathbf{y}, \xi, \eta; t)}{\partial x_j} \Big) ds \\
&= \sum_{k=1}^{n} \xi_k(s) \frac{\partial x_k(s; \mathbf{x}, \mathbf{y}, \xi, \eta; t)}{\partial x_j} \Big|_{s=0}^{s=t} + \sum_{\alpha=1}^{m} \eta_\alpha(s) \frac{\partial y_\alpha(s; \mathbf{x}, \mathbf{y}, \xi, \eta; t)}{\partial x_j} \Big|_{s=0}^{s=t}.
\end{aligned}$$

It follows that

$$\frac{\partial S}{\partial x_j}(t; \mathbf{x}, \mathbf{y}, \xi, \eta) = \xi_j(t) - \sum_{\alpha=1}^{m} \eta_\alpha(0) \frac{\partial y_\alpha(0; \mathbf{x}, \mathbf{y}, \xi, \eta; t)}{\partial x_j}.$$

Similarly, for $\beta = 1, \dots, m$,

$$\frac{\partial S}{\partial y_\beta}(t; \mathbf{x}, \mathbf{y}, \xi, \eta) = \eta_\beta(t) - \sum_{\alpha=1}^{m} \eta_\alpha(0) \frac{\partial y_\alpha(0; \mathbf{x}, \mathbf{y}, \xi, \eta; t)}{\partial y_\beta}.$$

Moreover,

$$\begin{aligned} \frac{\partial S}{\partial t}(t; \cdots) = & \sum_{k=1}^{n} \xi_k(t; \cdots)\dot{x}_k(t; \cdots) + \sum_{\alpha=1}^{m} \eta_\alpha(t; \cdots)\dot{y}_\alpha(t; \cdots) - H\big(\mathbf{x}, \mathbf{y}, \xi(t; \cdots), \eta(t; \cdots)\big) \\ & + \sum_{k=1}^{n} \xi_k(s; \cdots) \frac{\partial x_k(s; \cdots)}{\partial t}\Big|_{s=0}^{s=t} + \sum_{\alpha=1}^{m} \eta_\alpha(s; \cdots) \frac{\partial y_\alpha(s; \cdots)}{\partial t}\Big|_{s=0}^{s=t}. \end{aligned}$$

Differentiating $x_1 = x_1(t; \mathbf{x}, \mathbf{y}, \xi, \eta; t)$ yields

$$0 = \frac{d}{dt} x_1(t; \mathbf{x}, \mathbf{y}, \xi, \eta; t) = \dot{x}_1(t; \cdots) + \frac{\partial x_1(s; \mathbf{x}, \mathbf{y}, \xi, \eta; t)}{\partial t}\Big|_{s=t}.$$

On the other hand, one has

$$\xi_k(s; \cdots) \frac{\partial x_k(s; \cdots)}{\partial t}\Big|_{s=0}^{s=t} = -\xi_k(t; \cdots)\dot{x}_k(t; \cdots), \qquad k = 1, \dots, n,$$

and

$$\eta_\alpha(s; \cdots) \frac{\partial y_\alpha(s; \cdots)}{\partial t}\Big|_{s=0}^{s=t} = -\eta_\alpha(t; \cdots)\dot{y}_\alpha(t; \cdots) - \eta_\alpha(0; \cdots) \frac{\partial y_\alpha(0; \cdots)}{\partial t}, \qquad \alpha = 1, \dots, n,$$

therefore,

$$\frac{\partial S}{\partial t} = -H(t; \cdots) - \sum_{\alpha=1}^{m} \eta_\alpha(0; \cdots) \frac{\partial y_\alpha(0; \cdots)}{\partial t}.$$

It follows that if we set as in the statement of the theorem

$$h(t; \mathbf{x}, \mathbf{y}, \xi, \eta) = \sum_{\alpha=1}^{m} \eta_\alpha(0) y_\alpha(0) + S(t; \mathbf{x}, \mathbf{y}, \xi, \eta),$$

then it satisfies

$$\begin{aligned} \frac{\partial h}{\partial x_k} &= \xi_k(t; \mathbf{x}, \mathbf{y}, \xi, \eta; t), \qquad k = 1, \dots, n \\ \frac{\partial h}{\partial y_\alpha} &= \eta_\alpha(t; \mathbf{x}, \mathbf{y}, \xi, \eta; t), \qquad \alpha = 1, \dots, m, \end{aligned}$$

and

$$\frac{\partial h}{\partial t} + H\Big(\mathbf{x}, \mathbf{y}, \xi(t), \eta(t)\Big) = 0 \quad \Rightarrow \quad \frac{\partial h}{\partial t} + H\Big(\mathbf{x}, \mathbf{y}, \nabla_{\mathbf{x}} h, \nabla_{\mathbf{y}} h\Big) = 0.$$

This completes the proof of the theorem. □

We note that the derivation that (2.1) satisfies the Hamilton-Jacobi equation was complete general, not restriction to $H\Big(\mathbf{x}, \mathbf{y}, \nabla_{\mathbf{x}} h, \nabla_{\mathbf{y}} h\Big)$ being (1.3). In particular we did not assume that $\eta_\alpha(s)$ =constant for $\alpha = 1, \dots, m$. The action integral S is not a solution of the Hamilton-Jacobi equation because some of our free parameters are dual variables $\eta_\alpha(0)$ instead of $y_\alpha(0)$. For the Heisenberg sub-Laplacian or the Grusin operator, $\eta(0) = \eta$ cannot be switched to $y(0)$. As we know, $\dot{y} = 2(\dot{x}_1 x_2 - x_1 \dot{x}_2)$. From (1.5) – (1.8), one has

$$\dot{y} = 2\Big[\dot{x}_1 x_2(0) - x_1(0)\dot{x}_2 + \frac{1}{2}\big(\zeta_1^2(0) + \zeta_2^2(0)\big)\frac{1 - \cos(4\eta s)}{2\eta}\Big],$$

and

$$y(s) = 2\big(x_1(s)x_2(0) - x_1(0)x_2(s)\big) + \frac{E}{4\eta^2}\big(4\eta s - \sin(4\eta s)\big) + C.$$

At $s = t$, one has $x_1(t) = x_1$, $x_2(t) = x_2$ and

$$y = 2\big(x_1x_2(0) - x_1(0)x_2\big) + \frac{E}{4\eta^2}\big(4\eta t - \sin(4\eta t)\big) + C.$$

Hence, one has

$$\begin{aligned} y(s) =& y - 2\Big[\big(x_1 - x_1(s)\big)x_2(0) - x_1(0)\big(x_2 - x_2(s)\big)\Big] \\ &- \frac{E}{4\eta^2}\big[4\eta(t-s) - (\sin(4\eta t) - \sin(4\eta s))\big]. \end{aligned}$$

At $s = 0$,

$$y(0) = y + 2\big(x_1(0)x_2 - x_1x_2(0)\big) + |\mathbf{x} - \mathbf{x}_0|^2\mu(2\eta t),$$

where we set

$$\mu(\phi) = \frac{\phi}{\sin^2\phi} - \cot\,\phi.$$

To replace η by $y(0)$, one needs to invert μ,

$$\mu(2\eta t) = \frac{y - y(0) + 2\big(x_1(0)x_2 - x_1x_2(0)\big)}{|\mathbf{x} - \mathbf{x}_0|^2}.$$

This is impossible since for most of the values on the right hand side μ^{-1} is a many valued function [2]. Therefore we must leave η as one of the free parameters which does not permit S to be a solution of the Hamilton-Jacobi equation.

Before we go further, we present a scaling property of the solution to the Hamiltonian system

$$\frac{dx_j}{ds} = \frac{\partial H}{\partial \xi_j}, \quad \frac{dy_\alpha}{ds} = \frac{\partial H}{\partial \eta_\alpha}, \quad \frac{d\xi_j}{ds} = -\frac{\partial H}{\partial x_j}, \quad \frac{d\eta_\alpha}{ds} = -\frac{\partial H}{\partial y_\alpha},$$

$s \in [0, t]$ with the boundary conditions

$$\mathbf{x}(0) = \mathbf{x}_0, \quad \mathbf{x}(t) = \mathbf{x}, \quad \mathbf{y}(t) = \mathbf{y}, \quad \eta(0) = \eta(0).$$

Lemma 2.1. *One has the following scaling property*

$$\begin{aligned} x_j(s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \eta(0); t) =& x_j\big(\lambda s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big), \;\; j = 1, \dots, n \\ y_\alpha(s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \eta(0); t) =& y_\alpha\big(\lambda s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big), \;\; \alpha = 1, \dots, m \\ \xi_j(s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \eta(0); t) =& \lambda\xi_j\big(\lambda s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big), \;\; j = 1, \dots, n \\ \eta_\alpha(s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \eta(0); t) =& \lambda\eta_\alpha\big(\lambda s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big), \;\; \alpha = 1, \dots, m \end{aligned} \tag{2.2}$$

for $\lambda > 0$, if the two sides of (2.2) *stays in the domain of unique solvability of the Hamiltonian system.*

Proof. Denote the curve on the right-hand side of (2.2) by $\{\tilde{\mathbf{x}}(s), \tilde{\mathbf{y}}(s), \tilde{\xi}(s), \tilde{\eta}(s)\}$. Note that $s \in (0,t)$. Then for $j = 1, \dots, n$

$$\begin{aligned}\frac{\partial \tilde{x}_j}{\partial s} &= \lambda \dot{x}_j\big(\lambda s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big)\\ &= \lambda \frac{\partial H}{\partial \xi_j}\big(x_1\big(\lambda s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big), x_2\big(\lambda s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big), \dots\big)\\ &= \frac{\partial H}{\partial \xi_j}\big(\tilde{\mathbf{x}}(s), \tilde{\mathbf{y}}(s), \tilde{\xi}(s), \tilde{\eta}(s)\big),\end{aligned}$$

since $\frac{\partial H}{\partial \xi_j}$, $j = 1 \dots, n$, are homogeneous of degree 1 in $\xi_1, \dots, \xi_n$ and $\eta_1, \dots, \eta_m$. Similar calculations and homogeneity of degree 2 of $\frac{\partial H}{\partial x_j}$ and $\frac{\partial H}{\partial y_\alpha}$ in $\xi_1, \dots, \xi_n$ and $\eta_1, \dots, \eta_m$ yield

$$\frac{\partial \tilde{y}_\alpha}{\partial s} = \frac{\partial H}{\partial \eta_\alpha}, \qquad \frac{\partial \tilde{\xi}_j}{\partial s} = -\frac{\partial H}{\partial x_j}, \qquad \frac{\partial \tilde{\eta}_\alpha}{\partial s} = -\frac{\partial H}{\partial y_\alpha}.$$

Clearly,

$$\tilde{x}_j(0) = x_j\big(0; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big) = x_j(0), \qquad \tilde{x}_j(t) = x_j\big(\lambda t; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big) = x_j,$$

for $j = 1, \dots, n$ and

$$\begin{aligned}\tilde{y}_\alpha(t) &= y_\alpha(\lambda t; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big) = y_\alpha,\\ \tilde{\eta}_\alpha(0) &= \lambda \eta_\alpha(0; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big) = \lambda \frac{\eta_\alpha(0)}{\lambda} = \eta_\alpha(0)\end{aligned}$$

for $\alpha = 1, \dots, m$. The bicharacteristic curves are unique, so the two sides of (2.2) agree. □

Corollary 2.2. *One has*

$$h(\mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \eta(0); t) = \lambda h\big(\mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big).$$

Proof. In the case of Heisenberg group, the corollary is a direct consequence of the explicit formula (1.11) and in this case, $\eta(0) = \eta$ is a constant. Here we would like to give a proof which applies in more general case. We know that for $j = 1, \dots, m$,

$$\begin{aligned}\dot{x}_j(s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \eta(0); t) &= \frac{dx_j}{ds}(s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \eta(0); t)\\ &= \frac{dx_j}{ds}\big(\lambda s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big)\\ &= \lambda \dot{x}_j\big(\lambda s; \mathbf{x}, \mathbf{x}_0, \mathbf{y}, \xi, \frac{\eta(0)}{\lambda}; \lambda t\big).\end{aligned}$$

Similar result holds for $\dot{y}_\alpha$ for $\alpha = 1, \ldots, m$. Therefore,

$$\int_0^t \big[\xi(s)\cdot\dot{\mathbf{x}}(s) + \eta(s)\cdot\dot{\mathbf{y}}(s) - H(\mathbf{x}(s;\ldots),\ldots)\big]\,ds$$

$$= \int_0^t \Big[\lambda\xi\big(\lambda s;\mathbf{x},\mathbf{x}_0,\mathbf{y},\xi,\frac{\eta(0)}{\lambda};\lambda t\big)\cdot\lambda\dot{\mathbf{x}}(\lambda s;\ldots) + \sum_{\alpha=1}^m \lambda\eta_\alpha(\lambda s;\ldots)\cdot\lambda\dot{y}_\alpha(\lambda s;\ldots)$$

$$- \lambda^2 H(\mathbf{x}(\lambda s;\ldots),\ldots)\Big]\,ds$$

$$= \frac{1}{\lambda}\int_0^t \Big[\lambda^2\sum_{k=1}^n \xi_k(\lambda s;\ldots)\dot{x}_k(\lambda s;\ldots) + \lambda^2\sum_{\alpha=1}^m \eta_\alpha(\lambda s;\ldots)\dot{y}_\alpha(\lambda s;\ldots) - \lambda^2 H(\mathbf{x}(\lambda s;\ldots),\ldots)\Big]\,d(\lambda s)$$

$$= \lambda\int_0^t \Big[\xi\big(s';\mathbf{x},\mathbf{x}_0,\mathbf{y},\frac{\eta(0)}{\lambda},\lambda t\big)\cdot\dot{\mathbf{x}}(s';\ldots) + \eta(s';\ldots)\cdot\dot{\mathbf{y}}(s';\ldots) - H(\mathbf{x}(s';\ldots),\ldots)\Big]\,ds'$$

$$= \lambda S\big(\mathbf{x},\mathbf{x}_0,\mathbf{y},\xi,\frac{\eta(0)}{\lambda},\lambda t\big).$$

Also,

$$\sum_{\alpha=1}^m \eta_\alpha(0)y_\alpha(0;\mathbf{x},\mathbf{x}_0,\mathbf{y},\xi,\eta(0);t) = \lambda\sum_{\alpha=1}^m \frac{\eta_\alpha(0)}{\lambda}y_\alpha\big(0;\mathbf{x},\mathbf{x}_0,\mathbf{y},\xi,\frac{\eta(0)}{\lambda};\lambda t\big)$$

and the proof of the corollary is therefore complete. □

Set

$$f(\mathbf{x},\mathbf{x}_0,\mathbf{y},\xi,\eta(0)) = h(\mathbf{x},\mathbf{x}_0,\mathbf{y},\xi,\eta(0),t)\Big|_{t=1}.$$

Then

Theorem 2.2. *f is a solution of the generalized Hamilton-Jacobi equation*

$$\sum_{\alpha=1}^m \eta_\alpha(0)\frac{\partial f}{\partial\eta_\alpha(0)} + H\Big(\mathbf{x},\mathbf{y},\nabla_{\mathbf{x}}f,\nabla_{\mathbf{y}}f\Big) = f. \tag{2.3}$$

Proof. By homogeneity property of the function h, one has

$$h(\mathbf{x},\mathbf{x}_0,\mathbf{y},\xi,\eta(0),t) = \frac{1}{t}h(\mathbf{x},\mathbf{x}_0,\mathbf{y},\xi,t\eta(0),1) = \frac{1}{t}f(\mathbf{x},\mathbf{x}_0,\mathbf{y},\xi,t\eta(0)),$$

so,

$$\frac{\partial h}{\partial t} = -\frac{1}{t^2}f + \frac{1}{t}\sum_{\alpha=1}^m \eta_\alpha(0)\frac{\partial f}{\partial\eta_\alpha(0)} \tag{2.4}$$

on one hand. On the other hand,

$$\frac{\partial h}{\partial t} = -H\big(\mathbf{x},\mathbf{y},\nabla_{\mathbf{x}}h,\nabla_{\mathbf{y}}h\big) \tag{2.5}$$

from Theorem 2.1. Since (2.4) agrees with (2.5) for all t so we may set $t = 1$ which yields the proposition. □

At the rest of the sectionwe present some examples that revealthe geometrical nature of functions h and f.

2.3. **Laplace operator.** We start from the Laplace operator $\Delta = \sum_{k=1}^{n} \frac{\partial^2}{\partial x_k^2}$ in $\mathbb{R}^n$. The Hamiltonian function $H(\xi)$ is

$$H(\xi) = \frac{1}{2}\sum_{k=1}^{n} \xi_k^2$$

and hence we need to deal with $F(\xi, \gamma) = H + \gamma = 0$. The Hamilton's system is

$$\dot{\mathbf{x}} = \xi, \qquad \dot{\xi} = 0, \qquad \dot{\gamma} = 0.$$

with initial-boundary conditions $\mathbf{x}(0) = \mathbf{x}_0$, $\mathbf{x}(t) = \mathbf{x}$. Since $\dot{\xi} = 0$, it follows that $\xi(s) = \xi(0) =$ constants, is a constant vector. Then

$$\ddot{\mathbf{x}} = \dot{\xi} = 0 \quad \Rightarrow \quad \mathbf{x}(s) = \xi(0)s + \mathbf{x}_0.$$

Moreover,

$$\mathbf{x} = \mathbf{x}(t) = \xi(0)t + \mathbf{x}_0 \quad \Rightarrow \quad \xi(0) = \frac{\mathbf{x} - \mathbf{x}_0}{t}$$

and

$$\frac{\partial h}{\partial t} = \frac{1}{2}\sum_{k=1}^{n} \xi_k^2 = \sum_{k=1}^{n} \frac{(x_k - x_k^{(0)})^2}{2t^2} = \frac{|\mathbf{x} - \mathbf{x}_0|^2}{2t^2}$$

or,

$$h(\mathbf{x}, \mathbf{x}_0, t) = h(0) + \frac{|\mathbf{x} - \mathbf{x}_0|^2}{2t^2} t = h(0) + \frac{|\mathbf{x} - \mathbf{x}_0|^2}{2t}.$$

Since this is a translation invariant case, we may assume that $h(0) = 0$. Therefore,

$$f(\mathbf{x}, \mathbf{x}_0) = h(\mathbf{x}, \mathbf{x}_0, t)\Big|_{t=1} = \frac{|\mathbf{x} - \mathbf{x}_0|^2}{2}$$

gives us the Euclidean action function.

2.4. **Grusin operator.** We are in $\mathbb{R}^2$ now and the horizontal vector fields X_1, X_2 are given by

$$X_1 = \frac{\partial}{\partial x}, \quad \text{and} \quad X_2 = x\frac{\partial}{\partial y}.$$

The Grusin operator is given as follows: $\Delta_X = \frac{1}{2}\left(\frac{\partial}{\partial x}\right)^2 + \frac{1}{2}x^2\left(\frac{\partial}{\partial y}\right)^2$. It is obvious that Δ_X is elliptic away from the y-axis but degenerate on the y-axis. Since $[X_1, X_2] = \frac{\partial}{\partial y}$, hence $\{X_1, X_2, [X_1, X_2]\}$ spanned the tangent bundle of $\mathbb{R}^2$ everywhere. By Hörmander's theorem [12], Δ_X is hypoelliptic.

The Hamiltonian function H for the Δ_X is

$$H(x, y, \xi, \eta) = \frac{1}{2}\xi^2 + \frac{1}{2}x^2\eta^2. \tag{2.6}$$

The Hamilton system can be obtained as follows;

$$\begin{aligned} \dot{x} &= H_\xi = \xi, \\ \dot{y} &= H_\eta = \eta x^2, \\ \dot{\xi} &= -H_x = -\eta^2 x, \\ \dot{\eta} &= -H_y = 0, \\ \dot{S} &= \xi\dot{x} + \eta\dot{y} - H. \end{aligned}$$

With $0 \le s \le t$,

$$\eta(s) = \eta(0) = \eta_0 = \text{constant},$$

"constant" means "*constant along the bicharacteristic curve*". Next,

$$\ddot{x} = \dot{\xi} = -x\eta^2,$$

so

$$\ddot{x} + \eta^2 x = 0.$$

It follows that

$$x(s) = A\cos(\eta s) + B\sin(\eta s) = x(0)\cos(\eta s) + \frac{\xi(0)}{\eta}\sin(\eta s) = x_0\cos(\eta s) + \frac{\xi(0)}{\eta}\sin(\eta s).$$

Hence,

$$\xi(s) = \dot{x}(s)$$

yields

$$\xi(s) = \xi(0)\cos(\eta s) - \eta x_0 \sin(\eta s).$$

We also have

$$x = x(t) = x_0\cos(\eta t) + \frac{\xi(0)}{\eta}\sin(\eta t),$$

and

$$\frac{\xi(0)}{\eta} = \frac{x - x_0\cos(\eta t)}{\sin(\eta t)}. \tag{2.7}$$

Consequently,

$$x(s) = x(0)\cos(\eta s) + \frac{x - x_0\cos(\eta t)}{\sin(\eta t)}\sin(\eta s).$$

The singularities occur at $\eta = \eta_0 = \frac{k\pi}{t}$ when $x = \pm x_0$; they are $\eta = \frac{(2k+1)\pi}{t}$ if $x = x_0$ and $\eta_0 = \frac{2k\pi}{t}$ if $x = -x_0$. Next,

$$\begin{aligned}
\dot{y}(s) =& \eta x^2(s) \\
=& \eta\Big[x_0\big(\frac{1}{2} + \frac{1}{2}\cos(2\eta s)\big) + 2x_0\frac{\xi(0)}{\eta}\sin(\eta s)\cos(\eta s) + \big(\frac{\xi(0)}{\eta}\big)^2\big(\frac{1}{2} - \frac{1}{2}\cos(2\eta s)\big)\Big] \\
=& \frac{d}{ds}\Big\{\eta\Big[\frac{x_0^2}{2}\big(s + \frac{\sin(2\eta s)}{2\eta}\big) + \frac{x_0\xi(0)}{\eta^2}\sin^2(\eta s) + \frac{1}{2}\big(\frac{\xi(0)}{\eta}\big)^2\big(s - \frac{\sin(2\eta s)}{2\eta}\big)\Big]\Big\} \\
=& \frac{d}{ds}\Big\{\frac{\eta}{2}\Big[x_0^2 + \big(\frac{\xi(0)}{\eta}\big)^2\Big]s + \frac{1}{4}\Big[x_0^2 - \big(\frac{\xi(0)}{\eta}\big)^2\Big]\sin(2\eta s) + \frac{x_0}{2}\frac{\xi(0)}{\eta}\big(1 - \cos(2\eta s)\big)\Big\}.
\end{aligned}$$

We replace $\frac{\xi(0)}{\eta}$ by (2.7) and collect terms with x_0^2:

$$\begin{aligned}
&\frac{x_0^2}{2}\Big\{\eta s + \frac{1}{2}\sin(2\eta s) + \eta s\frac{\cos^2(\eta t)}{\sin^2(\eta t)} - \frac{1}{2}\frac{\cos^2(\eta t)}{\sin^2(\eta t)}\sin(2\eta t) - \frac{\cos(\eta t)}{\sin(\eta t)}\big(1 - \cos(2\eta s)\big)\Big\} \\
=& \frac{x_0^2}{2}\Big\{\frac{\eta s}{\sin^2(\eta t)} - \frac{1}{2}\frac{\cos^2(\eta t) - \sin^2(\eta t)}{\sin^2(\eta t)}\sin(2\eta s) - \frac{\cos(\eta t)}{\sin(\eta t)}\big(1 - \cos(2\eta s)\big)\Big\} \\
=& \frac{x_0^2}{2\sin^2(\eta t)}\Big\{\eta s - \frac{1}{2}\big[\cos(2\eta t)\sin(2\eta s) + \sin(2\eta t)\big(1 - \cos(2\eta s)\big)\big]\Big\} \\
=& \frac{x_0^2}{4\sin^2(\eta t)}\Big\{2\eta s - \big[\sin(2\eta t) - \sin\big(2\eta(t-s)\big)\big]\Big\}.
\end{aligned}$$

The terms containing x^2 are:

$$\frac{1}{4}\frac{x^2}{\sin^2(\eta t)}\big(2\eta s - \sin(2\eta s)\big),$$

and the terms with $x_0 x$ are the following:

$$\frac{1}{2}\frac{2xx_0}{\sin^2(\eta t)}\Big\{\frac{1}{2}\big[\sin\big(\eta(2s-t)\big)+\sin(\eta t)\big]-\eta\, s\cos(\eta t)\Big\}.$$

So,

$$\begin{aligned}\dot y(s) = \frac{d}{ds}\Big\{&\frac{x_0^2}{4\sin^2(\eta t)}\Big[2\eta s-\big[(\sin(2\eta t)-\sin\big(2\eta(t-s)\big)\big])Big]\\ &+\frac{x^2}{4\sin^2(\eta t)}\big(2\eta s-\sin(2\eta s)\big)\\ &+\frac{2xx_0}{4\sin^2(\eta t)}\Big[\frac{1}{2}\big(\sin\big(\eta(2s-t)\big)+\sin(\eta t)\big)-\eta\, s\cos(\eta t)\Big]\Big\}.\end{aligned}$$

The action function has the form

$$S=\int_0^t(\xi\dot x+\eta\dot y-H)ds=\eta(y-y(0))+\int_0^t(\xi^2-H)ds.$$

We find ξ^2 as follows

$$\begin{aligned}\xi^2(s)&=\frac{\xi^2(0)}{2}\big(1+\cos(2\eta s)\big)-\xi(0)\eta x_0\sin(2\eta s)+\frac{1}{2}\eta^2x_0^2\big(1-\cos(2\eta s_)\big)\\ &=\underbrace{\frac{1}{2}\big[\xi^2(0)+\eta^2x_0^2\big]}_{=H(0)}+\frac{1}{2}\big[\xi^2(0)-\eta^2x_0^2\big]\cos(2\eta s)-\eta x_0\xi(0)\sin(2\eta s).\end{aligned}$$

Since H is constant along the bicharacteristic, one has

$$H=H(0)=\frac{1}{2}\big[\xi^2(0)+\eta^2x_0^2\big].$$

Continuing, we obtain the action function

$$\begin{aligned}S=&\,\eta(y-y(0))+\int_0^t\Big[(\xi^2(0)-\eta^2x_0^2)\frac{\cos(2\eta s)}{2}-\eta x_0\xi(0)\sin(2\eta s)\Big]ds\\ =&\,\eta(y-y(0))+\frac{1}{2}\big(\xi^2(0)-\eta^2x_0^2\big)\frac{\sin(2\eta t)}{2\eta}+\eta x_0\xi(0)\frac{\cos(2\eta t)-1}{2\eta}.\end{aligned}$$

We simplify this

$$\begin{aligned}&S-\eta(y-y(0))\\ &=\frac{\eta^2}{2}\Big(\frac{x-x_0\cos(\eta t)}{\sin(\eta t)}\Big)^2\frac{\sin(2\eta t)}{2\eta}-\frac{1}{2}\eta^2x_0^2\frac{\sin(2\eta t)}{2\eta}+\eta^2x_0\frac{x-x_0\cos(\eta t)}{\sin(\eta t)}\frac{\cos(2\eta t)-1}{2\eta}\\ &=\frac{\eta}{4}\Big\{\Big(\frac{x-x_0\cos(\eta t)}{\sin(\eta t)}\Big)^2\sin(2\eta t)-x_0^2\sin(2\eta t)-2x_0\frac{x-x_0\cos(\eta t)}{\sin(\eta t)}\big(1-\cos(2\eta t)\big)\Big\}.\end{aligned}\tag{2.8}$$

In the bracket $\{\cdots\}$ of (2.8), terms involved x_0^2 are

$$\begin{aligned}&x_0^2\Big[\Big(\frac{\cos^2(\eta t)}{\sin^2(\eta t)}-1\Big)\sin(2\eta t)+2\frac{\cos(\eta t)}{\sin(\eta t)}(1-\cos(2\eta t))\Big]\\ &=x_0^2\Big(\frac{\cos(2\eta t)\sin(2\eta t)}{\sin^2(\eta t)}+2\frac{\cos(\eta t)}{\sin(\eta t)}-\frac{\cos(2\eta t)\sin(2\eta t)}{\sin^2(\eta t)}\Big)\\ &=2x_0^2\cot(\eta t),\end{aligned}$$

terms involved x^2 are

$$x^2 \frac{\sin(2\eta t)}{\sin^2(\eta t)} = 2x^2 \cot(\eta t),$$

and terms containing $x_0 x$ are

$$\begin{aligned} & 2xx_0\Big(- \frac{\cos(\eta t)}{\sin^2(\eta t)} \sin(2\eta t) - \frac{1-\cos(2\eta t)}{\sin(\eta t)}\Big) \\ = & - 2xx_0\Big(\frac{2\cos^2(\eta t)}{\sin(\eta t)} + 2\sin(\eta t)\Big) \\ = & - \frac{4xx_0}{\sin(\eta t)}. \end{aligned}$$

Hence,

$$\begin{aligned} \{\cdots\} = & 2(x^2 + x_0^2)\cot(\eta t) - \frac{4xx_0}{\sin(\eta t)} \\ = & \big[(x+x_0)^2 + (x-x_0)^2\big]\cot(\eta t) - \frac{(x+x_0)^2 - (x-x_0)^2}{\sin(\eta t)} \\ = & (x+x_0)^2\Big(\cot(\eta t) - \frac{1}{\sin(\eta t)}\Big) + (x-x_0)^2\Big(\cot(\eta t) + \frac{1}{\sin(\eta t)}\Big) \\ = & (x+x_0)^2 \frac{\cos(\eta t) - 1}{\sin(\eta t)} + (x-x_0)^2 \frac{\cos(\eta t)+1}{\sin(\eta t)} \\ = & - (x+x_0)^2 \tan\big(\frac{\eta t}{2}\big) + (x-x_0)^2 \cot\big(\frac{\eta t}{2}\big). \end{aligned}$$

Thus S has the following form:

$$S = \eta(y - y(0)) - \frac{\eta}{4}\Big[(x+x_0)^2 \tan\big(\frac{\eta t}{2}\big) - (x-x_0)^2 \cot\big(\frac{\eta t}{2}\big)\Big].$$

By Theorem 2.1, we know that

$$\begin{aligned} h(t;x,x_0,y,\eta) = & \eta y(0) + S(t;x,y,\eta) \\ = & \eta y(0) + \eta(y - y(0)) - \frac{\eta}{4}\Big[(x+x_0)^2 \tan\big(\frac{\eta}{2}\big) - (x-x_0)^2 \cot\big(\frac{\eta}{2}\big)\Big] \\ = & \eta y - \frac{\eta}{4}\Big[A^2 \tan\big(\frac{\eta t}{2}\big) - B^2 \cot\big(\frac{\eta t}{2}\big)\Big] \end{aligned}$$

is a solution of the Hamilton-Jacobi equation. Here $A = x + x_0$ and $B = x - x_0$. Now by Theorem 2.2, the function

$$f(x,x_0,y,\eta) = h(t;x,x_0,y,\eta)\Big|_{t=1} = \frac{1}{2}\frac{\eta}{2}\Big\{4y - A^2 \tan\big(\frac{\eta}{2}\big) + B^2 \cot\big(\frac{\eta}{2}\big)\Big\}$$

is a solution of the generalized Hamilton-Jacobi equation

$$\eta \frac{\partial f}{\partial \eta} + H\Big(x, x_0, y, \partial_x f, \partial_y f\Big) = f.$$

We set

$$\frac{\eta}{2} = \widetilde{\eta}\tau,$$

where $\tau \in \mathbb{R}$ yields the domain of integration and $\widetilde{\eta}$ is a fixed complex number.

Lemma 2.5. *Suppose f is a smooth function of $\tau \in \mathbb{R}$ and*

$$\lim_{\tau\to\pm\infty} Re(f)(\tau) = \infty$$

off the canonical curve $x_0^2 + x^2 = 0$. Then $\widetilde{\eta}$ is pure imaginary.

Proof. Let $\widetilde{\eta} = \eta_1 + i\eta_2$. An elementary calculation yields

$$f = \frac{1}{2}(\eta_1 + i\eta_2)\tau\Big\{4y + \frac{\sin(2\eta_1\tau)\big[(B^2 - A^2)\cosh(2\eta_2\tau) + (B^2 + A^2)\cos(2\eta_1\tau)\big]}{\cosh^2(2\eta_2\tau) - \cos^2(2\eta_1\tau)}$$
$$- i\frac{\sinh(2\eta_2\tau)\big[(B^2 + A^2)\cosh(2\eta_2\tau) + (B^2 - A^2)\cos(2\eta_1\tau)\big]}{\cosh^2(2\eta_2\tau) - \cos^2(2\eta_1\tau)}\Big\}$$

(i). $\eta_1 = 0$, *i.e.*, $\eta \in i\mathbb{R}$. When $\tau \approx \pm\infty$,

$$f \approx \frac{1}{2}i\eta_2\tau\Big\{4y - i2(x_0^2 + x^2)\tanh(2\eta_2\tau)\Big\},$$

and

$$\mathrm{Re}(f) \approx \frac{1}{4}(x_0^2 + x^2)2\eta_2\tau\tanh(2\eta_2\tau) \;\to\; \pm\infty$$

as $\tau \to \pm\infty$ as long as $x_0^2 + x^2 \neq 0$.
(ii). $\eta_2 = 0$, that is $\eta \in \mathbb{R}$. Then

$$f = 2\eta_1\tau y + \frac{1}{4}\frac{2\eta_1\tau}{\sin(2\eta_1\tau)}\Big[B^2 - A^2 + (B^2 + A^2)\cos(2\eta_1\tau)\Big]$$

is singular in $\tau \in \mathbb{R}$ when $x_0^2 + x^2 \neq 0$, otherwise

$$\mathrm{Re}(f) = f = 2\eta_1\tau y \underbrace{\longrightarrow}_{\tau\to\pm\infty} \pm(\mathrm{sgn}(y))\infty.$$

(iii). $\eta_1 \neq 0$, $\eta_2 \neq 0$. Here

$$f \approx \frac{1}{2}(\eta_1 + i\eta_2)\tau\Big\{4y - i(A^2 + B^2)\tanh(2\eta_2\tau)\Big\}$$

as $\tau \to \pm\infty$, and

$$\begin{aligned}\mathrm{Re}(f) &\approx 2\eta_1\tau y + (x_0^2 + x^2)\big|\eta_2\tau\big| \\ &= |\tau|\big[2(\mathrm{sgn}(\tau))\eta_1 y + (x_0^2 + x^2)|\eta_2|\big]\end{aligned}$$

and choosing x_0, x, y so that

$$2\eta_1 y > (x_0^2 + x^2)|\eta_2|$$

we have

$$\lim_{\tau\to\pm\infty} \mathrm{Re}(f) = \pm\infty$$

which we do not want. This complete the proof of Lemma (2.5). □

Following the tradition, we shall choose

$$\widetilde{\eta} = -\frac{i}{2}.$$

Then

$$f = -i\tau y + \frac{1}{2}(x_0^2 + x^2)\tau\coth\tau - \frac{\tau x_0 x}{\sinh\tau}.$$

2.6. **Sub-Laplace operator on step 2 nilpotent Lie groups.** Let $\mathcal{M}$ be a simply connected 2-step nilpotent Lie group $\mathbb{G}$ equipped with a left invariant metric. Let $\mathcal{G}$ be its Lie algebra and it is identified with the group $\mathbb{G}$ by the exponential map:

$$\exp : \mathcal{G} \to \mathbb{G}.$$

We assume

$$\mathcal{G} = [\mathcal{G},\mathcal{G}] \oplus [\mathcal{G},\mathcal{G}]^{\perp} = \mathcal{C} \oplus [\mathcal{G},\mathcal{G}]^{\perp} = \mathcal{C} \oplus \mathcal{H},$$

where $\mathcal{H}$ and $\mathcal{C}$ are vector spaces over $\mathbb{R}$ with an skew-symmetric bilinear form

$$B : \mathcal{H} \times \mathcal{H} \to \mathcal{C}$$

such that $B(\mathcal{H},\mathcal{H}) = \mathcal{C}$. The group law is given by

$$(\mathcal{H} \oplus \mathcal{C}) \times (\mathcal{H} \oplus \mathcal{C}) \to \mathcal{H} \oplus \mathcal{C}$$

with

$$(\mathbf{x},\mathbf{y}) * (\mathbf{x}',\mathbf{y}') = \big(\mathbf{x}+\mathbf{x}', \mathbf{y}+\mathbf{y}' + \frac{1}{2}B(\mathbf{x},\mathbf{x}')\big)$$

and then the exponential map is the identity map. Let $\{X_1,\dots,X_n\}$ be a basis of $\mathcal{H}$ and let $\{Y_1,\dots,Y_m\}$ be a basis of the center $[\mathcal{G},\mathcal{G}] = \mathcal{C}$. We assume $\{X_1,\dots,X_n\}$ and $\{Y_1,\dots,Y_m\}$ are orthonormal, and introduce a left invariant Riemannian metric on the group $\mathbb{G}$ in an obvious way.

We write the vector fields X_j, $j = 1,\dots,n$ by:

$$X_j = \frac{\partial}{\partial x_j} + \sum_{k=1}^{n}\sum_{\alpha=1}^{m} a_{jk}^{\alpha} x_k \frac{\partial}{\partial y_\alpha}$$

where the a_{jk}^{α} are real numbers and form skew-symmetric matrices $\big[a_{jk}^{\alpha}\big]_{j,k}$, *i.e.*, $a_{jk}^{\alpha} = -a_{kj}^{\alpha}$. We are interested in the sub-Laplacian Δ_X which can be defined as follows:

$$\Delta_X = \frac{1}{2}\sum_{j=1}^{n} X_j^2$$

It is easy to see that

$$\big[X_j, X_k\big] = 2\sum_{k=1}^{n}\sum_{\alpha=1}^{m} a_{jk}^{\alpha}\frac{\partial}{\partial y_\alpha}. \tag{2.9}$$

Lemma 2.7. *The operator Δ_X is hypoelliptic if and only if the rectangular matrix of order $\frac{n(n-1)}{2} \times m$ with element $\big[a_{jk}^{\alpha}\big]_{\{(j<k),\alpha\}}$ is of rank m (which implies that $m \le \frac{n(n-1)}{2}$).*

Proof. The operator Δ_X is hypoelliptic when the vector fields $\{X_j\}_{j=1}^{n}$ satisfy the "first" bracket generating condition. This implies that we can recover all the $\frac{\partial}{\partial y_\alpha}$ from the $\frac{n(n-1)}{2}$ relations (2.9). If we consider $\big[a_{jk}^{\alpha}\big]$ as a matrix with indices $\alpha = 1,\dots,m$ and the couples (j,k) where $j<k$, this means that this matrix should have rank m. □

We may define a Lie group structure on $\mathbb{R}^n \times \mathbb{R}^m$ with the following group law:

$$(\mathbf{x},\mathbf{y}) \circ (\mathbf{x}',\mathbf{y}') = \Big(x_1 + x_1', \dots, x_n + x_n', y_1 + y_1' + \sum_{j,k=1}^{n} a_{jk}^{1} x_j' x_k, \dots, y_m + y_m' + \sum_{j,k=1}^{n} a_{jk}^{m} x_j' x_k\Big). \tag{2.10}$$

It is easy to see that the X_j are left invariant vector fields such that

$$\big(X_j f\big)(\mathbf{x},\mathbf{y}) = \frac{\partial}{\partial x'_j}\big(f \circ \mathcal{L}_{(\mathbf{x},\mathbf{y})}\big)(\mathbf{x}',\mathbf{y}')\Big|_{\mathbf{x}'=0,\mathbf{y}'=0}$$

where

$$\mathcal{L}_{(\mathbf{x},\mathbf{y})}(\mathbf{x}',\mathbf{y}') = (\mathbf{x},\mathbf{y}) \circ (\mathbf{x}',\mathbf{y}')$$

is the left translation by the element $(\mathbf{x},\mathbf{y})$. In particular, Δ_X is a left invariant operator for this group structure (see [1] and [16]).

Let $\xi_1,\dots,\xi_n$ be the dual variables of $\mathbf{x}$ and $\eta_1,\dots,\eta_m$ be the dual variables of $\mathbf{y}$. We define the symbols ζ_j of the vector field X_j by

$$\zeta_j = \xi_j + \sum_{k=1}^{n}\sum_{\alpha=1}^{m} a_{jk}^{\alpha} x_k \eta_\alpha.$$

We shall try to find a solution of the following equation:

$$\frac{\partial h}{\partial t} + \frac{1}{2}\sum_{j=1}^{n}\Big(\frac{\partial h}{\partial x_j} + \sum_{k=1}^{n}\sum_{\alpha=1}^{m} a_{jk}^{\alpha} x_k \frac{\partial h}{\partial y_\alpha}\Big)^2 = 0.$$

Thus we start with

$$\frac{\partial z}{\partial t} + H(\nabla z) = 0, \tag{2.11}$$

where $H(\mathbf{x},\mathbf{y};\xi,\eta)$ is the Hamiltonian function as the full symbol of Δ_X,

$$H(\mathbf{x},\mathbf{y};\xi,\eta) = \frac{1}{2}\sum_{j=1}^{n}\big(\xi_j + \sum_{k=1}^{n}\sum_{\alpha=1}^{m} a_{jk}^{\alpha} x_k \eta_\alpha\big)^2 = \frac{1}{2}\sum_{j=1}^{n}\big(\xi_j + \sum_{k=1}^{n}\mathcal{A}_{kj}(\eta)\cdot x_k\big)^2. \tag{2.12}$$

Here

$$\mathcal{A}_{kj}(\eta) = \sum_{\alpha=1}^{m} a_{kj}^{\alpha}\eta_\alpha.$$

We shall find the bicharacteristic curves which are solutions to the corresponding Hamilton's system. The solutions define a one parameter family of symplectic isomorphism of the (punctures) cotangent bundle $T^*(\mathbb{R}^n\times\mathbb{R}^m)\setminus\{\mathbf{0}\}$. Since $\mathcal{A}^t(\eta) = -\mathcal{A}(\eta)$, the Hamilton's system can be written explicitly as follows:

$$\begin{aligned}
\dot{x}_j &= H_{\xi_j} = \xi_j - \sum_{k=1}^{n}\mathcal{A}_{jk}(\eta)\cdot x_k = \zeta_j, \quad \text{for } j=1,\dots,n\\
\dot{y}_\alpha &= H_{\eta_\alpha} = \sum_{j=1}^{n}\sum_{k=1}^{n} a_{jk}^{\alpha} x_k \zeta_j, \quad \text{for } \alpha=1,\dots,m\\
\dot{\xi}_j &= -\,H_{x_j} = -\sum_{k=1}^{n}\mathcal{A}_{jk}(\eta)\cdot\zeta_k = \sum_{k=1}^{n}\mathcal{A}_{kj}(\eta)\cdot\zeta_k, \quad \text{for } j=1,\dots,n\\
\dot{\eta}_\alpha &= -\,H_{y_\alpha} = 0, \quad \text{for } \alpha=1,\dots,m
\end{aligned} \tag{2.13}$$

with the initial-boundary conditions such that

$$\begin{cases}
\mathbf{x}(0) = 0\\
\mathbf{x}(t) = \mathbf{x} = (x_1,\dots,x_n)\\
\mathbf{y}(t) = \mathbf{y} = (y_1,\dots,y_m)\\
\eta(0) = i\tau = i(\tau_1,\dots,\tau_m)
\end{cases} \tag{2.14}$$

where $t \in \mathbb{R}$, $\mathbf{x}$ and $\mathbf{y}$ are arbitrarily given. With $0 \le s \le t$,

$$\eta_\alpha(s) = \eta_\alpha = \text{constant}, \quad \text{for } \alpha = 1, \dots, m$$

"constant" means "*constant along the bicharacteristic curve*". Also

$$H = \frac{1}{2}\sum_{j=1}^n \dot{x}_j^2 = \frac{1}{2}\sum_{j=1}^n \zeta^2 = E = \text{energy}.$$

Another way to see that E is constant along the bicharacteristic, note that

$$\begin{aligned} \ddot{x}_j =& \dot{\zeta}_j = \dot{\xi}_j - \sum_{k=1}^n \mathcal{A}_{jk}(\eta) \cdot \dot{x}_k \\ =& -\sum_{k=1}^n \mathcal{A}_{jk}(\eta) \cdot \zeta_k - \sum_{k=1}^n \mathcal{A}_{jk}(\eta) \cdot \zeta_k \\ =& -2\sum_{k=1}^n \mathcal{A}_{jk}(\eta) \cdot \zeta_k \end{aligned} \tag{2.15}$$

for $j = 1, \dots, n$. Hence

$$\ddot{\mathbf{x}} = \dot{\zeta} = \dot{\xi} + \mathcal{A}(\eta)\dot{\mathbf{x}} = -2\mathcal{A}(\eta)\zeta. \tag{2.16}$$

Therefore,

$$\ddot{\mathbf{x}} \cdot \dot{\mathbf{x}} = -2\mathcal{A}(\eta)\zeta \cdot \zeta = 0$$

since $\mathcal{A}$ is skew-symmetric. It follows that

$$\frac{1}{2}\sum_{j=1}^n \dot{x}_j^2 = \frac{1}{2}\dot{\mathbf{x}} \cdot \dot{\mathbf{x}} = E = \text{energy}.$$

Since $\dot{\mathbf{x}}(s) = e^{-2s\mathcal{A}(\eta)}\xi(0)$, by integrating the equation

$$\mathcal{A}(\eta)\dot{\mathbf{x}}(s) = \mathcal{A}(\eta)e^{-2s\mathcal{A}(\eta)}\xi(0),$$

one has

$$\mathcal{A}(\eta)\mathbf{x}(s) = -\frac{1}{2}\Big(e^{-2s\mathcal{A}(\eta)} - I\Big)\xi(0)$$

where I is the $n \times n$ identity matrix. Since $\eta_\alpha = \eta(0) = i\tau_\alpha$ is pure imaginary, the matrix $i\mathcal{A}(\tau)$ is self-adjoint. It follows that the matrix

$$\frac{is\mathcal{A}(\tau)}{\sinh(it\mathcal{A}(\tau))} = \frac{1}{2\pi i}\int_\gamma \frac{\lambda}{\sinh(\lambda)}\Big(\lambda - it\mathcal{A}(\tau)\Big)^{-1} d\lambda$$

is well defined and invertible for any $t \in \mathbb{R}$ and $\tau \in \mathbb{R}^m$. Here γ is a suitable contour surrounding the spectrum of the matrix $it\mathcal{A}(\tau)$. The matrix

$$\frac{1}{2\pi i}\int_\gamma \frac{\lambda}{\sinh(\lambda)}\Big(\lambda - it\mathcal{A}(\tau)\Big)^{-1} d\lambda$$

has an inverse:

$$\frac{1}{2\pi i}\int_\gamma \frac{\sinh(\lambda)}{\lambda}\Big(\lambda - it\mathcal{A}(\tau)\Big)^{-1} d\lambda$$

We write it as

$$\frac{\sinh(i\mathcal{A}(\tau))}{i\mathcal{A}(\tau)} = \sum_{k=0}^\infty \frac{(i\mathcal{A}(\tau))^{2k}}{(2k+1)!}.$$

Then for any fixed $t \in \mathbb{R}$, we have one-to-one correspondence between the initial condition $\xi(0)$ and boundary condition $\mathbf{x}$:

$$\xi(0) = e^{it\mathcal{A}(\tau)} \cdot \frac{i\mathcal{A}(\tau)}{\sinh(it\mathcal{A}(\tau))} \cdot \mathbf{x}, \qquad t \neq 0.$$

Now we may solve the initial value problem:

$$\begin{cases} \dot{x}_j(s) = & \frac{\partial H}{\partial \xi_j} = \xi_j + i\sum_{k=1}^n \sum_{\alpha=1}^m a_{jk}^\alpha x_k \tau_\alpha = \xi_j + i\sum_{k=1} \mathcal{A}_{kj}(\tau) x_k, \\ \dot{\xi}_j(s) = & -\frac{\partial H}{\partial x_j} = -i\sum_{k=1}^n \Big(\xi_k + i\sum_{\ell=1}^n \mathcal{A}_{\ell k}(\tau) x_\ell\Big) \cdot \mathcal{A}_{jk}(\tau) \end{cases}$$

with the initial conditions

$$\begin{cases} \mathbf{x}(0) = 0 \\ \xi(0) = e^{it\mathcal{A}(\tau)} \cdot \frac{i\mathcal{A}(\tau)}{\sinh(it\mathcal{A}(\tau))}\mathbf{x}. \end{cases}$$

Straightforward computations show that

$$\begin{aligned} \mathbf{x}(s) =& \mathbf{x}(s;\mathbf{x},\tau,t) = e^{i(t-s)\mathcal{A}(\tau)} \frac{\sinh(is\mathcal{A}(\tau))}{\sinh(it\mathcal{A}(\tau))} \cdot \mathbf{x} \\ \xi(s) =& \xi(s;\mathbf{x},\tau,t) \\ =& \frac{i\mathcal{A}(\tau)}{\sinh(it\mathcal{A}(\tau))} \cdot e^{it\mathcal{A}(\tau)} \Big(I - e^{-is\mathcal{A}(\tau)} \sinh(is\mathcal{A}(\tau))\Big) \cdot \mathbf{x} \\ =& \Big(e^{-is\mathcal{A}(\tau)} \cosh(is\mathcal{A}(\tau))\Big) \cdot \Big(e^{it\mathcal{A}(\tau)} \frac{i\mathcal{A}(\tau)}{\sinh(it\mathcal{A}(\tau))}\Big)\mathbf{x} \\ =& \Big(e^{-is\mathcal{A}(\tau)} \cosh(is\mathcal{A}(\tau))\Big) \cdot \xi(0). \end{aligned}$$

Hence we obtain solutions for the initial-boundary problem (2.13) under the condition (2.14). We also have the following solutions for $\mathbf{y}(s)$:

$$y_\alpha(s) = y_\alpha(0) + \int_0^s \sum_{k=1}^n \Big(\big(e^{-2iu\mathcal{A}(\tau)}\xi(0)\big)_k \cdot \sum_{\ell=1}^n a_{\ell k}^\alpha x_\ell(u)\Big) du, \quad \alpha = 1, \dots, m.$$

Again by Theorem 2.2, the function

$$f(\mathbf{x},\mathbf{y},\tau) = h(\mathbf{x},\mathbf{y},\tau,t)\Big|_{t=1}$$

is a solution of the generalized Hamilton-Jacobi equation. In our case, the function f can be calculated explicitly.

$$\begin{aligned} f(\mathbf{x},\mathbf{y},\tau) =& h(\mathbf{x},\mathbf{y},\tau,t)\Big|_{t=1} \\ =& \sum_{\alpha=1}^m \eta_\alpha(0) y_\alpha(0) + \int_0^1 \big(\xi \cdot \dot{\mathbf{x}} + \eta \cdot \dot{\mathbf{y}} - H\big) ds \\ =& \eta_0 \sum_{\alpha=1}^m \tau_\alpha y_\alpha + \int_0^1 \big(\xi \cdot \dot{\mathbf{x}} - H\big) ds. \end{aligned}$$

Here η_0 is a pure imaginary number. This choice can be motivated by Lemma 2.5.

Since

$$\xi \cdot \dot{\mathbf{x}} - H = \frac{1}{2}\langle \zeta, \zeta \rangle - \langle \zeta, \mathcal{A}\mathbf{x} \rangle,$$

then

$$\begin{aligned}\langle \zeta, \mathcal{A}\mathbf{x}\rangle &= \Big\langle \zeta, \frac{\mathcal{A}(\tau)e^{2s\mathcal{A}(\tau)}}{e^{2\mathcal{A}(\tau)}-I}\mathbf{x}\Big\rangle - \Big\langle \zeta, \frac{\mathcal{A}(\tau)}{e^{2\mathcal{A}(\tau)}-I}\mathbf{x}\Big\rangle \\ &= \frac{1}{2}\langle \zeta,\zeta\rangle - \Big\langle \frac{2\mathcal{A}(\tau)e^{2s\mathcal{A}(\tau)}}{e^{2\mathcal{A}(\tau)}-I}\mathbf{x}, \frac{\mathcal{A}(\tau)}{e^{2\mathcal{A}(\tau)}-I}\mathbf{x}\Big\rangle.\end{aligned}$$

It follows that

$$\xi\cdot\dot{\mathbf{x}} - H = \Big\langle \frac{2\mathcal{A}(\tau)e^{2s\mathcal{A}(\tau)}}{e^{2\mathcal{A}(\tau)}-I}\mathbf{x}, \frac{\mathcal{A}(\tau)}{e^{2\mathcal{A}(\tau)}-I}\mathbf{x}\Big\rangle = \Big\langle \frac{2\mathcal{A}(\tau)\cosh(2s\mathcal{A}(\tau))}{e^{2\mathcal{A}(\tau)}-I}\mathbf{x}, \frac{\mathcal{A}(\tau)}{e^{2\mathcal{A}(\tau)}-I}\mathbf{x}\Big\rangle.$$

The second equality due to $\mathcal{A}$ is skew-symmetric. Now we can integrate from $s=0$ to $s=1$ to obtain

$$\int_0^1 \big(\xi\cdot\dot{\mathbf{x}} - H\big)ds = \frac{1}{2}\Big\langle \big(\mathcal{A}(\tau)\coth(\mathcal{A}(\tau))\big)\mathbf{x},\mathbf{x}\Big\rangle.$$

It follows that

$$f(\mathbf{x},\mathbf{y},\tau) = -i\sum_{\alpha=1}^{m}\tau_\alpha y_\alpha + \frac{1}{2}\Big\langle \big(\mathcal{A}(\tau)\coth(\mathcal{A}(\tau))\big)\mathbf{x},\mathbf{x}\Big\rangle. \tag{2.17}$$

Using equation (2.17), we may complete the discuss in Section 2.

Example 2.8. When

$$\mathcal{A} = \begin{bmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ & & \cdots & \\ 0 & 0 & \cdots & a_{2n}\end{bmatrix} \in M_{2n\times 2n}, \quad \text{with } a_j = a_{j+n}, \quad j=1,\dots,n,$$

i.e., the group is an anisotropic Heisenberg group. In this case, $m=1$ and

$$f(\mathbf{x},y,\tau) = -i\tau y + \tau\sum_{k=1}^{n} a_k\coth(2a_k\tau)\big(x_k^2 + x_{n+k}^2\big).$$

Example 2.9. In $\mathbb{R}^4$, the basis of quaternion numbers $\mathbb{H} = \{a + b\mathbf{i} + c\mathbf{j} + d\mathbf{k} : \ a,b,c,d\in\mathbb{R}\}$ can be given by real matrices

$$M_0 = \begin{bmatrix} 1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{bmatrix}, \qquad M_1 = \begin{bmatrix} 0&1&0&0\\-1&0&0&0\\0&0&0&1\\0&0&-1&0\end{bmatrix},$$

$$M_2 = \begin{bmatrix} 0&0&0&-1\\0&0&-1&0\\0&1&0&0\\1&0&0&0\end{bmatrix}, \qquad M_3 = \begin{bmatrix} 0&0&-1&0\\0&0&0&1\\1&0&0&0\\0&-1&0&0\end{bmatrix}.$$

We have

$$q = \begin{bmatrix} a&b&-d&-c\\-b&a&-c&d\\d&c&a&b\\c&-d&-b&a\end{bmatrix} = aM_0 + bM_1 + cM_2 + dM_3.$$

The number a is called the *real part* and denoted by $a = \mathrm{Re}(q)$. The vector $\mathbf{u} = (b,c,d)$ is the *imaginary part* of q. We use the notations

$$b = \mathrm{Im}_1(q), \quad c = \mathrm{Im}_2(q), \quad d = \mathrm{Im}_3(q), \quad \text{and} \quad \mathrm{Im}(q) = \mathbf{u} = (b,c,d).$$

We introduce the quaternionic H-type group denoted by $\mathcal{Q}$. This group consists of the set

$$\mathbb{H} \times \mathbb{R}^3 = \{[\mathbf{x}, \mathbf{y}] : \ \mathbf{x} \in \mathbb{H}, \ \mathbf{y} = (y_1, y_2, y_3) \in \mathbb{R}^3\}$$

with the multiplication law defined in (2.10) with $[a_{jk}^{\alpha}] = M_\alpha$, $\alpha = 1, 2, 3$. The horizontal vector fields $X = (X_1, X_2, X_3, X_4)$ of the group $\mathcal{Q}$ can be written as follows:

$$X = \nabla_{\mathbf{x}} + \frac{1}{2}\Big(M_1 \mathbf{x} \frac{\partial}{\partial y_1} + M_2 \mathbf{x} \frac{\partial}{\partial y_2} + M_3 \mathbf{x} \frac{\partial}{\partial y_3}\Big),$$

with $\mathbf{x} = (x_1, x_2, x_3, x_4)$ and

$$\nabla_{\mathbf{x}} = \Big(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}, \frac{\partial}{\partial x_4}\Big).$$

In this case, the solution for the generalized Hamilton-Jacobi equation is

$$f(\mathbf{x}, y_1, y_2, y_3, \tau_1, \tau_2, \tau_3) = -i \sum_{\alpha=1}^{3} \tau_\alpha y_\alpha + \frac{|\mathbf{x}|^2}{2} |\tau| \coth(2|\tau|)$$

See details in [6] In general multidimensional case, the matrix $\mathcal{A}$ can be defined as follows:

$$\mathcal{A} = \begin{bmatrix} \sum_{\alpha=1}^{3} a_1^\alpha M_\alpha & 0 & \dots & 0 \\ 0 & \sum_{\alpha=1}^{3} a_2^\alpha M_\alpha & \dots & 0 \\ & & \dots & \\ 0 & 0 & \dots & \sum_{\alpha=1}^{3} a_n^\alpha M_\alpha \end{bmatrix}.$$

In this case we obtain the so called anisotropic quaternion Carnot group considered in [7]. The complex action is given by

$$f(x, y, \tau) = -i \sum_{\alpha} \tau_\alpha y_\alpha + \frac{1}{2} \sum_{l=1}^{n} |x_l|^2 |\tau|_l \coth(2|\tau|_l),$$

where $|x_l|^2 = \sum_{j=0}^{3} x_{4l-j}^2$, $|\tau|_l = \big(\sum_{\alpha=1}^{3} (a_l^\alpha)^2 \tau_\alpha^2\big)^{1/2}$. If all a_l^α, $l = 1, \dots, n$ are equal, we get the example of multidimensional quaternion H-type group. More information about H-type groups can be found in [5, 13, 14, 15].

3. **Heat kernel and transport equation**

Let us return to the heat kernel. We consider the sub-Laplacian

$$\Delta_X = \frac{1}{2} \sum_{k=1}^{n} X_k^2 \quad \text{with} \quad X_k = \frac{\partial}{\partial x_k} + \sum_{j=1}^{n} \sum_{\alpha=1}^{m} a_{kj}^\alpha x_j \frac{\partial}{\partial y_\alpha}.$$

Assume that $\{X_1, \dots, X_n\}$ is an orthonormal basis of the "*horizontal subbundle*" on a simply connected nilpotent 2 step Lie group. The Hamiltonian of the operator Δ_X is

$$H(\mathbf{x}, \mathbf{y}, \xi, \eta) = \frac{1}{2} \sum_{k=1}^{n} \Big(\xi_k + \sum_{j=1}^{n} \sum_{\alpha=1}^{m} a_{kj}^\alpha x_j \eta_\alpha\Big)^2.$$

By Theorem 2.2, the function f associated with H is a solution of the generalized Hamilton-Jacobi equation:

$$H(\mathbf{x}, \mathbf{y}, \nabla_{\mathbf{x}} f, \nabla_{\mathbf{y}} f) + \sum_{\alpha=1}^{m} \tau_\alpha \frac{\partial f}{\partial \tau_\alpha} = f(\mathbf{x}, \mathbf{y}; \eta_1, \dots, \eta_m).$$

As we know, the function f depends on free variables η_α, $\alpha = 1, \dots, m$. To this end we shall sum over η_α, or for convenience $\tau_\alpha = t\eta_\alpha$, $\alpha = 1, \dots, m$; an extra t can always be absorbed in the power q which can be determined after we solve the generalized Hamilton-Jacobi equation. Thus we write heat kernel of $\Delta_X - \frac{\partial}{\partial t}$ as following

$$K(\mathbf{x}, \mathbf{y}; t) = K_t(\mathbf{x}, \mathbf{y}) = \frac{1}{t^q} \int_{\mathbb{R}^m} e^{-\frac{f(\mathbf{x},\mathbf{y},\tau)}{t}} V(\tau) d\tau. \tag{3.1}$$

Here V is the volume element. To see whether (3.1) is a representation of the heat kernel we apply the heat operator to K and take it across the integral.

$$\Big(\Delta_X - \frac{\partial}{\partial t}\Big) \frac{e^{-\frac{f(\mathbf{x},\mathbf{y},\tau)}{t}}}{t^q} = \frac{e^{-\frac{f(\mathbf{x},\mathbf{y},\tau)}{t}}}{t^{q+2}} \big(H(\mathbf{x}, \mathbf{y}, \nabla_{\mathbf{x}} f, \nabla_{\mathbf{y}} f) - f\big) - \frac{e^{-\frac{f(\mathbf{x},\mathbf{y},\tau)}{t}}}{t^{q+1}} \big(\Delta_X(f) - q\big),$$

and the eiconal equation (2.3) implies that

$$\begin{aligned} &\Big(\Delta_X - \frac{\partial}{\partial t}\Big) \frac{e^{-\frac{f(\mathbf{x},\mathbf{y},\tau)}{t}} V(\tau)}{t^q} \\ &= \frac{e^{-\frac{f(\mathbf{x},\mathbf{y},\tau)}{t}}}{t^{q+1}} \sum_{\alpha=1}^m \tau_\alpha \Big(-\frac{1}{t}\frac{\partial f}{\partial \tau_\alpha}\Big) V(\tau) - \frac{e^{-\frac{f(\mathbf{x},\mathbf{y},\tau)}{t}}}{t^{q+1}} \big(\Delta_X f - q\big) V(\tau) \\ &= -\frac{e^{-\frac{f(\mathbf{x},\mathbf{y},\tau)}{t}}}{t^{q+1}} \Big[\sum_{\alpha=1}^m \tau_\alpha \frac{\partial V}{\partial \tau_\alpha} + \big(\Delta_X f - q + m\big) V(\tau)\Big] + \sum_{\alpha=1}^m \frac{\partial}{\partial \tau_\alpha} \Big(\frac{e^{-\frac{f(\mathbf{x},\mathbf{y},\tau)}{t}} \tau_\alpha V(\tau)}{t^{q+1}}\Big). \end{aligned}$$

Assuming

$$\frac{e^{-\frac{f(u)}{t}} \tau_\alpha V(\tau)}{t^{q+1}} \to 0$$

as $\tau_\alpha \to$ the ends of an appropriate contour Γ_α for $\alpha = 1, \dots, m$, one has

$$\begin{aligned} &\Big(\Delta_X - \frac{\partial}{\partial t}\Big) K_t(\mathbf{x}, \mathbf{y}) \\ &= \Big(\Delta_X - \frac{\partial}{\partial t}\Big) \Big\{\frac{1}{t^q} \int_{\cup_{\alpha=1}^m \Gamma_\alpha} e^{-\frac{f(\mathbf{x},\mathbf{y},\tau)}{t}} V(\tau) d\tau\Big\} \\ &= -\frac{1}{t^{q+1}} \int_{\cup_{\alpha=1}^m \Gamma_\alpha} e^{-\frac{f(\mathbf{x},\mathbf{y},\tau)}{t}} \Big[\sum_{\alpha=1}^m \tau_\alpha \frac{\partial V}{\partial \tau_\alpha} + \big(\Delta_X f - q + m\big) V(\tau)\Big] d\tau = 0 \end{aligned}$$

if $t \neq 0$ and

$$\sum_{\alpha=1}^m \tau_\alpha \frac{\partial V}{\partial \tau_\alpha}(\tau) + \big(\Delta_X f - q + m\big) V(\tau) = 0. \tag{3.2}$$

The equation (3.2) is called the first order transport equation.

Remark 3.1. Here we have made a crucial assumption on the volume element, *i.e.,* V does not depend on the space variables $\mathbf{x}$ and $\mathbf{y}$. That simplify the transport equation significantly. Under a more general situation a function V will found among co-dimension one form

$$V d\tau = \sum_{\ell=1}^m (-1)^{\ell-1} V_\ell d\tau_1 \wedge \cdots \wedge \widehat{d\tau_\ell} \wedge \cdots \wedge d\tau_m$$

which satisfies a so-called "generalized transport equation":

$$df\wedge\Delta_X(V)+\sum_{\ell=1}^{n}X_\ell(f)X_\ell(dV)+\mathcal{D}(dV)-\big(\Delta_X f+n-m-1\big)dV=0,$$

where $\mathcal{D}(V)$ is defined by

$$\mathcal{D}(V)=\sum_{k=1}^{m}\tau_k\frac{\partial}{\partial\tau_k}(V)=\sum_{k=1}^{m}\sum_{\ell=1}^{m}(-1)^{\ell-1}\tau_k\frac{\partial V_\ell}{\partial\tau_k}d\tau_1\wedge\cdots\wedge\widehat{d\tau_\ell}\wedge\cdots\wedge d\tau_m.$$

Detailed discussion can be found in Furutani [9] and Greiner [11].

With f given by (2.17), one has

$$\Delta_X f=\frac{1}{2}\mathrm{tr}\big(\mathcal{A}(\tau)\coth(\mathcal{A}(\tau))\big)=\frac{1}{2}\mathrm{tr}\Big(\frac{1}{2\pi i}\int_{\mathcal{C}}\lambda\frac{\cosh(\lambda)}{\sinh(\lambda)}\big(\lambda-i\mathcal{A}(\tau)\big)^{-1}d\lambda\Big). \tag{3.3}$$

Then (3.2) becomes

$$\begin{aligned}&\sum_{\alpha=1}^{m}\tau_\alpha\frac{\partial V}{\partial\tau_\alpha}(\tau)+\big(\Delta_X f-q+m\big)V(\tau)=0\quad\Leftrightarrow\\&\sum_{\alpha=1}^{m}\tau_\alpha\frac{\partial V}{\partial\tau_\alpha}(\tau)=\Big(q-m-\frac{1}{2}\mathrm{tr}\big(\mathcal{A}(\tau)\coth(\mathcal{A}(\tau))\big)\Big)V.\end{aligned} \tag{3.4}$$

Fix τ and define for $0\le\lambda\le1$

$$W(\lambda)=V(\lambda\tau).$$

Hence, (3.4) reduces to

$$\lambda\frac{dW}{d\lambda}=\Big[q-m-\frac{1}{2}\mathrm{tr}\big(\lambda\mathcal{A}(\tau)\coth(\lambda\mathcal{A}(\tau))\big)\Big]W.$$

Here we are using the fact that $\mathcal{A}(\tau)$ is linear in τ. It follows that

$$\frac{dW}{W}=\Big(\frac{q-m}{\lambda}-\frac{1}{2}\mathrm{tr}\big(\mathcal{A}(\tau)\coth(\lambda\mathcal{A}(\tau))\big)\Big)d\lambda.$$

Hence,

$$\log W=(q-m)\big(\log\lambda+\log C\big)-\frac{1}{2}\log(\sinh(\mathcal{A}(\lambda\tau))).$$

Therefore,

$$V(\tau)=\frac{(\det\mathcal{A}(\tau))^{q-m}}{\sqrt{\big(\det\sinh(\mathcal{A}(\tau))\big)}}.$$

If we propose the volume element V is real analytic and non-vanish at 0, then we have $q=\frac{n}{2}+m$.

Consequently,

$$P=\frac{A}{(2\pi t)^q}\int_{\mathbb{R}^m}e^{-\frac{f(\mathbf{x},\mathbf{y},\tau)}{t}}V(\tau)d\tau, \tag{3.5}$$

where f is given by (3.3) and

$$V(\tau)=\frac{(\det\mathcal{A}(\tau))^{\frac{n}{2}}}{\sqrt{\big(\det\sinh(\mathcal{A}(\tau))\big)}}$$

where the branch is taken to be $V(0)=1$. Finally we can write down the second main results on this paper.

Theorem 3.2. *The equation*

$$P_t(\mathbf{x},\mathbf{y}) = \frac{A}{(2\pi t)^q}\int_{\mathbb{R}^m} e^{-\frac{f(\mathbf{x},\mathbf{y},\tau)}{t}} V(\tau)d\tau,$$

represents the heat kernel for Δ_X *if and only if* $q = \frac{n}{2}+m$, *in which case* $A = 1$.

We clearly have

$$\frac{\partial P}{\partial t} - \Delta_X P = 0, \qquad t>0$$

and

$$\lim_{t\to 0} P(\mathbf{x},\mathbf{y},t) = \delta(\mathbf{x})\delta(\mathbf{y}).$$

The calculation is long but straightforward. Readers can find the proof of this theorem in many places, see *e.g.,* [1, 2, 3, 4, 8, 10]. We skip the proof here. Instead, we list some examples.

Example 3.1. The Heisenberg sub-Laplacian: $\Delta_X = \frac{1}{2}\Big(\frac{\partial}{\partial x_1}+2x_2\frac{\partial}{\partial y}\Big)^2+\frac{1}{2}\Big(\frac{\partial}{\partial x_2}-2x_1\frac{\partial}{\partial y}\Big)^2$ which is defined as (1.1). The action function is $f(\mathbf{x},y) = -i\tau y + (x_1^2+x_2^2)\tau\coth(2\tau)$. The volume is $V(\tau) = \frac{2\tau}{\sinh(2\tau)}$. In this case $n=2$, $m=1$ and (3.5) has the following expression:

$$P_t(\mathbf{x},y) = \frac{2}{(2\pi t)^2}\int_{-\infty}^{+\infty} e^{-\frac{f(\mathbf{x},y,\tau)}{t}}\frac{\tau}{\sinh(2\tau)}d\tau. \tag{3.6}$$

Example 3.2. The Grusin operator: $\Delta_G = \frac{1}{2}\Big(\frac{\partial}{\partial x}\Big)^2+\frac{1}{2}x^2\Big(\frac{\partial}{\partial y}\Big)^2$. There is no group structure in this case. However, this operator has connection with the Heisenberg sub-Laplacian. Let $\mathbf{H}_1$ be the Heisenberg group whose Lie algebra has a basis $\{X_1, X_2, T\}$ with the bracket relation $[X_1, X_2] = -4T$. As in (1.1),

$$\Delta_X = -\frac{1}{2}(X_1^2+X_2^2)$$

is the sub-Laplacian on $\mathbf{H}_1$. Let $\mathbf{N}_{X_2} = \langle X_2\rangle = [\{aX_2\}_{a\in\mathbb{R}}]$ be a subgroup generated by the element X_2. The map $\rho:\mathbf{H}_1\to\mathbb{R}^2$ defined by

$$\begin{aligned}\rho:\mathbf{H}_1\to\mathbb{R}^2\cong\mathbf{h}\ni g =& x_1X_1+x_2X_2+zZ\\ =&(x_1,x_2,z)\mapsto(u,v)\in\mathbb{R}^2\end{aligned}$$

where

$$u = x_1, \qquad v = z+\frac{1}{2}x_1x_2$$

realizes the projection map

$$\mathbf{H}_1\cong\mathbb{R}^3 \;\to\; \mathbf{N}_{X_2}\setminus\mathbf{H}_1\cong\mathbb{R}^2.$$

In fact, this is a principal bundle and the trivialization is given by the map

$$\mathbf{N}_{X_2}\times(\mathbf{N}_{X_2}\setminus\mathbf{H}_1)\cong\mathbb{R}\times\mathbb{R}^2\ni(a;u,v)\mapsto(x_1,x_2,z)\in\mathbb{R}^3\cong\mathbf{H}_1$$

where

$$(a;u,v)\;\mapsto\;\big(u,a,v-\frac{1}{2}au\big).$$

So the sub-Laplacian Δ_X on $\mathbf{H}_1$ and Grusin operator Δ_G commutes each other through the map ρ:

$$\Delta_H\circ\rho^* = \rho^*\circ\Delta_G.$$

The heat kernel $P_t(\mathbf{x},y)\in C^\infty(\mathbb{R}_+\times\mathbf{H}_1)$ is given by (3.6). Hence,

$$\int_{-\infty}^{+\infty} P_t\big((x_1,x_2,y),(u,a,v-\frac{1}{2}ua)\big) = P_t^G((x_1+y+\frac{1}{2}x_1x_2),(u,v))$$

that is, the fiber integration of the function $P_t(g,h)$ along the fiber of the map ρ gives the heat kernel of the Grusin operator.

$$P_t^G((x_0,0),(x,y)) = \frac{1}{(2\pi t)^{\frac{3}{2}}} \int_{-\infty}^{+\infty} e^{-\frac{f(x,x_0,y,\tau)}{t}} \sqrt{\frac{|\tau|}{\sinh|\tau|}} d\tau$$

Example 3.3. Step 2 nilpotent Lie group: $\Delta_X = -\frac{1}{2}\sum_{j=1}^n X_j^2$ where

$$X_j = \frac{\partial}{\partial x_j} + \sum_{k=1}^n \Big(\sum_{\alpha=1}^m a_{jk}^\alpha x_k \Big) \frac{\partial}{\partial y_\alpha}$$

with $\mathcal{A}_{jk}^{(\alpha)} = \big[a_{jk}^\alpha\big]_{j,k}$ is a skew-symmetric and orthogonal matrix. The heat kernel is

$$P_t(\mathbf{x},\mathbf{y}) = \frac{1}{(2\pi t)^{\frac{n}{2}+m}} \int_{\mathbb{R}^m} e^{-\frac{2i\mathbf{y}\cdot\tau - \langle \mathcal{A}(\tau)\coth(\mathcal{A}(\tau))\mathbf{x},\mathbf{x}\rangle}{2t}} \sqrt{\det \frac{\mathcal{A}(\tau)}{\sinh(\mathcal{A}(\tau))}} d\tau.$$

Here $\mathcal{A}_{jk}(\tau) = \sum_{\alpha=1}^m a_{jk}^\alpha \tau_\alpha$. In particular, if $\mathcal{A}_{jk}^{(\alpha)}$ satisfies further assumption: $\mathcal{A}_{jk}^{(\alpha)}\mathcal{A}_{jk}^{(\gamma)} + \mathcal{A}_{jk}^{(\gamma)}\mathcal{A}_{jk}^{(\alpha)} = 0$, *i.e.*, the group in a H-type group. Then the heat kernel has the following form:

$$P_t(\mathbf{x},\mathbf{y}) = \frac{1}{(2\pi t)^{\frac{n}{2}+m}} \int_{\mathbb{R}^m} e^{-\frac{2i\mathbf{y}\cdot\tau + |\mathbf{x}|^2|\tau|\coth(|\tau|)}{2t}} \Big(\frac{|\tau|}{\sinh|\tau|}\Big)^{\frac{n}{2}} d\tau.$$

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Department of Mathematics, Eastern Michigan University, Ypsilanti, MI, 48197, USA
E-mail address: ocalin@emunix.emich.edu

Department of Mathematics, Georgetown University, Washington D.C. 20057, USA

Department of Mathematics, National Tsing Hua University, Hsinchu, Taiwan 30013, ROC
E-mail address: chang@georgetown.edu

Department of Mathematics, University of Bergen, Johannes Brunsgate 12, Bergen 5008, Norway
E-mail address: irina.markina@uib.no