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Gradient estimates, Harnack inequalities and estimates for heat kernels of the sum of squares of vector fields

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1 Introduction

In this paper we shall study the equations

$$\left(L - \frac{\partial}{\partial t}\right) u(x, t) = 0 \tag{1.1}$$

and

$$Lu(x) = 0 \tag{1.2}$$

associated to the operator $L = \sum_i X_i^2 - X_0$ on a compact manifold M with a positive measure μ, where $X_1, X_2, \ldots, X_m$ are smooth vector fields on M and $X_0 = \sum_i c_i X_i$. Our main purpose is to prove (Theorem 3.1 and Theorem 3.2) Harnack inequalities for positive solutions of Eq. (1.1) and Eq. (1.2) and to derive (Theorem 4.1) an upper estimate for the fundamental solution of the operator $L - \frac{\partial}{\partial t}$.

Since Hömander's work [3], many people have investigated various properties of such an operator L (see, e.g., [2, 4, 11, 12]). Recently Nagel et al. [10] studied the geometries associated to the operator L. On the other hand, Jerison and Sanchez-Calle [5], Kusuoka and Stroock [6] obtained upper and lower estimates for the heat kernel of $L - \frac{\partial}{\partial t}$ for small time t. Similar upper bounds for the heat kernel was also proved by Melrose [9] using the wave equation method. More recently Kusuoka and Stroock [7] have also investigated the long time behavior of the heat kernel of $L - \frac{\partial}{\partial t}$.

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One of the standard ways in studying the sum of squares of vector fields is to use Rothschild–Stein lifting and reduce the problem to the model cases. In this paper we shall explore a different approach, the method of gradient estimates. The method of gradient estimates, originated first in Yau [13] and Cheng and Yau [1] and further developed in Li and Yau [8], has been used very successfully in studying elliptic and parabolic operators. In §2 we derive gradient estimates (Theorem 2.1 and Theorem 2.2) for positive solutions of Eq. (1.1) and Eq. (1.2) under the assumption that, for $1 \leqq i, j, k \leqq m$, $[X_i, [X_j, X_k]]$ can be expressed as linear combinations of $X_1, \ldots, X_m$ and their brackets $[X_1, X_2], \ldots, [X_{m-1}, X_m]$. It is not surprising that our gradient estimates are more delicate due to the fact that the operator L is only weakly elliptic. Once the gradient estimates are derived the proof of Harnack inequalities and the upper estimate for the heat kernel follows essentially the same way as in [8]. These are given in §3 and §4 respectively.

We hope that the method of gradient estimates can be applied to study other problems related to the sum of squares of vector fields and can be extended to any family of vector fields $X_1, \ldots, X_m$ satisfying the more general condition: the commutators of $X_1, \ldots, X_m$ of order r can be expressed as the linear combinations of $X_1, \ldots, X_m$ and their commutators up to the order $r-1$.

2 Gradient estimates

Let $X_1, X_2, \ldots, X_m$ be smooth vector fields on a compact manifold M. Let

$$L = \sum_i X_i^2 - X_0$$

with

$$X_0 = \sum_i c_i X_i$$

where c_i are some smooth functions on M. Our goal in this section is to derive an estimate on the derivatives of positive solutions $u(x, t)$ on $M \times [0, \infty)$ of the equation

$$\left(L - \frac{\partial}{\partial t}\right) u(x, t) = 0 . \tag{2.1}$$

Throughout this section we shall assume that $X_1, \ldots, X_m$ satisfy the following condition: for $1 \leqq i, j, k \leqq m$, $[X_i, [X_j, X_k]]$ can be expressed as linear combinations of $X_1, \ldots, X_m$ and their brackets $[X_1, X_2], \ldots, [X_{m-1}, X_m]$. i.e., we have

$$[X_i, [X_j, X_k]] = \sum_l a_{ijk}^l X_l + \sum_\alpha b_{ijk}^\alpha Y_\alpha \tag{2.2}$$

where we have set $\{Y_\alpha\} = \{[X_i, X_j]\}$, $\{a_{ijk}^l\}$ and $\{b_{ijk}^\alpha\}$ are some functions on M. Let us denote by

$$\begin{aligned} a &= \max |a_{ijk}^l| & a' &= \max |X_h a_{ijk}^l| \\ b &= \max |b_{ijk}^\alpha| & b' &= \max |X_h b_{ijk}^\alpha| \\ c &= \max |c_i| & c' &= \max\{|X_j c_i|, |Y_\alpha c_i|, |X_j^2 c_i|\} . \end{aligned} \tag{2.3}$$

First we need the following

Lemma 2.1 *Let $u(x, t)$ be a positive solution of Eq. (2.1) and $f = \log u$. For any given constants $\frac{1}{2} < \lambda < 1$ and $\delta > 1$, the function*

$$F = t\left\{\sum_j |X_j f|^2 + \sum_\alpha [1 + |Y_\alpha f|^2]^\lambda - \delta(X_0 f + f_t)\right\}$$

satisfies the inequality

$$\begin{aligned}\left(L - \frac{\partial}{\partial t}\right)F \geqq & -\frac{F}{t} + \frac{t}{m}\left(\sum_i |X_i f|^2 - X_0 f - f_t\right)^2 + t\sum_{i,j}|X_i X_j f|^2 + \frac{t}{2}\sum_\alpha |Y_\alpha f|^2 \\ & + 2\lambda(2\lambda - 1)t\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1}|X_i Y_\alpha f|^2 + 2t\sum_i X_i f[L, X_i]f \\ & - \delta t[L, X_0]f + 2\delta t\sum_i X_i f[X_i, X_0]f \\ & + 2\lambda t\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} Y_\alpha f[L, Y_\alpha]f \\ & + 4\lambda t\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} X_i f Y_\alpha f[X_i, Y_\alpha]f - 2\sum_i X_i f X_i F\,.\end{aligned}$$

Proof. Differentiating F in the direction of X_0, we have

$$\begin{aligned}X_0 F = t\Bigg\{& 2\sum_j X_j f X_0 X_j f + 2\lambda\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} Y_\alpha f X_0 Y_\alpha f \\ & - \delta(X_0^2 f + X_0 f_t)\Bigg\}\,.\end{aligned} \tag{2.4}$$

Similarly, for $i = 1, 2, \ldots, m$, we have

$$\begin{aligned}X_i F = t\Bigg\{& 2\sum_j X_j f X_i X_j f + 2\lambda\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} Y_\alpha f X_i Y_\alpha f \\ & - \delta(X_i X_0 f + X_i f_t)\Bigg\}\,.\end{aligned} \tag{2.5}$$

Differentiating (2.5) once more in the direction X_i and summing over $i = 1, \ldots, m$, we get

$$\begin{aligned}\sum_i X_i^2 F = t\Bigg\{& 2\sum_{i,j}|X_i X_j f|^2 + 2\sum_{i,j} X_j f X_j(X_i^2 f) + 2\sum_{i,j} X_j f[X_i^2, X_j]f \\ & + 2\lambda\sum_{i,\alpha}[1 + |Y_\alpha f|^2]^{\lambda-1} Y_\alpha f[X_i^2, Y_\alpha]f \\ & + 2\lambda\sum_{i,\alpha}[1 + |Y_\alpha f|^2]^{\lambda-1} Y_\alpha f Y_\alpha(X_i^2 f) \\ & + 2\lambda\sum_{i,\alpha}[1 + |Y_\alpha f|^2]^{\lambda-2}(X_i Y_\alpha f)^2[1 + (2\lambda - 1)|Y_\alpha f|^2] \\ & - \delta\left(\sum_i X_i^2 X_0 f + \sum_i X_i^2 f_t\right)\Bigg\}\,.\end{aligned} \tag{2.6}$$

On the other hand, we have

$$F_t = \frac{F}{t} + t\left\{2\sum_j X_j f X_j f_t + 2\lambda \sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} Y_\alpha f Y_\alpha f_t \right.$$
$$\left. - \delta(X_0 f_t + f_{tt})\right\}. \tag{2.7}$$

Combining (2.4), (2.6) and (2.7), we obtain

$$\left(L - \frac{\partial}{\partial t}\right)F = -\frac{F}{t} + t\left\{2\sum_{i,j}|X_i X_j f|^2 + 2\sum_j X_j f X_j\left(L - \frac{\partial}{\partial t}\right)f\right.$$
$$+ 2\sum_j X_j f[L, X_j]f - \delta[L, X_0]f$$
$$+ 2\lambda\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} Y_\alpha f[L, Y_\alpha]f$$
$$+ 2\lambda\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} Y_\alpha f Y_\alpha\left(L - \frac{\partial}{\partial t}\right)f$$
$$+ 2\lambda\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-2}(X_i Y_\alpha f)^2[1 + (2\lambda - 1)|Y_\alpha f|^2]$$
$$\left. - \delta X_0\left(L - \frac{\partial}{\partial t}\right)f - \delta\frac{\partial}{\partial t}\left(L - \frac{\partial}{\partial t}\right)f\right\}. \tag{2.8}$$

Notice that $f = \log u$ satisfies the equation

$$\left(L - \frac{\partial}{\partial t}\right)f = -\sum_i (X_i f)^2 . \tag{2.9}$$

Also

$$\sum_{i,j}|X_i X_j f|^2 = \sum_i |X_i^2 f|^2 + \sum_{i \neq j}|X_i X_j f|^2$$
$$\geqq \frac{1}{m}\left(\sum_i X_i^2 f\right)^2 + \frac{1}{2}\sum_\alpha |Y_\alpha f|^2$$
$$= \frac{1}{m}\left(\sum_i |X_i f|^2 - X_0 f - f_t\right)^2 + \frac{1}{2}\sum_\alpha |Y_\alpha f|^2 . \tag{2.10}$$

Moreover, by (2.4), (2.5), (2.9) and direct computation, we get

$$t\left\{2\sum_j X_j f X_j\left(L - \frac{\partial}{\partial t}\right)f + 2\lambda\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} Y_\alpha f Y_\alpha\left(L - \frac{\partial}{\partial t}\right)f\right.$$
$$\left. - \delta X_0\left(L - \frac{\partial}{\partial t}\right)f - \delta\frac{\partial}{\partial t}\left(L - \frac{\partial}{\partial t}\right)f\right\}$$
$$= -2\sum_i X_i F X_i f + 2\delta t\sum_i X_i f[X_i, X_0]f$$
$$+ 4\lambda t\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} X_i f Y_\alpha f[X_i, Y_\alpha]f . \tag{2.11}$$

Plugging (2.9), (2.10) and (2.11) into (2.8) we obtain Lemma 2.1.

For later purpose we are going to compute certain terms that appear in Lemma 2.1. First

$$[X_0, X_j]f = \sum_i c_i[X_i, X_j]f - \sum_i (X_j c_i)X_i f$$

and

$$\begin{aligned}[L, X_j]f &= \sum_i [X_i^2, X_j]f + [X_0, X_j]f \\ &= \sum_i \{X_i[X_i, X_j]f + [X_i, X_j]X_i f\} + [X_0, X_j]f \\ &= 2\sum_i X_i[X_i, X_j]f - \sum_i [X_i, [X_i, X_j]]f + [X_0, X_j]f .\end{aligned}$$

From (2.2) and (2.3) we have

$$\begin{aligned}|[L, X_j]f| \leqq 2\sum_i |[X_i[X_i, X_j]f| + (ma + c')\sum_i |X_i f| \\ + (mb + c)\sum_\alpha |Y_\alpha f|\end{aligned} \tag{2.12}$$

and

$$|[X_0, X_j]f| \leqq c\sum_\alpha |Y_\alpha f| + c'\sum_i |X_i f| . \tag{2.13}$$

Similarly

$$\begin{aligned}|[L, Y_\alpha]f| &\leqq \left|\sum_i X_i[X_i, Y_\alpha]f\right| + \left|\sum_i [X_i, Y_\alpha]X_i f\right| + |[X_0, Y_\alpha]f| \\ &\leqq 2a\sum_{i,j} |X_i X_j f| + 2b\sum_{i,\beta} |X_i Y_\beta f| + c\sum_i |[X_i, Y_\alpha]f| \\ &\quad + (ma' + C_4 ab + c')\sum_i |X_i f| + (mb' + C_5 b^2)\sum_\alpha |Y_\alpha f| .\end{aligned} \tag{2.14}$$

Also

$$|[X_i, Y_\alpha]f| \leqq a\sum_j |X_j f| + b\sum_\beta |Y_\beta f| . \tag{2.15}$$

Finally

$$\begin{aligned}|[L, X_0]f| &= \left|\sum_i [X_i^2, X_0]f\right| \\ &= \left|\sum_{i,j} c_j[X_i^2, X_j]f + (X_i^2 c_j)X_j f\right| \\ &\leqq 2c\sum_{i,j} |X_i[X_i, X_j]f| + (ma + c')\sum_i |X_i f| + mb\sum_\alpha |Y_\alpha f| .\end{aligned} \tag{2.16}$$

Now we are ready to present our first result in this section.

Proposition 2.1 *Let $u(x, t)$ be a positive solution of Eq. (2.1) on $M \times [0, \infty)$. Then for $1/2 < \lambda < 2/3$, there exists a constant $\delta_0 = \delta_0(\lambda) > 1$ such that for any $\delta > \delta_0$ and $t > 0$, $u(x, t)$ satisfies the estimate*

$$\frac{1}{u^2}\sum_i |X_i u|^2 + \sum_\alpha \left(1 + \frac{1}{u^2}|Y_\alpha u|^2\right)^\lambda - \delta\frac{X_0 u}{u} - \delta\frac{u_t}{u} \leqq C_1 t^{-1} + C_2 + C_3 t^{\frac{\lambda}{\lambda - 1}} \tag{2.17}$$

where C_1, C_2 and C_3 are positive constants depending only on $m, \delta, \lambda, a, a', b, b', c, c'$.

Proof. Consider the function

$$F = t\left\{\sum_j |X_j f|^2 + \sum_\alpha [1 + |Y_\alpha f|^2]^\lambda - \delta(X_0 f + f_t)\right\}, \quad t \geqq 0$$

where

$$f = \log u .$$

We claim that there exist positive constants C_1, C_2 and C_3 such that

$$F \leqq C_1 + C_2 t + C_3 t^{\frac{2\lambda - 1}{\lambda - 1}} . \tag{2.18}$$

If not, then for arbitrary such C_1, C_2 and C_3 we have

$$F > C_1 + C_2 t + C_3 t^{\frac{2\lambda - 1}{\lambda - 1}} \tag{2.19}$$

at the maximum point (x_0, t_0) of F on $M \times [0, T]$ for some $T > 0$. Clearly, $t_0 > 0$, since $F(x, 0) = 0$ by its definition. Then at (x_0, t_0), we have

$$X_i F = 0, \quad \text{for } i = 1, 2, \ldots, m$$

$$\frac{\partial F}{\partial t} \geqq 0 ,$$

and

$$LF \leqq 0 .$$

Applying Lemma 2.1 to F and evaluating at (x_0, t_0), we get

$$\begin{aligned} 0 &\geqq \left(L - \frac{\partial}{\partial t}\right) F(x_0, t_0) \\ &\geqq -\frac{F}{t_0} + \frac{t_0}{m}\left(\sum_i |X_i f|^2 - X_0 f - f_t\right)^2 + t_0 \sum_{i,j} |X_i X_j f|^2 + \frac{t_0}{2}\sum_\alpha |Y_\alpha f|^2 \\ &\quad + 2\lambda(2\lambda - 1)t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda - 1} |X_i Y_\alpha f|^2 + 2t_0 \sum_i X_i f [L, X_i] f \\ &\quad - \delta t_0 [L, X_0] f + 2\delta t_0 \sum_i X_i f [X_i, X_0] f \\ &\quad + 2\lambda t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda - 1} Y_\alpha f [L, Y_\alpha] f \\ &\quad + 4\lambda t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda - 1} X_i f Y_\alpha f [X_i, Y_\alpha] f . \end{aligned}$$

By the estimates (2.12)–(2.16) we see that at (x_0, t_0),

$$
\begin{aligned}
0 \geqq &-\frac{F}{t_0} + \frac{t_0}{m}\Big(\sum_i |X_i f|^2 - X_0 f - f_t\Big)^2 + t_0 \sum_{i,j} |X_i X_j f|^2 + \frac{t_0}{2}\sum_\alpha |Y_\alpha f|^2 \\
&+ 2\lambda(2\lambda - 1)t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} |X_i Y_\alpha f|^2 - 4t_0 \sum_{i,j} |X_i f|\,|X_j[X_j, X_i]f| \\
&- 2(ma + c' + \delta c')t_0 \Big(\sum_i |X_i f|\Big)^2 - 2(mb + c + \delta c)t_0 \sum_i |X_i f| \sum_\alpha |Y_\alpha f| \\
&- 2c\delta \sum_{i,j} |X_i[X_i, X_j]f| - \delta(m^2 a + mc')\sum_i |X_i f| \\
&- \delta(m^2 b + mc)\sum_\alpha |Y_\alpha f| - 4a\lambda t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f| \sum_{i,j}|X_i X_j f| \\
&- 4b\lambda t_0 \sum_{\alpha,i,\beta} [1 + |Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f|\,|X_i Y_\beta f| \\
&- 2(ma' + C_4 ab + c')\lambda t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f| \sum_i |X_i f| \\
&- 2(mb' + C_5 b^2)\lambda t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f| \sum_\beta |Y_\beta f| \\
&- 4a\lambda t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f| \Big(\sum_i |X_i f|\Big)^2 \\
&- 4b\lambda t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f| \sum_i |X_i f| \sum_\beta |Y_\beta f|\,. \qquad (2.20)
\end{aligned}
$$

We need to estimate the right hand side of (2.20). In the following, inequalities of the type

$$
xy \leqq ax^2 + \frac{1}{4a}y^2 \quad (a > 0)
$$

will be used repeatedly. First

$$
\begin{aligned}
\sum_{i,j} |X_i f|\,|X_j[X_j, X_i]f| &\leqq \sum_{i,j,\alpha} |X_i f|\,|X_j Y_\alpha f| \\
&= \sum_{\alpha,j}\Big(\sum_i |X_i f|\Big)[1 + |Y_\alpha f|^2]^{\frac{1-\lambda}{2}} \\
&\quad \times [1 + |Y_\alpha f|^2]^{\frac{\lambda-1}{2}}|X_j Y_\alpha f| \\
&\leqq \frac{m}{\lambda(2\lambda - 1)}\Big(\sum_i |X_i f|\Big)^2\Big(\sum_\alpha [1 + |Y_\alpha f|^2]^{\frac{1-\lambda}{2}}\Big)^2 \\
&\quad + \frac{\lambda(2\lambda - 1)}{4}\sum_{\alpha,i} [1 + |Y_\alpha f|^2]^{\lambda-1}|X_i Y_\alpha f|^2 \qquad (2.21)
\end{aligned}
$$

Hence

$$\sum_{i,j} |X_i f||X_j[X_j, X_i]f| \leqq \varepsilon\left(\sum_i |X_i f|^2\right)^2 + m^2\varepsilon^{-1}(2\lambda-1)^{-2}\left(\sum_\alpha [1+|Y_\alpha f|^2]^{\frac{1-\lambda}{2}}\right)^4 + \frac{\lambda(2\lambda-1)}{4}\sum_{\alpha,i}[1+|Y_\alpha f|^2]^{\lambda-1}|X_i Y_\alpha f|^2 \tag{2.22}$$

where $\varepsilon > 0$ is some constant to be determined.

Similarly

$$2c\delta\sum_{i,j}|X_i[X_i, X_j]f| \leqq \frac{2mc\delta}{\lambda(2\lambda-1)}\left(\sum_\alpha [1+|Y_\alpha f|^2]^{\frac{1-\lambda}{2}}\right)^2 + \frac{\lambda(2\lambda-1)}{2}\sum_{\alpha,i}[1+|Y_\alpha f|^2]^{\lambda-1}|X_i Y_\alpha f|^2 \tag{2.23}$$

$$2(mb+c+\delta c)\sum_i |X_i f|\sum_\alpha |Y_\alpha f| \leqq 16(mb+c+\delta c)^2\left(\sum_i |X_i f|\right)^2 + \frac{1}{16}\left(\sum_\alpha |Y_\alpha f|\right)^2 \tag{2.24}$$

and

$$\begin{aligned} &4a\sum_\alpha [1+|Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f|\sum_{i,j}|X_i X_j f| \\ &\leqq \frac{1}{m^2}\sum_{i,j}|X_i X_j f|^2 + 4a^2m^2\left(\sum_\alpha [1+|Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f|\right)^2 \\ &\leqq \sum_{i,j}|X_i X_j f|^2 + 4a^2m^2\left(\sum_\alpha [1+|Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f|\right)^2 . \end{aligned} \tag{2.25}$$

We also have

$$\begin{aligned} &4b\sum_{\alpha,i,\beta}[1+|Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f||X_i Y_\beta f| \\ &\leqq 8mb^2(2\lambda-1)^{-1}\left(\sum_\alpha [1+|Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f|\right)^2\left(\sum_\beta [1+|Y_\beta f|^2]^{\frac{1-\lambda}{2}}\right)^2 \\ &\quad + \frac{(2\lambda-1)}{2}\sum_{\alpha,i}[1+|Y_\alpha f|^2]^{\lambda-1}|X_i Y_\alpha f| \end{aligned} \tag{2.26}$$

and

$$\begin{aligned} &4a\sum_\alpha [1+|Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f|\left(\sum_i |X_i f|\right)^2 \\ &\leqq \frac{\varepsilon}{m^2}\left(\sum_i |X_i f|\right)^4 + 4m^2a^2\varepsilon^{-1}\left(\sum_\alpha [1+|Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f|\right)^2 \\ &\leqq \varepsilon\left(\sum_i |X_i f|^2\right)^2 + 4m^2a^2\varepsilon^{-1}\left(\sum_\alpha [1+|Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f|\right)^2 . \end{aligned} \tag{2.27}$$

Finally

$$\begin{aligned}
&4b\sum_\alpha [1+|Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f|\sum_i |X_i f|\sum_\beta |Y_\beta f|\\
&\leqq 64m^2b^2\Big(\sum_i |X_i f|\Big)^2\Big(\sum_\alpha [1+|Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f|\Big)^2+\frac{1}{16m^2}\Big(\sum_\beta |Y_\beta f|\Big)^2\\
&\leqq \frac{\varepsilon}{m^2}\Big(\sum_i |X_i f|\Big)^4+C_6b^4\varepsilon^{-1}\Big(\sum_\alpha [1+|Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f|\Big)^4+\frac{1}{16}\sum_\beta |Y_\beta f|^2\\
&\leqq \varepsilon\Big(\sum_i |X_i f|^2\Big)^2+C_6b^4\varepsilon^{-1}\Big(\sum_\alpha [1+|Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f|\Big)^4+\frac{1}{16}\sum_\beta |Y_\beta f|^2 .
\end{aligned}\tag{2.28}$$

We have to divide our discussion into two cases.

Case 1

$$\sum_i |X_j f|^2-\frac{\delta}{\delta_0}(X_0 f+f_t)>0 \tag{2.29}$$

where $\delta_0>1$ is some fixed constant to be chosen and $\delta>\delta_0$.

In this case we observe that

$$\begin{aligned}
\Big(\sum_j |X_j f|^2-X_0 f-f_t\Big)^2&=\Big\{\frac{\delta_0}{\delta}\Big(\sum_j |X_j f|^2-\frac{\delta}{\delta_0}(X_0 f+f_t)\Big)+\Big(1-\frac{\delta_0}{\delta}\Big)\sum_j |X_j f|^2\Big\}^2\\
&\geqq \frac{1}{\delta^2}\Big(\delta_0\sum_j |X_j f|^2-\delta(X_0 f+f_t)\Big)^2+\frac{(\delta-\delta_0)^2}{\delta^2}\Big(\sum_j |X_j f|^2\Big)^2 .
\end{aligned}\tag{2.30}$$

Plug (2.22)–(2.28) and (2.30) into (2.20) and compute. We obtain, at (x_0, t_0),

$$\begin{aligned}
0\geqq &-\frac{F}{t_0}+\frac{t_0}{m\delta^2}\Big(\delta_0\sum_i |X_i f|^2-\delta(X_0 f+f_t)\Big)^2+\frac{(\delta-\delta_0)^2}{m\delta^2}t_0\Big(\sum_j |X_j f|^2\Big)^2\\
&+\frac{3t_0}{8}\sum_\alpha |Y_\alpha f|^2-6\varepsilon t_0\Big(\sum_i |X_i f|^2\Big)^2\\
&-4m^2\varepsilon^{-1}(2\lambda-1)^{-2}t_0\Big(\sum_\alpha [1+|Y_\alpha f|^2]^{\frac{1-\lambda}{2}}\Big)^4\\
&-C_6t_0\Big(\sum_i |X_i f|\Big)^2-\frac{2mc\delta}{\lambda(2\lambda-1)}t_0\Big(\sum_\alpha [1+|Y_\alpha f|^2]^{\frac{1-\lambda}{2}}\Big)^2\\
&-\delta(m^2a+mc')t_0\sum_i |X_i f|-\delta(m^2b+mc)t_0\sum_\alpha |Y_\alpha f|\\
&-8mb^2(2\lambda-1)^{-1}t_0\Big(\sum_\alpha [1+|Y_\alpha f|^2]^{\lambda-1}|Y_\alpha f|\Big)^2\Big(\sum_\beta [1+|Y_\beta f|^2]^{\frac{1-\lambda}{2}}\Big)^2
\end{aligned}$$

$$- 2(mb' + C_5 b^2 + mbc) t_0 \sum_{\alpha,\beta} [1 + |Y_\alpha f|^2]^{\lambda-1} |Y_\alpha f| |Y_\beta f|$$

$$- C_6 b^4 \varepsilon^{-1} \left(\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} |Y_\alpha f| \right)^4$$

$$- C_9 t_0 \left(\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} |Y_\alpha f| \right)^2 . \tag{2.31}$$

Let us denote

$$x = \delta_0 \sum_i |X_i f|^2 - \delta(X_0 f + f_t)$$

and

$$y = \max |Y_\alpha f| .$$

Without loss of generality we may assume that $y > 1$. Then (2.31) becomes

$$0 \geqq -\frac{F}{t_0} + \frac{t_0}{m\delta^2} x^2 + \frac{t_0}{4} y^2 + t_0 \left\{ \frac{(\delta - \delta_0)^2}{m\delta^2} \left(\sum_j |X_j f|^2 \right)^2 - 6\varepsilon \left(\sum_j |X_j f|^2 \right)^2 \right.$$

$$\left. - \delta(m^2 a + mc') \sum_i |X_i f| - C_6 \sum_i |X_i f|^2 \right\}$$

$$+ t_0 \left\{ \frac{1}{8} y^2 - C_7 y^{4(1-\lambda)} - C_8 y^{2(1-\lambda)} - C_9 y^{2(2\lambda-1)} - C_{10} y^{4(2\lambda-1)} \right.$$

$$\left. - C_{11} y^{2\lambda} - C_{12} y \right\} , \tag{2.32}$$

where C_i, $i = 6, 7, \ldots, 12$ are positive constants depending on m, a, a', b, b', c, c', δ, λ.

From the fact that z^2 grows faster than z^a for $0 < a < 2$ and the assumption that $1/2 < \lambda < 2/3$, we see that there exists a constant C_{13} such that the last two terms in (2.32) are bounded from below by $-C_{13} t_0$ provided we choose $\varepsilon < (\delta - \delta_0)^2 / 12 m\delta^2$.

Therefore we obtain the following inequality:

$$0 \geqq \frac{-F}{t_0} + \frac{t_0}{m\delta^2} x^2 + \frac{t_0}{4} y^2 - C_{13} t_0 . \tag{2.33}$$

At (x_0, t_0), we have either

$$x = \delta_0 \sum_i |X_i f|^2 - \delta(X_0 f + f_t) \geqq \sum_\alpha [1 + |Y_\alpha f|^2]^\lambda$$

or

$$\sum_\alpha [1 + |Y_\alpha f|^2]^\lambda \geqq x .$$

In the first case we get, from (2.33),

$$0 \geqq -2 t_0 x + \frac{t_0^2}{m\delta^2} x^2 - C_{13} t_0^2 .$$

This implies that

$$t_0 x \leqq 2m\delta^2 + C_{14} t_0 .$$

Since $\delta_0 > 1$, we have

$$F \leqq t_0 x + t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^\lambda \leqq 2t_0 x \leqq 4m\delta^2 + Ct_0 \tag{2.34}$$

for some constant C depending on $m, \lambda, \delta, a, a', b, b', c, c'$. This is a contradiction to (2.19).

In the second case we have

$$0 \geqq -2C_{15} y^{2\lambda} + \frac{t_0}{4} y^2 - C_{13} t_0 . \tag{2.35}$$

(i) If $t_0 < 1$ then we must have

$$y \leqq C_2 t_0^{\frac{1}{2(\lambda-1)}} .$$

Hence

$$t_0 y^{2\lambda} \leqq C_2 t_0^{\frac{2\lambda-1}{\lambda-1}} ;$$

(ii) If $t_0 \geqq 1$ then

$$0 \geqq -2C_{15} t_0 y^{2\lambda} + \frac{t_0}{4} y^2 - C_{13} t_0 .$$

Therefore

$$0 \geqq -2C_{15} y^{2\lambda} + \frac{y^2}{4} - C_{13} .$$

This implies that

$$y \leqq C_{16}$$

and

$$t_0 y^{2\lambda} \leqq C_{17} t_0$$

for some constant C_{17}. So we conclude that, for $t_0 > 0$,

$$t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^\lambda \leqq C_{18} t_0 y^{2\lambda} \leqq C_{19} t_0 + C_{20} t_0^{\frac{2\lambda-1}{\lambda-1}} .$$

It follows that

$$F \leqq 2t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^\lambda \leqq C_2 t_0 + C_3 t_0^{\frac{2\lambda-1}{\lambda-1}}$$

for some positive constants C_2 and C_3 depending on $m, \lambda, \delta, a, a', b, b', c, c'$, again contradicting (2.19). Together with (2.34) this shows that (2.18) holds under the assumption (2.29).

Case 2

$$\sum_i |X_j f|^2 - \frac{\delta}{\delta_0}(X_0 f + f_t) \leqq 0 .$$

In this case we may assume that

$$(\delta_0 - 1)\sum_i |X_i f|^2 \leqq \sum_\alpha [1 + |Y_\alpha f|^2]^\lambda . \tag{2.36}$$

Otherwise (2.18) follows trivially, since

$$\begin{aligned} F &= t_0 \left\{ \sum_i |X_i f|^2 + \sum_\alpha [1 + |Y_\alpha f|^2]^\lambda - \delta(X_0 f + f_t) \right\} \\ &\leqq t_0 \left\{ \delta_0 \sum_i |X_i f|^2 - \delta(X_0 f + f_t) \right\} \\ &= \delta_0 t_0 \left\{ \sum_i |X_j f|^2 - \frac{\delta}{\delta_0} (X_0 f + f_t) \right\} \leqq 0 . \end{aligned}$$

Plugging (2.2), (2.23)–(2.26) into (2.20) and using (2.36) we obtain, at (x_0, t_0),

$$\begin{aligned} 0 \geqq & -\frac{F}{t_0} + \frac{3t_0}{8} \sum_\alpha |Y_\alpha f|^2 - \frac{4m}{\lambda(2\lambda - 1)} t_0 \left(\sum_i |X_i f| \right)^2 \left(\sum_\alpha [1 + |Y_\alpha f|^2]^{\frac{1-\lambda}{2}} \right)^2 \\ & - C_6 t_0 \left(\sum_i |X_i f| \right)^2 - \frac{2mc\delta}{\lambda(2\lambda - 1)} t_0 \left(\sum_\alpha [1 + |Y_\alpha f|^2]^{\frac{1-\lambda}{2}} \right)^2 \\ & - \delta(m^2 a + mc') t_0 \sum_i |X_i f| \\ & - \delta(m^2 b + mc) t_0 \sum_\alpha |Y_\alpha f| - C_9 t_0 \left(\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda - 1} |Y_\alpha f| \right)^2 \\ & - 8mb^2 (2\lambda - 1)^{-1} t_0 \left(\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda - 1} |Y_\alpha f| \right)^2 \left(\sum_\beta [1 + |Y_\beta f|^2]^{\frac{1-\lambda}{2}} \right)^2 \\ & - 2(mb' + C_5 b^2 + mbc) t_0 \sum_{\alpha, \beta} [1 + |Y_\alpha f|^2]^{\lambda - 1} |Y_\alpha f| |Y_\beta f| \\ & - 4a t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda - 1} |Y_\alpha f| \left(\sum_i |X_i f| \right)^2 \\ & - 4b t_0 \sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda - 1} |Y_\alpha f| \sum_i |X_i f| \sum_\beta |Y_\beta f| \\ \geqq & -\frac{F}{t_0} + \frac{t_0}{4} y^2 + t_0 \left\{ \frac{1}{8} y^2 - \frac{C_{21}}{(\delta_0 - 1)} y^2 - C_{22} y^{2\lambda} - \delta C_{23} y^{2(1-\lambda)} - \delta C_{24} y^\lambda \right. \\ & \left. - \delta C_{25} y - C_{26} y^{2(2\lambda - 1)} - C_{27} y^{4\lambda - 1} - C_{28} y^{3\lambda} \right\} \end{aligned} \tag{2.37}$$

where C_{21} is a positive constant depending only on λ and m.

Choose δ_0 so that $\delta_0 \geqq 16C_{21} + 1$ then for $1/2 < \lambda < 2/3$ there exists some constant C_{29} such that the last term in (2.37) is bounded by $-C_{29} t_0$. Therefore, at (x_0, t_0),

$$0 \geqq -\frac{F}{t_0} + \frac{t_0}{4} y^2 - C_{29} t_0 \geqq -C_{15} y^{2\lambda} + \frac{t_0}{4} y^2 - C_{29} t_0 .$$

Then the same argument as in treating (2.35) implies (2.18). Thus the proof of Proposition 2.1 is completed.

For small t we have a slightly different estimate

Proposition 2.2 *For $0 < t \leqq 1$ and $1/2 < \lambda < 2/3$, there exists a constant C such that*

$$\frac{1}{u^2}\sum_i |X_i u|^2 + t^{2\lambda-1}\sum_\alpha \left(1 + \frac{1}{u^2}|Y_\alpha u|^2\right)^\lambda - \delta\frac{X_0 u}{u} - \delta\frac{u_t}{u} \leqq Ct^{-1}.$$

Proof. The arguement is essentially the same as in the proof of Proposition 2.1. In this case we consider instead the function

$$F = F_1 + F_2 = t\left\{\sum_j |X_j f|^2 - \delta(X_0 f + f_t)\right\} + t^{2\lambda}\sum_\alpha [1 + |Y_\alpha f|^2]^\lambda$$

with $1/2 < \lambda < 2/3$.

At the maximum point (x_0, t_0) for F on $M \times [0, 1]$ we have the following inequality

$$\begin{aligned}
0 &\geqq \left(L - \frac{\partial}{\partial t}\right) F(x_0, t_0) \\
&\geqq -\frac{F_1}{t_0} - \frac{2\lambda F_2}{t_0} + \frac{t_0}{m}\left(\sum_i |X_i f|^2 - X_0 f - f_t\right)^2 \\
&\quad + t_0 \sum_{i,j} |X_i X_j f|^2 + \frac{t_0}{2}\sum_\alpha |Y_\alpha f|^2 \\
&\quad + 2\lambda(2\lambda - 1)t_0^{2\lambda}\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1}|X_i Y_\alpha f|^2 + 2t_0\sum_i X_i f[L, X_i] f \\
&\quad + 2\lambda t_0^{2\lambda}\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} Y_\alpha f[L, Y_\alpha] f \\
&\quad + 4\lambda\varepsilon t_0^{2\lambda}\sum_\alpha [1 + |Y_\alpha f|^2]^{\lambda-1} X_i f Y_\alpha f[X_i, Y_\alpha] f.
\end{aligned}$$

For case 1, all we need to modify are the estimates (2.22) and (2.23). We have instead

$$\begin{aligned}
\sum_{i,j} |X_i f||X_j[X_j, X_i] f| &\leqq \sum_{i,j,\alpha} |X_i f||X_j Y_\alpha f| \\
&\leqq \varepsilon\left(\sum_i |X_i f|^2\right)^2 + m^2\varepsilon^{-1}(2\lambda - 1)^{-2} t_0^{2-4\lambda}\left(\sum_\alpha [1 + |Y_\alpha f|^2]^{\frac{1-\lambda}{2}}\right)^4 \\
&\quad + \frac{\lambda(2\lambda - 1)}{4} t_0^{2\lambda-1}\sum_{\alpha,i} [1 + |Y_\alpha f|^2]^{\lambda-1}|X_i Y_\alpha f|^2,
\end{aligned}$$

and

$$\begin{aligned}
2c\delta\sum_{i,j} |X_i[X_i, X_j] f| &\leqq \frac{2mc\delta}{\lambda(2\lambda - 1)} t_0^{1-2\lambda}\left(\sum_\alpha [1 + |Y_\alpha f|^2]^{\frac{1-\lambda}{2}}\right)^2 \\
&\quad + \frac{\lambda(2\lambda - 1)}{2} t_0^{2\lambda-1}\sum_{\alpha,i} [1 + |Y_\alpha f|^2]^{\lambda-1}|X_i Y_\alpha f|^2.
\end{aligned}$$

Corresponding to (2.33), we have

$$0 \geqq -\frac{F_1}{t_0} - \frac{2\lambda F_2}{t_0} + \frac{t_0}{m\delta^2} x^2 + \frac{t_0}{4} y^2 - C_{30} t_0^{3-4\lambda} y^{4-4\lambda}$$
$$- C_{31} t_0^{2-2\lambda} y^{2-2\lambda} - C_{32} t_0 \tag{2.38}$$

because $t_0 \leqq 1$.

Multiplying t_0 to (2.38), we get

$$0 \geqq -t_0 x - C_{33}(t_0 y)^{2\lambda} + \frac{t_0^2}{m\delta^2} x^2 + \frac{t_0^2}{4} y^2 - C_{30}(t_0 y)^{4-4\lambda}$$
$$- C_{31}(t_0 y)^{2-2\lambda} - C_{32} t_0^2 .$$

Since $1/2 < \lambda < 2/3$, there exists a positive constant C_{34} such that

$$\frac{t_0^2}{4} y^2 - C_{33}(t_0 y)^{2\lambda} - C_{30}(t_0 y)^{4-4\lambda} - C_{31}(t_0 y)^{2-2\lambda} \leqq -C_{34} .$$

Hence

$$0 \geqq -t_0 x + \frac{t_0^2}{m\delta^2} x^2 - C_{35} .$$

It follows that $F \leqq C'$ for some positive constant C'.

For case 2 the modification is similar and we again have $F \leqq C'$. This finishes the proof of Proposition 2.2.

Combining Proposition 2.1 with Proposition 2.2, we obtain the following main result of this section.

Theorem 2.1 *Let $X_1, X_2, \ldots, X_m$ be smooth vector fields on a compact manifold M satisfying the condition (2.2). Then there exists a constant $\delta_0 > 1$ such that for any positive solution $u(x, t)$ of Eq. (1.1) on $M \times [0, \infty)$, any $\delta > \delta_0$ and $t > 0$, we have the estimate*

$$\frac{1}{u^2} \sum_i |X_i u|^2 - \delta \frac{X_0 u}{u} - \delta \frac{u_t}{u} \leqq C_1' t^{-1} + C_2'$$

where C_1' and C_2' are positive constants depending on m, δ_0, δ, a, a', b, b', c, c'.

For positive solutions of Eq. (1.2) we have

Theorem 2.2 *Let $u(x, t)$ be a positive solution of the equation*

$$Lu(x) = 0$$

on M. Then for $0 < \lambda < 2/3$, there exists a constant $\delta_0 = \delta_0(\lambda)$ such that for any $\delta > \delta_0$, $u(x)$ satisfies the estimate

$$\frac{1}{u^2} \sum_i |X_i u|^2 + \sum_\alpha \left[1 + \frac{1}{u^2} |Y_\alpha u|^2\right]^\lambda - \delta \frac{X_0 u}{u} \leqq C_3'$$

where C_3' is a positive constant depending on m, λ, δ, a, a', b, b', c, c'.

The proof of Theorem 2.2 follows from Proposition 2.1.

3 Harnack inequalities

In this section we shall derive Harnack inequalities for positive solutions of Eq. (1.1) and Eq. (1.2). Let $X_1, \ldots, X_m$ be smooth vector fields on a compact manifold M with a positive measure μ. We assume that $X_1, \ldots, X_m$ satisfy Hörmander's condition: the vector fields $X_1, \ldots, X_m$ together with their commutators up to certain finite order r span the tangent space at every point of M.

In this case there is a natural distance $d(x, y)$ on M associated to the operator L:

$$d(x, y) = \inf\{b \mid \exists \text{ an admissible curve } \gamma\colon [0, b] \to M \text{ with } \gamma(0) = x, \gamma(b) = y\} \tag{3.1}$$

where an admissible curve γ is a Lipschitz curve such that

$$\gamma'(s) = \sum_i a_i(s) X_i(\gamma(s))$$

for some functions $a_i(s)$ satisfying $\sum_i a_i(s)^2 \leqq 1$. Balls for the metric d are denoted by

$$B_x(r) = \{ y \in M \mid d(x, y) < r\} . \tag{3.2}$$

Theorem 3.1 *Let $X_1, X_2, \ldots, X_m$ be smooth vector fields on a compact manifold M satisfying the condition* (2.2) *and Hörmander's condition. Then there exists a constant $\delta_0 > 1$ such that for any positive solution $u(x, t)$ of Eq.* (1.1) *on $M \times [0, \infty)$ and any $\delta > \delta_0$, $0 < t_1 < t_2$, and $x, y \in M$, we have*

$$u(x, t_1) \leqq u(y, t_2) \left(\frac{t_2}{t_1}\right)^{C_4'} \exp\left(\frac{\delta}{2(t_2 - t_1)} d^2(x, y) + C_5'(t_2 - t_1)\right),$$

where C_4' and C_5' are positive constants depending on m, δ_0, δ, a, a', b, b', c, c'.

Proof. Let γ be an admissible curve given by γ: $[0, b] \to M$, with $\gamma(0) = y$ and $\gamma(b) = x$. We define η: $[0, b] \to M \times [t_1, t_2]$ by

$$\eta(s) = \left(\gamma(s), \frac{(b - s)t_2 + st_1}{b}\right).$$

Clearly $\eta(0) = (y, t_2)$ and $\eta(b) = (x, t_1)$. Integrating $(d/ds)(\log u)$ along γ, we have

$$\begin{aligned}\log u(x, t_1) - \log u(y, t_2) &= \int_0^b \left(\frac{d}{ds} \log u\right) ds \\ &= \int_0^b \left\{\sum_i a_i X_i \log u - \frac{(t_2 - t_1)}{b} (\log u)_t\right\} ds .\end{aligned}$$

Applying Theorem 2.1, we get

$$\begin{aligned}\log\left(\frac{u(x, t_1)}{u(y, t_2)}\right) \leqq \int_0^b &\left\{\sum_i |a_i| |X_i \log u| + \frac{(t_2 - t_1)}{b\delta} (C_1' t^{-1} + C_2') \right. \\ &\left. - \frac{(t_2 - t_1)}{b}\left(\delta^{-1} \sum_i |X_i \log u|^2 - X_0 \log u\right)\right\} ds\end{aligned}$$

$$\leqq \int_0^b \left\{ \sum_i (|a_i||X_i \log u| - \frac{(t_2 - t_1)}{2b\delta}|X_i \log u|^2) \right.$$

$$+ \frac{(t_2 - t_1)}{b\delta}(C_1' t^{-1} + C_2')$$

$$\left. + \frac{(t_2 - t_1)}{b\delta} \sum_i \left(c\delta |X_i \log u| - \frac{1}{2}|X_i \log u|^2 \right) \right\} ds$$

$$\leqq \int_0^b \left\{ \frac{\delta b}{2(t_2 - t_1)} \sum_i |a_i|^2 \right.$$

$$\left. + \frac{(t_2 - t_1)}{b\delta}\left(C_1' t^{-1} + C_2' + \frac{mc^2\delta^2}{2} \right) \right\} ds . \tag{3.3}$$

Since $t = (b - s)t_2/b + st_1/b$, and γ is admissible, (3.3) gives

$$\log\left(\frac{u(x, t_1)}{u(y, t_2)}\right) \leqq \frac{\delta b^2}{2(t_2 - t_1)} + C_1' \delta^{-1} \log\left(\frac{t_2}{t_1}\right) + \left(C_2' \delta^{-1} + \frac{mc^2 \delta}{2} \right)(t_2 - t_1) .$$

Because γ is an arbitrary admissible curve between x and y we therefore obtain

$$\log\left(\frac{u(x, t_1)}{u(y, t_2)}\right) \leqq \frac{\delta d(x, y)^2}{2(t_2 - t_1)} + C_1' \delta^{-1} \log\left(\frac{t_2}{t_1}\right) + \left(C_2' \delta^{-1} + \frac{mc^2 \delta}{2} \right)(t_2 - t_1) .$$

The theorem follows by taking exponentials of the above inequality.

If we apply Theorem 2.2 instead, the same method yields

Theorem 3.2 *Let $u(x)$ be a positive solution of the equation*

$$Lu(x) = 0$$

on M. Then there exists a constant $\delta_0 > 1$ such that for any $\delta > \delta_0$ and $x, y \in M$, we have

$$u(x) \leqq \exp(Cd(x, y))u(y)$$

for some positive constant C.

Various mean value type inequalities can be obtained from Theorem 3.1 and Theorem 3.2. For example, we have

$$u(x, t_1) \leqq \left(\int_{B_x(r)} u^2(y, t_2)dy \right)^{1/2} \left(\frac{t_2}{t_1}\right)^{C_4'} \exp\left(\frac{\delta r^2}{2(t_2 - t_1)} + C_5'(t_2 - t_1) \right) . \tag{3.4}$$

4 An upper estimate for the heat kernel

Let M be a compact manifold with a positive measure μ. Let $X_1, X_2, \ldots, X_m$ be smooth vector fields on M satisfying Hörmander's condition and condition (2.2). We assume that the operator $L = \sum_i X_i^2 - X_0$ is self-adjoint with respect to the measure μ. Our goal in this section is to derive an upper estimate for the fundamental solution $H(x, y, t)$ of Eq. (1.1) on $M \times M \times (0, \infty)$.

Let $d(x, y)$ be the distance function on M as defined in (3.1) and

$$\rho(x, y, t) = \frac{1}{2t} d^2(x, y), \quad (t > 0) . \tag{4.1}$$

For $d(x, y)$ we have

$$\sum_i |X_i d|^2(x, y) \leqq 1$$

in the weak sense on M. Therefore $\rho(x, y, t)$ satisfies

$$\frac{1}{2}\sum_i |X_i \rho|^2 + \rho_t \leqq 0 . \tag{4.2}$$

Define

$$g(x, y, t) = -\rho(x, y, (1 + 2\alpha)T - t) . \tag{4.3}$$

Then we also have

$$\frac{1}{2}\sum_i |X_i g|^2 + g_t \leqq 0 . \tag{4.4}$$

Following [8] we set

$$F(y, t) = \int_{S_1} H(y, z, t) H(x, z, T) dz$$

for $x \in M$, $0 \leqq t \leqq \tau < (1 + 2\alpha)T$, and $S_1 \subseteq M$. Then for any subset $S_2 \subseteq M$, we have

Lemma 4.1

$$\int_{S_2} F^2(z, \tau) dz \leqq \int_{S_1} H^2(x, z, T) dz \sup_{z \in S_2} \exp(-\rho(x, z, (1 + 2\alpha)T))$$
$$\times \sup_{z \in S_2} \exp(\rho(x, z, (1 + 2\alpha)T - \tau)) .$$

Proof. As a function of y, $F(y, t)$ satisfies Eq. (1.1), therefore

$$0 = 2\int_0^\tau \int_M e^{g(x, y, t)} F(y, t)\left(L_y - \frac{\partial}{\partial t}\right) F(y, t) . \tag{4.5}$$

Integrating the right hand side of (4.5) by parts and using (4.4) we get

$$\begin{aligned}
0 &= -2\int_0^\tau \int_M e^g |X_i F|^2 - 2\int_0^\tau e^g F \sum_i X_i F X_i g \\
&\quad + \int_0^\tau \int_M e^g F^2 g_t - \int_M e^g F^2|_{t=\tau} + \int_M e^g F^2|_{t=0} \\
&\leqq -\int_M e^g F^2|_{t=\tau} + \int_M e^g F^2|_{t=0} \\
&\quad - 2\int_0^\tau \int_M e^g \sum_i \left(X_i F + \frac{1}{2} F X_i g\right)^2 .
\end{aligned}$$

Hence

$$\int_M e^{g(x,y,\tau)}F^2(y,\tau) \leqq \int_M e^{g(x,y,0)}F^2(y,0) .$$

But

$$F(y,0) = \begin{cases} H(x,y,T), & \text{if } y \in S_1 ; \\ 0, & \text{otherwise} . \end{cases}$$

Thus

$$\int_M e^{g(x,y,0)}F^2(y,0) \leqq \sup_{z \in S_1} \exp(-\rho(x,z,(1+2\alpha)T) \int_{S_1} H^2(x,z,T)dz .$$

On the other hand

$$\begin{aligned}\int_M e^{g(x,y,\tau)}F^2(y,\tau) &\geqq \int_{S_2} e^{g(x,y,\tau)}F^2(y,\tau) \\ &\geqq \inf_{z \in S_2} \exp(-\rho(x,z,(1+2\alpha)T-\tau)) \int_{S_2} F^2(z,\tau)dz .\end{aligned}$$

This proves Lemma 4.1.

Theorem 4.1 *Let $X_1, X_2, \ldots, X_m$ be smooth vector fields on a compact manifold M satisfying Hörmander's condition and the condition* (2.2). *Let L be self-adjoint with respect to the measure μ on M. Then for some $\delta > 1$ and $0 < \varepsilon < 1$, the fundamental solution $H(x,y,t)$ of Eq.* (1.1) *satisfies the estimate*

$$H(x,y,t) \leqq C(\varepsilon)^{\delta} V^{-1/2}(B_x(\sqrt{t}))V^{-1/2}(B_y(\sqrt{t}))\exp\left(C_5'\varepsilon t - \frac{d^2(x,y)}{(4+\varepsilon)t}\right)$$

where $C(\varepsilon)$ depends on ε with $C(\varepsilon) \to \infty$ as $\varepsilon \to 0$.

Proof. Applying Theorem 3.1 to the function $F(y,t)$ in Lemma 4.1 and take $S_1 = B_y(\sqrt{t})$, $S_2 = B_x(\sqrt{t})$ with $\tau = (1+\alpha)T$, we have

$$\begin{aligned}\left(\int_{B_y(\sqrt{t})} H^2(x,z,T)dz\right)^2 &= F^2(x,T) \\ &\leqq V^{-1}(B_x(\sqrt{t})) \int_{B_x(\sqrt{t})} F^2(z,(1+\alpha)T)dz \\ &\quad \times (1+\alpha)^{2C_4'} \exp\left(\frac{\delta t}{\alpha T} + 2C_5'\alpha T\right) \\ &\leqq V^{-1}(B_x(\sqrt{t})) \int_{B_y(\sqrt{t})} H^2(x,z,T)dz(1+\alpha)^{2C_4'} \\ &\quad \times \exp\left(\frac{\delta t}{\alpha T} + 2C_5'\alpha T + \frac{t}{2\alpha T}\right. \\ &\quad \left. - \inf_{z \in B_y(\sqrt{t})} \rho(x,z,(1+2\alpha)T)\right) .\end{aligned}$$

So we obtain

$$\int_{B_y(\sqrt{t})} H^2(x, z, T)dz \leqq V^{-1}(B_x(\sqrt{t}))(1 + \alpha)^{2C'_4}\exp\left(\frac{(2\delta + 1)t}{2\alpha T} + 2C'_5\alpha T\right)$$
$$\times \exp\left(- \inf_{z \in B_y(\sqrt{t})} \rho(x, z, (1 + 2\alpha)T)\right).$$

Applying Theorem 3.1 once more to $H(x, z, t)$ and setting $T = (1 + \alpha)t$, this yields

$$\begin{aligned} H^2(x, y, t) &\leqq V^{-1}(B_y(\sqrt{t})) \int_{B_y(\sqrt{t})} H^2(x, z, T)dz(1 + \alpha)^{2C'_4}\exp\left(\frac{\delta}{\alpha} + 2C'_5\alpha t\right) \\ &\leqq V^{-1}(B_x(\sqrt{t}))V^{-1}(B_y(\sqrt{t}))(1 + \alpha)^{4C_1}\exp\left(\frac{(4\delta + 2\alpha + 1)}{2\alpha(1 + \alpha)}\right. \\ &\quad \left. + 2C'_5\alpha(2 + \alpha)t\right) \\ &\quad \times \exp\left(- \inf_{z \in B_y(\sqrt{t})} \rho(x, z, (1 + \alpha)(1 + 2\alpha)t)\right). \end{aligned} \tag{4.6}$$

If $x \in B_y(\sqrt{t})$, then

$$\inf_{z \in B_y(\sqrt{t})} \rho(x, z, (1 + \alpha)(1 + 2\alpha)t) = 0 \geqq \frac{d^2(x, y)}{2t} - \frac{1}{2}. \tag{4.7}$$

Otherwise, $d(x, y) > \sqrt{t}$ and we have

$$\inf_{z \in B_y(\sqrt{t})} \rho(x, z, (1 + \alpha)(1 + 2\alpha)t) = \inf_{z \in B_y(\sqrt{t})} \frac{d^2(x, z)}{2(1 + \alpha)(1 + 2\alpha)t} \geqq \frac{(d(x, y) - \sqrt{t})^2}{2(1 + \alpha)(1 + 2\alpha)t}.$$

Applying the inequality

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

to the above and setting $2(1 + \alpha)^2(1 + 2\alpha) = 2 + \varepsilon/2$ we obtain

$$\inf_{z \in B_y(\sqrt{t})} \rho(x, z, (1 + \alpha)(1 + 2\alpha)t) \geqq \frac{2d^2(x, y)}{(4 + \varepsilon)t} - \frac{2(1 + \alpha)}{\alpha(4 + \varepsilon)}.$$

This together with (4.6) and (4.7) proves Theorem 4.1.

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