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SUBGRADIENT ESTIMATE AND LIOUVILLE-TYPE THEOREM FOR THE CR HEAT EQUATION ON HEISENBERG GROUPS*

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Abstract. In this paper, we first get a subgradient estimate of the CR heat equation on a closed pseudohermitian $(2n+1)$-manifold. Secondly, by deriving the CR version of sub-Laplacian comparison theorem on an $(2n+1)$-dimensional Heisenberg group H^n, we are able to establish a subgradient estimate and then the Liouville-type theorem for the CR heat equation on H^n.

Key words. Subgradient estimate, Liouville-type Theorem, Heat Kernel, Pseudohermitian manifold, Heisenberg Group, CR-pluriharmonic, CR-Paneitz operator, Sub-Laplacian, Li-Yau Harnack inequality.

AMS subject classifications. Primary 32V05, 32V20; Secondary 53C56

1. Introduction. In the paper of [Y], S.-T. Yau derived a gradient estimate for positive harmonic functions on a complete noncompact Riemannian manifold. As a consequence, Liouville-type theorems can be proved for manifolds of nonnegative Ricci curvature. Moreover, in the paper of [LY], P. Li and S.-T. Yau established the parabolic Li-Yau gradient estimate and Li-Yau Harnack inequality for the positive solution of the heat equation on a complete Riemannian manifold.

However for a pseudohermitian $(2n+1)$-manifold (M, J, θ), the corresponding estimates are not clear due to a lack of sub-Laplacian comparison theorem and CR Bochner formula. In this paper, we consider the CR heat equation (1.6) with respect to the sub-Laplacian on (M, J, θ). By using the arguments of [LY] and CR Bochner formula (2.1), we are able to derive the CR version of parabolic Li-Yau gradient estimate and the so-called reversed Li-Yau Harnack inequality for the positive solution of CR heat equation. Then by combining the standard parabolic Li-Yau gradient estimate, we derive a subgradient estimate of the CR heat equation on closed pseudohermitian $(2n+1)$-manifolds. Moreover, by deriving the CR version of sub-Laplacian comparison theorem on $(2n+1)$-dimensional Heisenberg groups H^n, we are able to establish the subgradient estimate and the Liouville-type theorem for the CR heat equation on H^n.

The main key step is to derive the CR version of Bochner formula. This formula (2.1) involving a third order operator P which characterizes CR-pluriharmonic functions ([L1]), is hard to control. However after integrating by parts (see 1.5), we are able to relate this extra term to the CR Paneitz operator P_0.

We first give a brief introduction to pseudohermitian geometry (see [L1] for more details). Let (M, ξ) be a $(2n+1)$-dimensional, orientable, contact manifold with contact structure ξ, $\dim_R \xi = 2n$. A CR structure compatible with ξ is an endomorphism $J : \xi \to \xi$ such that $J^2 = -1$. We also assume that J satisfies the following integrability condition: If X and Y are in ξ, then so is $[JX, Y] + [X, JY]$

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and $J([JX,Y]+[X,JY])=[JX,JY]-[X,Y]$. A CR structure J can extend to $\mathbb{C}\otimes\xi$ and decomposes $\mathbb{C}\otimes\xi$ into the direct sum of $T_{1,0}$ and $T_{0,1}$ which are eigenspaces of J with respect to i and $-i$, respectively. A manifold M with a CR structure is called a CR manifold. A pseudohermitian structure compatible with ξ is a CR structure J compatible with ξ together with a choice of contact form θ. Such a choice determines a unique real vector field T transverse to ξ, which is called the the characteristic vector field of θ, such that $\theta(T)=1$ and $\mathcal{L}_T\theta=0$ or $d\theta(T,\cdot)=0$. Let $\{T,Z_\alpha,Z_{\bar\alpha}\}$ be a frame of $TM\otimes\mathbb{C}$, where Z_α is any local frame of $T_{1,0}$, $Z_{\bar\alpha}=\overline{Z_\alpha}\in T_{0,1}$ and T is the characteristic vector field. Then $\{\theta,\theta^\alpha,\theta^{\bar\alpha}\}$, which is the coframe dual to $\{T,Z_\alpha,Z_{\bar\alpha}\}$, satisfies

$$d\theta=ih_{\alpha\bar\beta}\theta^\alpha\wedge\theta^{\bar\beta}, \tag{1.1}$$

for some hermitian matrix of functions $(h_{\alpha\bar\beta})$. Actually we can always choose Z_α such that $h_{\alpha\bar\beta}=\delta_{\alpha\beta}$; hence, throughout this paper, we assume $h_{\alpha\bar\beta}=\delta_{\alpha\beta}$.

The Levi form $\langle\ ,\ \rangle_{L_\theta}$ is the Hermitian form on $T_{1,0}$ defined by

$$\langle Z,W\rangle_{L_\theta}=-i\left\langle d\theta,Z\wedge\overline{W}\right\rangle.$$

We can extend $\langle\ ,\ \rangle_{L_\theta}$ to $T_{0,1}$ by defining $\left\langle\overline{Z},\overline{W}\right\rangle_{L_\theta}=\overline{\langle Z,W\rangle}_{L_\theta}$ for all $Z,W\in T_{1,0}$. The Levi form induces naturally a Hermitian form on the dual bundle of $T_{1,0}$, denoted by $\langle\ ,\ \rangle_{L_\theta^*}$, and hence on all the induced tensor bundles. Integrating the Hermitian form (when acting on sections) over M with respect to the volume form $d\mu=\theta\wedge d\theta$, we get an inner product on the space of sections of each tensor bundle. We denote the inner product by the notation $\langle\ ,\ \rangle$. For example

$$\langle\varphi,\psi\rangle=\int_M\varphi\bar\psi\ d\mu,$$

for functions φ and ψ.

The pseudohermitian connection of (J,θ) is the connection ∇ on $TM\otimes\mathbb{C}$ (and extended to tensors) given in terms of a local frame $Z_\alpha\in T_{1,0}$ by

$$\nabla Z_\alpha=\theta_\alpha{}^\beta\otimes Z_\beta,\quad\nabla Z_{\bar\alpha}=\theta_{\bar\alpha}{}^{\bar\beta}\otimes Z_{\bar\beta},\quad\nabla T=0,$$

where $\theta_\alpha{}^\beta$ are the 1-forms uniquely determined by the following equations:

$$\begin{aligned}d\theta^\beta&=\theta^\alpha\wedge\theta_\alpha{}^\beta+\theta\wedge\tau^\beta,\\0&=\tau_\alpha\wedge\theta^\alpha,\\0&=\theta_\alpha{}^\beta+\theta_{\bar\beta}{}^{\bar\alpha},\end{aligned}\tag{1.2}$$

We can write (by Cartan lemma) $\tau_\alpha=A_{\alpha\gamma}\theta^\gamma$ with $A_{\alpha\gamma}=A_{\gamma\alpha}$. The curvature of the Webster-Stanton connection, expressed in terms of the coframe $\{\theta=\theta^0,\theta^\alpha,\theta^{\bar\alpha}\}$, is

$$\begin{aligned}\Pi_\beta{}^\alpha&=\overline{\Pi_{\bar\beta}{}^{\bar\alpha}}=d\theta_\beta{}^\alpha-\theta_\beta{}^\gamma\wedge\theta_\gamma{}^\alpha,\\\Pi_0{}^\alpha&=\Pi_\alpha{}^0=\Pi_0{}^{\bar\beta}=\Pi_{\bar\beta}{}^0=\Pi_0{}^0=0.\end{aligned}$$

Webster showed that $\Pi_\beta{}^\alpha$ can be written

$$\Pi_\beta{}^\alpha=R_\beta{}^\alpha{}_{\rho\bar\sigma}\theta^\rho\wedge\theta^{\bar\sigma}+W_\beta{}^\alpha{}_\rho\theta^\rho\wedge\theta-W^\alpha{}_{\beta\bar\rho}\theta^{\bar\rho}\wedge\theta+i\theta_\beta\wedge\tau^\alpha-i\tau_\beta\wedge\theta^\alpha$$

where the coefficients satisfy

$$R_{\beta\bar{\alpha}\rho\bar{\sigma}} = \overline{R_{\alpha\bar{\beta}\sigma\bar{\rho}}} = R_{\bar{\alpha}\beta\bar{\sigma}\rho} = R_{\rho\bar{\alpha}\beta\bar{\sigma}}, \quad W_{\beta\bar{\alpha}\gamma} = W_{\gamma\bar{\alpha}\beta}.$$

We will denote components of covariant derivatives with indices preceded by comma; thus write $A_{\alpha\beta,\gamma}$. The indices $\{0, \alpha, \bar{\alpha}\}$ indicate derivatives with respect to $\{T, Z_\alpha, Z_{\bar{\alpha}}\}$. For derivatives of a scalar function, we will often omit the comma, for instance, $f_\alpha = Z_\alpha f,\ f_{\alpha\bar{\beta}} = Z_{\bar{\beta}} Z_\alpha f - \theta_\alpha{}^\gamma (Z_{\bar{\beta}}) Z_\gamma f,\ f_0 = Tf$ for a (smooth) function.

For a real function f, the subgradient ∇_b is defined by $\nabla_b f \in \xi$ and $\langle Z, \nabla_b f\rangle_{L_\theta} = df(Z)$ for all vector fields Z tangent to contact plane. Locally $\nabla_b f = \sum_\alpha f_{\bar{\alpha}} Z_\alpha + f_\alpha Z_{\bar{\alpha}}$. We can use the connection to define the subhessian as the complex linear map

$$(\nabla^H)^2 f : T_{1,0} \oplus T_{0,1} \to T_{1,0} \oplus T_{0,1},$$

by

$$(\nabla^H)^2 f(Z) = \nabla_Z \nabla_b f.$$

Also

$$\Delta_b f = Tr\left((\nabla^H)^2 f\right) = \textstyle\sum_\alpha (f_{\alpha\bar{\alpha}} + f_{\bar{\alpha}\alpha}).$$

The Webster-Ricci tensor and the torsion tensor on $T_{1,0}$ are defined by

$$Ric(X, Y) = R_{\alpha\bar{\beta}} X^\alpha Y^{\bar{\beta}},$$

and

$$Tor(X, Y) = i \textstyle\sum_{\alpha,\beta} (A_{\bar{\alpha}\bar{\beta}} X^{\bar{\alpha}} Y^{\bar{\beta}} - A_{\alpha\beta} X^\alpha Y^\beta),$$

where $X = X^\alpha Z_\alpha,\ Y = Y^\beta Z_\beta,\ R_{\alpha\bar{\beta}} = R_\gamma{}^\gamma{}_{\alpha\bar{\beta}}$. The Webster scalar curvature is $R = R_\alpha{}^\alpha = h^{\alpha\bar{\beta}} R_{\alpha\bar{\beta}}$.

Next we recall some definitions.

Definition 1.1. *(i) A piecewise smooth curve $\gamma : [0, 1] \to M$ is said to be horizontal if $\gamma'(t) \in \xi$ whenever $\gamma'(t)$ exists. The length of γ is then defined by*

$$l(\gamma) = \int_0^1 \langle \gamma'(t), \gamma'(t)\rangle^{\frac{1}{2}} dt.$$

The Carnot-Carathéodory distance between two points $p,\ q \in M$ is

$$d_c(p, q) = \inf\left\{l(\gamma)|\ \gamma \in C_{p,q}\right\},$$

where $C_{p,q}$ is the set of all horizontal curves joining p and q.

(ii) By Chow connectivity theorem [Cho], there always exists a horizontal curve joining p and q, so the distance is finite. We say M is complete if it is complete as a metric space.

Definition 1.2. *A smooth real-valued function u in M is said to be CR-pluriharmonic function if for any point $p \in M$, there is an open neighborhood U of p in M and a smooth real-valued function v on U such that $\overline{\partial}_b(u + iv) = 0$.*

Definition 1.3. *([L1]) Let (M^{2n+1}, J, θ) be a complete pseudohermitian manifold. Define*

$$P\varphi = \sum_{\alpha=1}^{n} (\varphi_{\overline{\alpha}}{}^{\overline{\alpha}}{}_{\beta} + inA_{\beta\alpha}\varphi^{\alpha})\theta^{\beta} = (P_{\beta}\varphi)\theta^{\beta}, \quad \beta = 1, 2, \cdots, n$$

which is an operator that characterizes CR-pluriharmonic functions. Here

$$P_{\beta}\varphi = \sum_{\alpha=1}^{n} (\varphi_{\overline{\alpha}}{}^{\overline{\alpha}}{}_{\beta} + inA_{\beta\alpha}\varphi^{\alpha}) \tag{1.3}$$

and $\overline{P}\varphi = (\overline{P}_{\beta}\varphi)\theta^{\overline{\beta}}$, the conjugate of P. Moreover we define

$$P_0\varphi = 4\left(\delta_b(P\varphi) + \overline{\delta}_b(\overline{P}\varphi)\right) \tag{1.4}$$

which is the so-called CR Paneitz operator P_0. Here δ_b is the divergence operator that takes $(1,0)$-forms to functions by $\delta_b(\sigma_{\alpha}\theta^{\alpha}) = \sigma_{\alpha,}{}^{\alpha}$ and $\bar{\delta}_b(\sigma_{\overline{\alpha}}\theta^{\overline{\alpha}}) = \sigma_{\overline{\alpha}},{}^{\overline{\alpha}}$. If we define $\partial_b\varphi = \varphi_{\alpha}\theta^{\alpha}$ and $\bar{\partial}_b\varphi = \varphi_{\overline{\alpha}}\theta^{\overline{\alpha}}$, then the formal adjoint of ∂_b on functions (with respect to the Levi form and the volume form $d\mu$) is $\partial_b^* = -\delta_b$.

We observe that if (M, J, θ) is a closed pseudohermitian $(2n+1)$-manifold, then

$$-\int_M \langle P\varphi + \overline{P}\varphi, d_b\varphi\rangle \, d\mu = \frac{1}{4}\int_M P_0\varphi \cdot \varphi \, d\mu. \tag{1.5}$$

In particular if (M, J, θ) has zero torsion, we have

$$P_0\varphi = \mathcal{L}_n\mathcal{L}_{\overline{n}} = [\Delta_b^2\varphi + n^2T^2\varphi].$$

Here

$$\mathcal{L}_n\varphi = -\Delta_b\varphi + inT\varphi = -2\varphi_{\overline{\alpha}}{}^{\overline{\alpha}}.$$

For the details about these operators, the reader can make reference to [GL], [H] and [L1].

Remark 1.1. *([H], [GL]) (i) Let (M, J, θ) be a closed pseudohermitian $(2n+1)$-manifold with $n \geq 2$. Then a smooth real-valued function f satisfies $P_0 f = 0$ on M if and only if $P_{\beta}f = 0$ on M. It holds also for a closed pseudohermitian 3-manifold of zero torsion.*

(ii) Let $P_{\beta}f = 0$. If M is the boundary of a connected strictly pseudoconvex domain $\Omega \subset C^{n+1}$, then f is the boundary value of a pluriharmonic function u in Ω. That is, $\partial\overline{\partial}u = 0$ in Ω. Moreover, if Ω is simply connected, there exists a holomorphic function w in Ω such that $\mathrm{Re}(w) = u$ and $u|_M = f$.

In this paper, we consider the positive solution $u(x,t)$ of the CR heat equation with respect to the sub-Laplacian

$$\frac{\partial}{\partial t}u(x,t) = \Delta_b u(x,t) \tag{1.6}$$

on $M \times [0, T)$.

PROPOSITION 1.1. *Let (M, J, θ) be a closed pseudohermitian $(2n+1)$-manifold. If $u(x,t)$ is the positive smooth solution of (1.6) on $M \times [0, \infty)$. Suppose that*

$$[2Ric - (n+2)Tor](Z, Z) \geq -l_0 |Z|^2,$$

for all $Z \in T_{1,0}$ and l_0 is a nonnegative constant. Then the function

$$G = t\left[|\nabla_b \varphi|^2 + \left(1 + \frac{2}{n}\right)\varphi_t\right] \tag{1.7}$$

satisfies the inequality

$$\begin{array}{rcl}\left(\Delta_b - \frac{\partial}{\partial t}\right) G & \geq & -\frac{2n}{n+2}\langle \nabla_b \varphi, \nabla_b G\rangle \\ & & +\frac{2n}{(n+1)(n+2)^2 t} G\left(G - \frac{(n+1)(n+2)^2}{2n}\right) \\ & & -l_0 t \left|\nabla_b \varphi\right|^2 - \frac{8}{n} t u^{-2} \left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*}.\end{array}$$

Let $u(x,t)$ be a positive solution of (1.6) on $M \times [0, \infty)$. In section 2, it is proved that if $P_\beta u = 0$ at $t = 0$, then $P_\beta u = 0$ for all t on a closed pseudohermitian $(2n+1)$-manifold of zero torsion. Then the extra term of CR Bochner formula (2.1) becomes

$$\langle Pu + \overline{P}u, d_b u\rangle = 0 \tag{1.8}$$

on $M \times [0, \infty)$.

Now by using the arguments of [LY], (2.1) and (1.8), we are able to derive the CR version of parabolic Li-Yau gradient estimate for the positive solution $u(x,t)$ of (1.6) on $M \times [0, \infty)$.

COROLLARY 1.2. *Let (M, J, θ) be a closed pseudohermitian $(2n+1)$-manifold of zero torsion and nonnegative pseudohermitian Ricci tensors. If $u(x,t)$ is the positive solution of (1.6) on $M \times [0, \infty)$ such that*

$$P_\beta u = 0$$

at $t = 0$. Then u satisfies the estimate

$$\frac{|\nabla_b u|^2}{u^2} + \frac{n+2}{n}\frac{u_t}{u} \leq \frac{(n+1)(n+2)^2}{2n}\frac{1}{t} \tag{1.9a}$$

on $M \times [0, \infty)$.

By combining the result of [CY] and Corollary 1.2, we get the following subgradient estimate of the logarithm of a positive solution to (1.6).

THEOREM 1.3. *Let (M, J, θ) be a closed pseudohermitian $(2n+1)$-manifold of zero torsion and nonnegative pseudohermitian Ricci tensor. If $u(x,t)$ is the positive solution of (1.6) on $M \times [0, \infty)$ such that*

$$P_\beta u = 0, \quad \beta = 1, 2, \cdots, n$$

at $t = 0$. Then there exist constants C_1, C_2 such that u satisfies the subgradient estimate

$$t\left|\nabla_b \log u\right|^2 \leq C_1 + C_2 t \tag{1.10}$$

on $M \times [0, \infty)$.

Note that the arguments of [LY] can be extended easily to complete noncompact pseudohermitian $(2n+1)$-manifold if one can have the CR version of Laplacian comparison theorem. Indeed, this is the case for a $(2n+1)$-dimensional Heisenberg group H^n (see section 5 for details). Then we have

THEOREM 1.4. *If* $u(x,t)$ *be a positive smooth solution of (1.6)*

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

on $H^n \times [0,T)$ *with*

$$P_\beta u = 0$$

at $t = 0$, *then* u *satisfies the subgradient estimate*

$$t\,|\nabla_b \log u|^2 \le \frac{(n+2)(n^2+5n+2)}{4(n+1)} + \epsilon$$

on $H^n \times [0,T)$ *for any* $\epsilon > 0$.

REMARK 1.2. *For the CR Yamabe flow on a closed pseudohermitian* 3*-manifold of zero torsion and nonnegative Tanaka-Webster curvature, we have the similar result on CR version of Li-Yau-Hamilton inequality ([CCW]).*

As a consequence, we have the following Liouville-type theorems for CR heat equation on $H^n \times [0, \infty)$.

COROLLARY 1.5. *Let* (H^n, J, θ) *be the standard* $(2n+1)$*-dimensional Heisenberg group. If* $u(x,t)$ *is a positive solution of (1.6) on* $H^n \times [0,\infty)$ *with a positive smooth CR-pluriharmonic function as an initial. Then* u *is a constant.*

REMARK 1.3. *It is true that there are no nontrivial positive harmonic functions on* H^n*. See [KS] for details.*

Now for any L^2-function $u(x,t)$, we may write

$$u(x,t) = u_{\ker}(x,t) + u^{\perp}(x,t)$$

with $P_0(u_{\ker}(x,t)) = 0$. From Lemma 2.2, we may split the CR heat equation (1.6) into the following heat equations respectively :

$$\frac{\partial}{\partial t} u^{\perp} = \Delta_b u^{\perp} \tag{1.11}$$

and

$$\frac{\partial}{\partial t} u_{\ker} = \Delta_b u_{\ker} \tag{1.12}$$

on Heisenberg group (H^n, J, θ). Observe that $H(x,y,t) \in C^\infty(H^n \times H^n \times \mathbf{R}^+)$ and for any fixed y, t, $H(x,y,t) \in L^2(H^n)$. Then for any L^2-function $u(x,0) = f(x)$, we have

$$f(x) = f_{\ker}(x) + f^{\perp}(x)$$

and

$$H(x,y,t) = H_{\ker}(x,y,t) + H^{\perp}(x,y,t)$$

with $P_0(f_{\ker}(x)) = 0$ and $P_0(H_{\ker}(x,y,t)) = 0$. Hence

$$u^{\perp}(y,t) = \int H^{\perp}(x,y,t) f^{\perp}(x) dx$$

and

$$u_{\ker}(y,t) = \int H_{\ker}(x,y,t) f_{\ker}(x) dx.$$

As a consequence from Theorem 1.4 and Corollary 4.4, we have the following subgradient estimate of the heat kernel.

Corollary 1.6. *Let $H(x,y,t)$ be the heat kernel of (1.6) on $H^n \times [0,T)$ with $H(x,y,t) = H_{\ker}(x,y,t) + H^{\perp}(x,y,t)$. Then for some constant δ and $0 < \epsilon < 1$,*

$$|\nabla_b H_{\ker}(x,y,t)| \leq C(\epsilon)^{\frac{\delta}{2}} t^{-\frac{(2n+3)}{2}} \exp\left(-\frac{d_c^2(x,y)}{2(4+\epsilon)t} \right)$$

with $C(\epsilon) \to \infty$ as $\epsilon \to 0$.

For simplicity, we first prove Theorems of this paper on a pseudohermitian $(2n+1)$-manifold (M, J, θ) with $n = 1$ as in section $3, 4$. The higher dimensional cases will be given in section 5, 6.

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2. CR Bochner formula and preserving property. In this section, we will drive the CR version of Bochner formula and the preserving property for (1.6) on a pseudohermitian (M^{2n+1}, J, θ).

We first derive the following CR version of Bochner formula on a complete pseudohermitian (M^{2n+1}, J, θ).

Lemma 2.1. *Let (M^{2n+1}, J, θ) be a complete pseudohermitian manifold. For a real smooth function u on (M, J, θ),*

$$\begin{aligned} \tfrac{1}{2}\Delta_b|\nabla_b u|^2 &= |(\nabla^H)^2 u|^2 + (1+\tfrac{2}{n}) < \nabla_b u, \nabla_b \Delta_b u >_{L_\theta} \\ &\quad + [2Ric - (n+2)Tor]((\nabla_b u)_{\mathbf{C}}, (\nabla_b u)_{\mathbf{C}}) \\ &\quad - \tfrac{4}{n} < Pu + \overline{P}u, d_b u >_{L_\theta^*} . \end{aligned} \tag{2.1}$$

Here $(\nabla_b u)_{\mathbf{C}} = u_{\overline{\alpha}} Z_\alpha$ is the corresponding complex $(1,0)$-vector field of $\nabla_b u$ and $d_b u = u_\alpha \theta^\alpha + u_{\overline{\alpha}} \theta^{\overline{\alpha}}$.

Remark 2.1. *In [Chi] and [CC], the CR Bochner formulae (2.1) was derived for $n = 1$.*

Proof. First from [Gr], we have for a real function u

$$\begin{aligned} \tfrac{1}{2}\Delta_b|\nabla_b u|^2 &= |(\nabla^H)^2 u|^2 + <\nabla_b u, \nabla_b\Delta_b u>_{L_\theta} \\ &\quad +(2Ric - nTor)((\nabla_b u)_{\mathbf{C}}, (\nabla_b u)_{\mathbf{C}}) \\ &\quad -2i\textstyle\sum_{\alpha=1}^n (u_\alpha u_{\overline{\alpha}0} - u_{\overline{\alpha}}u_{\alpha 0}). \end{aligned} \tag{2.2}$$

We use the matrix $h_{\alpha\overline{\beta}}$ to raise and lower indices. In the following we always compute at one point. Then one may assume $h_{\alpha\overline{\beta}} = \delta_{\alpha\overline{\beta}}$ to lower the index. For instance,

$$P_\beta\varphi = \sum_{\alpha=1}^n (\varphi_{\overline{\alpha}\alpha\beta} + inA_{\beta\alpha}\varphi_{\overline{\alpha}})$$

and

$$u_{0\overline{\alpha}} - u_{\overline{\alpha}0} = \sum_{\gamma=1}^n A_{\overline{\gamma}\ \overline{\alpha}} u_\gamma$$

and

$$iu_0 = u_{\gamma\overline{\beta}} - u_{\overline{\beta}\gamma}.$$

Compute

$$\begin{aligned} & iu_\alpha u_{\overline{\alpha}0} \\ &= iu_\alpha u_{0\overline{\alpha}} - i\textstyle\sum_{\gamma=1}^n A_{\overline{\gamma}\ \overline{\alpha}} u_\alpha u_\gamma \\ &= \tfrac{1}{n}u_\alpha \textstyle\sum_{\beta=1}^n (u_{\beta\overline{\beta}\overline{\alpha}} - u_{\overline{\beta}\beta\overline{\alpha}}) - i\textstyle\sum_{\gamma=1}^n A_{\overline{\gamma}\ \overline{\alpha}} u_\gamma u_\alpha \\ &= \tfrac{1}{n}u_\alpha \overline{P}_\alpha u + i\textstyle\sum_{\gamma=1}^n A_{\overline{\gamma}\ \overline{\alpha}} u_\alpha u_\gamma - \tfrac{1}{n}\textstyle\sum_{\beta=1}^n (u_\alpha u_{\overline{\beta}\beta\overline{\alpha}}) \\ & -i\textstyle\sum_{\gamma=1}^n A_{\overline{\gamma}\ \overline{\alpha}} u_\gamma u_\alpha \\ &= \tfrac{1}{n}u_\alpha \overline{P}_\alpha u - \tfrac{1}{n}\textstyle\sum_{\beta=1}^n (u_\alpha u_{\overline{\beta}\beta\overline{\alpha}}) \end{aligned}$$

and

$$-iu_{\overline{\alpha}}u_{\alpha 0} = \mathrm{conj}(iu_\alpha u_{\overline{\alpha}0}).$$

Then

$$\begin{aligned} -2i\textstyle\sum_{\alpha=1}^n (u_\alpha u_{\overline{\alpha}0} - u_{\overline{\alpha}}u_{\alpha 0}) &= -\tfrac{2}{n} < Pu + \overline{P}u, d_b u >_{L_\theta^*} \\ &\quad +\tfrac{2}{n}\textstyle\sum_{\alpha,\beta=1}^n (u_\alpha u_{\overline{\beta}\beta\overline{\alpha}} + u_{\overline{\alpha}}u_{\beta\overline{\beta}\alpha}). \end{aligned}$$

But

$$\begin{aligned} & <\nabla_b u, \nabla_b\Delta_b u>_{L_\theta} \\ &= \textstyle\sum_{\alpha,\beta=1}^n [u_\alpha(u_{\overline{\beta}\beta} + u_{\beta\overline{\beta}})_{\overline{\alpha}} + u_{\overline{\alpha}}(u_{\overline{\beta}\beta} + u_{\beta\overline{\beta}})_\alpha] \\ &= \textstyle\sum_{\alpha,\beta=1}^n (u_\alpha u_{\overline{\beta}\beta\overline{\alpha}} + u_{\overline{\alpha}}u_{\beta\overline{\beta}\alpha}) + \textstyle\sum_{\alpha,\beta=1}^n (u_\alpha u_{\beta\overline{\beta}\overline{\alpha}} + u_{\overline{\alpha}}u_{\overline{\beta}\beta\alpha}) \\ &= \textstyle\sum_{\alpha,\beta=1}^n (u_\alpha u_{\overline{\beta}\beta\overline{\alpha}} + u_{\overline{\alpha}}u_{\beta\overline{\beta}\alpha}) + < Pu + \overline{P}u, d_b u >_{L_\theta^*} \\ & +in\textstyle\sum_{\gamma,\alpha=1}^n (A_{\overline{\gamma}\ \overline{\alpha}} u_\alpha u_\gamma - A_{\gamma\ \alpha} u_{\overline{\alpha}} u_{\overline{\gamma}}) \\ &= \textstyle\sum_{\alpha,\beta=1}^n (u_\alpha u_{\overline{\beta}\beta\overline{\alpha}} + u_{\overline{\alpha}}u_{\beta\overline{\beta}\alpha}) + < Pu + \overline{P}u, d_b u >_{L_\theta^*} \\ & +nTor((\nabla_b u)_{\mathbf{C}}, (\nabla_b u)_{\mathbf{C}}). \end{aligned}$$

It follows that

$$\begin{aligned} -2i\textstyle\sum_{\alpha=1}^n (u_\alpha u_{\overline{\alpha}0} - u_{\overline{\alpha}}u_{\alpha 0}) &= -\tfrac{4}{n} < Pu + \overline{P}u, d_b u >_{L_\theta^*} \\ &\quad -2Tor((\nabla_b u)_{\mathbf{C}}, (\nabla_b u)_{\mathbf{C}}) \\ &\quad +\tfrac{2}{n} <\nabla_b u, \nabla_b\Delta_b u>_{L_\theta}. \end{aligned} \tag{2.3}$$

Finally from (2.2) and (2.3), we have

$$\begin{array}{rcl}\frac{1}{2}\Delta_b|\nabla_b u|^2 & = & |(\nabla^H)^2u|^2+(1+\frac{2}{n})<\nabla_b u,\nabla_b\Delta_b u>_{L_\theta} \\ & & +[2Ric-(n+2)Tor]((\nabla_b u)_{\mathbf{C}},(\nabla_b u)_{\mathbf{C}}) \\ & & -\frac{4}{n}<Pu+\overline{P}u,d_b u>_{L_\theta^*}.\end{array}$$

□

LEMMA 2.2. *Let* (M,J,θ) *be a closed pseudohermitian* $(2n+1)$*-manifold of zero torsion. If* $u(x,t)$ *is a solution of*

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

on $M\times[0,\infty)$ *with* $P_\beta u(x,0)=0$*. Then* $P_\beta u(x,t)=0$ *for all* $t\in(0,\infty)$*.*

Proof. Let (M,J,θ) be a closed pseudohermitian $(2n+1)$-manifold of zero torsion. From Remark 1.1, we have $P_0u=0$ if and only if $P_\beta u=0$ and

$$P_0u=((\Delta_b)^2u+nT^2u).$$

It follows that $\Delta_bP_0u=P_0\Delta_bu$. Apply P_0 to the heat equation, we obtain

$$\left(\Delta_b-\frac{\partial}{\partial t}\right)P_0u(x,t)=0$$

on $M\times[0,\infty)$ with $P_0u(x,0)=0$. Hence the Lemma follows from the maximum principle and Remark 1.1. □

LEMMA 2.3. *Let* (H^n,J,θ) *be the standard* $(2n+1)$*-dimensional Heisenberg group. If* $u(x,t)$ *is a solution of*

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

on $M\times[0,\infty)$ *with* $P_\beta u(x,0)=0,\ \beta=1,...,n$*. Then* $P_\beta u(x,t)=0$ *for all* $t\in[0,\infty)$*.*

REMARK 2.2. *Since* (H^n,J,θ) *is complete noncompact,* $P_\beta u$ *is not necessarily vanishing even if* $P_0u=0$*. So we need to have a different proof from Lemma 2.2.*

Proof. We first do it for $n=1$. We need the following commutation relation ([L1])

$$\begin{array}{rcl}C_{I,01}-C_{I,10} & = & C_{I,\bar{1}}A_{11}-kC_IA_{11,\bar{1}}, \\ C_{I,0\bar{1}}-C_{I,\bar{1}0} & = & C_{I,1}A_{\bar{1}\bar{1}}+kC_IA_{\bar{1}\bar{1},1}, \\ C_{I,1\bar{1}}-C_{I,\bar{1}1} & = & iC_{I,0}+kWC_I,\end{array}\tag{2.4}$$

Here C_I denotes a coefficient of a tensor with multi-index I consisting of only 1 and $\bar{1}$, and k is the number of 1 minus the number of $\bar{1}$ in I.

For

$$\begin{array}{rcl}\frac{\partial}{\partial t}u_{\bar{1}11} & = & (\Delta_bu)_{\bar{1}11} \\ & = & (u_{\bar{1}1}+u_{1\bar{1}})_{\bar{1}11} \\ & = & (u_{\bar{1}1\bar{1}11}+u_{1\bar{1}\bar{1}11}),\end{array}$$

it follows from (2.4) that

$$u_{\bar{1}1\bar{1}11} = u_{\bar{1}11\bar{1}1} - iu_{\bar{1}101} = u_{\bar{1}11\bar{1}1} - iu_{\bar{1}110}$$

and

$$\begin{aligned} u_{1\bar{1}\bar{1}11} &= u_{\bar{1}1\bar{1}11} + iu_{0\bar{1}11} \\ &= (u_{\bar{1}11\bar{1}1} - iu_{\bar{1}101}) + iu_{0\bar{1}11} \\ &= (u_{\bar{1}111\bar{1}} - iu_{\bar{1}110}) - iu_{\bar{1}101} + iu_{0\bar{1}11} \\ &= u_{\bar{1}111\bar{1}} - iu_{\bar{1}110}. \end{aligned}$$

Thus for $\mathcal{L}_2 = -\Delta_b + 2iT$

$$\frac{\partial}{\partial t}u_{\bar{1}11} = \Delta_b u_{\bar{1}11} - 2iu_{\bar{1}110} = -\mathcal{L}_2 u_{\bar{1}11}. \tag{2.5}$$

This plus (2.5) imply

$$\frac{\partial}{\partial t}(P_1 u) = -\mathcal{L}_2(P_1 u).$$

Similarly for $n \geq 2$, we have

$$\frac{\partial}{\partial t}(P_\beta u) = \frac{\partial}{\partial t}(\sum_{\alpha=1}^{n} u_{\overline{\alpha}\alpha\beta}) = \sum_{\alpha=1}^{n}(\Delta_b u)_{\overline{\alpha}\alpha\beta} = \sum_{\gamma,\alpha=1}^{n}(u_{\gamma\overline{\gamma}} + u_{\overline{\gamma}\gamma})_{\overline{\alpha}\alpha\beta}.$$

Now by commutation relations

$$\begin{aligned} u_{\gamma\overline{\gamma}\overline{\alpha}\alpha\beta} &= u_{\overline{\gamma}\gamma\overline{\alpha}\alpha\beta} + iu_{0\overline{\alpha}\alpha\beta} \\ &= u_{\overline{\gamma}\gamma\overline{\alpha}\beta\alpha} + iu_{\overline{\alpha}\alpha\beta0} \\ &= u_{\overline{\gamma}\gamma\beta\overline{\alpha}\alpha} - iu_{\overline{\gamma}\gamma0\alpha} + iu_{\overline{\alpha}\alpha\beta0} \\ &= u_{\overline{\gamma}\gamma\beta\overline{\alpha}\alpha} - iu_{\overline{\gamma}\gamma\alpha0} + iu_{\overline{\alpha}\alpha\beta0} \end{aligned} \tag{2.6}$$

and

$$\begin{aligned} u_{\overline{\gamma}\gamma\overline{\alpha}\alpha\beta} &= u_{\overline{\gamma}\gamma\overline{\alpha}\beta\alpha} \\ &= u_{\overline{\gamma}\gamma\beta\overline{\alpha}\alpha} - iu_{\overline{\gamma}\gamma0\alpha} \\ &= u_{\overline{\gamma}\gamma\beta\alpha\overline{\alpha}} - iu_{\overline{\gamma}\gamma\beta0} - iu_{\overline{\gamma}\gamma\alpha0}. \end{aligned} \tag{2.7}$$

It follows from (2.6) and (2.7) that

$$\begin{aligned} \tfrac{\partial}{\partial t}(P_\beta u) &= \textstyle\sum_{\gamma,\alpha=1}^{n}(u_{\gamma\overline{\gamma}\overline{\alpha}\alpha\beta} + u_{\overline{\gamma}\gamma\overline{\alpha}\alpha\beta}) \\ &= \Delta_b(P_\beta u) - 2i\textstyle\sum_{\gamma,\alpha=1}^{n} u_{\overline{\gamma}\gamma\alpha0} + i\sum_{\gamma,\alpha=1}^{n} u_{\overline{\alpha}\alpha\beta0} - i\sum_{\gamma,\alpha=1}^{n} u_{\overline{\gamma}\gamma\beta0} \\ &= \Delta_b(P_\beta u) - 2i\textstyle\sum_{\gamma,\alpha=1}^{n} u_{\overline{\gamma}\gamma\alpha0} \\ &= \Delta_b(P_\beta u) - 2iT(\textstyle\sum_{\alpha=1}^{n} P_\alpha u). \end{aligned}$$

Hence

$$\frac{\partial}{\partial t}(\sum_{\beta=1}^{n} P_\beta u) = \Delta_b(\sum_{\beta=1}^{n} P_\beta u) - i2nT(\sum_{\beta=1}^{n} P_\beta u).$$

That is

$$\frac{\partial}{\partial t}(\sum_{\beta=1}^{n} P_\beta u) = -\mathcal{L}_{2n}(\sum_{\beta=1}^{n} P_\beta u).$$

Here $\mathcal{L}_{2n} = -\Delta_b + i2nT$. Since $2n$ is not an odd integer, $-\mathcal{L}_{2n}$ is a subelliptic operator again. Then by the uniqueness of solution to subelliptic parabolic equation, $P_\beta u(x,t) = 0$ for all $t \in [0,\infty)$ if $P_\beta u(x,0) = 0$, $\beta = 1, ..., n$. $\square$

3. Subgradient estimate of the CR heat equation. In this section, we first establish the subgradient estimate of Theorem 1.3 for $n = 1$. For $n \geq 2$, we refer it to section 6.

Let (M, J, θ) be a closed pseudohermitian 3-manifold. By using the arguments of [LY], we are able to derive the CR version of parabolic Li-Yau gradient estimate for the positive solution $u(x, t)$ of (1.6) on $M \times [0, \infty)$.

Let $\varphi = \log u$. Then φ satisfies

$$\left(\Delta_b - \frac{\partial}{\partial t}\right)\varphi = -\left|\nabla_b \varphi\right|^2.$$

On the other hand, from Cao-Yau's ([CY]) paper, one has the standard parabolic Li-Yau gradient estimate.

Proposition 3.1. *([CY, Theorem 2.1]) Let (M, J, θ) be a closed pseudohermitian $(2n+1)$-manifold and $u(x,t)$ be a positive smooth solution of (1.6) on $M \times [0, \infty)$. Then there exist constants $C^{'}, C^{''}$ and $\delta_0 > 1$ such that for any $\delta \geq \delta_0$, u satisfies the estimate*

$$\frac{\left|\nabla_b u\right|^2}{u^2} - \delta \frac{u_t}{u} \leq \frac{C^{'}}{t} + C^{''} \tag{3.1}$$

on $M \times [0, \infty)$.

Now we derive the CR version of parabolic Li-Yau gradient estimate for the positive solution of the CR heat equation. First, we need the following Lemma.

Lemma 3.2. *Let (M, J, θ) be a closed pseudohermitian $(2n+1)$-manifold. Let $\varphi = \ln f$, for $f > 0$. Then*

$$\begin{aligned} &\left\langle P\varphi + \bar{P}\varphi, d_b\varphi \right\rangle_{L_\theta^*} \\ &= f^{-2}\left\langle Pf + \bar{P}f, d_b f\right\rangle_{L_\theta^*} - \tfrac{1}{2}\left\langle \nabla_b\varphi, \nabla_b|\nabla_b\varphi|^2\right\rangle - \tfrac{1}{2}f^{-1}\Delta_b f|\nabla_b\varphi|^2. \end{aligned} \tag{3.2}$$

Proof. In the following, we use the Einstein convention notation. Let $Q(x) = \left|\nabla_b\varphi\right|^2(x)$. We compute

$$\begin{aligned} \nabla_b Q &= Q_{\overline{\alpha}} Z_\alpha + Q_\alpha Z_{\overline{\alpha}} = 2\nabla_b(\varphi_\alpha \varphi_{\overline{\alpha}}) \\ &= 2f^{-4}(f^2 f_\alpha f_{\overline{\alpha}\overline{\beta}} + f^2 f_{\overline{\alpha}} f_{\alpha\overline{\beta}} - 2f_\alpha f_{\overline{\alpha}} f_{\overline{\beta}}) Z_\beta + \text{complex conjugate.} \end{aligned}$$

It follows that

$$\begin{aligned} &P_\beta\varphi \\ &= \varphi_{\overline{\alpha}\alpha\beta} + inA_{\beta\alpha}\varphi_{\overline{\alpha}} \\ &= f^{-4}(f^3 f_{\overline{\alpha}\alpha\beta} - f^2 f_\alpha f_{\overline{\alpha}\beta} - f^2 f_{\overline{\alpha}} f_{\alpha\beta} - f^2 f_\beta f_{\overline{\alpha}\alpha} + 2f f_\alpha f_\beta f_{\overline{\alpha}}) + inA_{\beta\alpha} f^{-1} f_{\overline{\alpha}} \\ &= f^{-1}(P_\beta f - \frac{1}{2} f Q_\beta - f^{-1} f_\beta f_{\overline{\alpha}\alpha}) \\ &= f^{-1}(P_\beta f - \frac{1}{2} f Q_\beta - \varphi_\beta f_{\overline{\alpha}\alpha}), \end{aligned}$$

thus

$$\begin{aligned}\left\langle P\varphi+\bar{P}\varphi,d_b\varphi\right\rangle_{L_\theta^*} &= \left\langle (P_\beta\varphi)\,\theta^\beta+\left(\bar{P}_\beta\varphi\right)\theta^{\overline{\beta}},\varphi_\beta\theta^\beta+\varphi_{\overline{\beta}}\theta^{\overline{\beta}}\right\rangle_{L_\theta^*}\\ &= (P_\beta\varphi)\,\varphi_{\overline{\beta}}+\left(\bar{P}_\beta\varphi\right)\varphi_\beta\\ &= f^{-1}(P_\beta f-\frac{1}{2}fQ_\beta-\varphi_\beta f_{\overline{\alpha}\alpha})\varphi_{\overline{\beta}}+\text{complex conjugate}\\ &= f^{-2}\left\langle Pf+\bar{P}f,d_bf\right\rangle_{L_\theta^*}-\frac{1}{2}\left\langle\nabla_b\varphi,\nabla_b|\nabla_b\varphi|^2\right\rangle-\frac{1}{2}f^{-1}\Delta_bf\left|\nabla_b\varphi\right|^2.\end{aligned}$$

This implies the Lemma. □

LEMMA 3.3. *Let (M,J,θ) be a closed pseudohermitian 3-manifold. If $u(x,t)$ is the positive smooth solution $u(x,t)$ of (1.6) on $M\times[0,\infty)$. Suppose that*

$$(2Ric-3Tor)(Z,Z)\geq -k_0|Z|^2,$$

for all $Z\in T_{1,0}$ and k_0 is a nonnegative constant. Then the function

$$F=t\left(\left|\nabla_b\varphi\right|^2+3\varphi_t\right) \tag{3.3}$$

satisfies the inequality

$$\begin{aligned}\left(\Delta_b-\frac{\partial}{\partial t}\right)F &\geq -\frac{2}{3}\langle\nabla_b\varphi,\nabla_bF\rangle+\frac{1}{9t}F(F-9)+\\ &\quad -k_0t\left|\nabla_b\varphi\right|^2-8tu^{-2}\left\langle Pu+\bar{P}u,d_bu\right\rangle_{L_\theta^*}.\end{aligned}$$

Proof. First differentiating (3.3) w.r.t. the t-variable, we have

$$\begin{aligned}F_t &= \frac{1}{t}F+t\left(\left|\nabla_b\varphi\right|^2+3\varphi_t\right)_t\\ &= \frac{1}{t}F+t\left(4\left|\nabla_b\varphi\right|^2+3\Delta_b\varphi\right)_t\\ &= \frac{1}{t}F+t\left[8\langle\nabla_b\varphi,\nabla_b\varphi_t\rangle+3\Delta_b\varphi_t\right].\end{aligned} \tag{3.4}$$

By using the CR version of Bochner formula (2.1) and Lemma 3.2, one obtains

$$\begin{aligned}\Delta_bF &= t\left(\Delta_b\left|\nabla_b\varphi\right|^2+3\Delta_b\varphi_t\right)\\ &= t[2|(\nabla^H)^2\varphi|^2+6\left\langle\nabla_b\varphi,\nabla_b\Delta_b\varphi\right\rangle\\ &\quad +2(2Ric-3Tor)((\nabla_b\varphi)_{\mathbf{C}},(\nabla_b\varphi)_{\mathbf{C}})\\ &\quad -8\langle P\varphi+\bar{P}\varphi,d_b\varphi\rangle_{L_\theta^*}+3\Delta_b\varphi_t]\\ &\geq t[4\left|\varphi_{11}\right|^2+(\Delta_b\varphi)^2+6\left\langle\nabla_b\varphi,\nabla_b\Delta_b\varphi\right\rangle-k_0\left|\nabla_b\varphi\right|^2\\ &\quad -8\langle P\varphi+\bar{P}\varphi,d_b\varphi\rangle_{L_\theta^*}+3\Delta_b\varphi_t]\\ &= t[4\left|\varphi_{11}\right|^2+(\Delta_b\varphi)^2+6\left\langle\nabla_b\varphi,\nabla_b\Delta_b\varphi\right\rangle-k_0\left|\nabla_b\varphi\right|^2\\ &\quad -8u^{-2}\left\langle Pu+\bar{P}u,d_bu\right\rangle_{L_\theta^*}+4\varphi_t|\nabla_b\varphi|^2\\ &\quad +4\left\langle\nabla_b\varphi,\nabla_b|\nabla_b\varphi|^2\right\rangle+3\Delta_b\varphi_t].\end{aligned} \tag{3.5}$$

Here we have used the inequalities

$$\left|(\nabla^H)^2\varphi\right|^2 = 2\left|\varphi_{11}\right|^2 + \frac{1}{2}(\Delta_b\varphi)^2 + \frac{1}{2}\varphi_0^2 \geq 2\left|\varphi_{11}\right|^2 + \frac{1}{2}(\Delta_b\varphi)^2, \tag{3.6}$$

$$(2Ric - 3Tor)((\nabla_b\varphi)_{\mathbb{C}}, (\nabla_b\varphi)_{\mathbb{C}}) \geq -k_0\left|(\nabla_b\varphi)_{\mathbb{C}}\right|^2 = -\frac{k_0}{2}\left|\nabla_b\varphi\right|^2,$$

and

$$\varphi_t = \frac{u_t}{u} = \frac{\Delta_b u}{u}.$$

Applying the formula

$$\Delta_b\varphi = \varphi_t - \left|\nabla_b\varphi\right|^2 = \frac{1}{3t}F - \frac{4}{3}\left|\nabla_b\varphi\right|^2 \tag{3.7}$$

and combining (3.4), (3.5), we conclude

$$\begin{aligned}
\left(\Delta_b - \frac{\partial}{\partial t}\right)F \geq & -\frac{1}{t}F + t[4\left|\varphi_{11}\right|^2 + (\Delta_b\varphi)^2 + 6\left\langle\nabla_b\varphi, \nabla_b\Delta_b\varphi\right\rangle \\
& +4\left\langle\nabla_b\varphi, \nabla_b|\nabla_b\varphi|^2\right\rangle - 8\langle\nabla_b\varphi, \nabla_b\varphi_t\rangle \\
& -k_0\left|\nabla_b\varphi\right|^2 + 4\varphi_t|\nabla_b\varphi|^2 - 8u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*}] \\
= & -\frac{1}{t}F + t[-\frac{2}{3t}\langle\nabla_b\varphi, \nabla_b F\rangle - \frac{4}{3}\left\langle\nabla_b\varphi, \nabla_b|\nabla_b\varphi|^2\right\rangle + 4\left|\varphi_{11}\right|^2 \\
& +(\Delta_b\varphi)^2 - k_0\left|\nabla_b\varphi\right|^2 + 4\varphi_t|\nabla_b\varphi|^2 - 8u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*}].
\end{aligned}$$

Now it is easy to see that

$$\left\langle\nabla_b\varphi, \nabla_b|\nabla_b\varphi|^2\right\rangle = 4\mathrm{Re}(\varphi_{11}\varphi_{\bar{1}}\varphi_{\bar{1}}) + \Delta_b\varphi|\nabla_b\varphi|^2.$$

Thus

$$\begin{aligned}
-\tfrac{4}{3}\left\langle\nabla_b\varphi, \nabla_b|\nabla_b\varphi|^2\right\rangle &= -\tfrac{16}{3}\mathrm{Re}(\varphi_{11}\varphi_{\bar{1}}\varphi_{\bar{1}}) - \tfrac{4}{3}\Delta_b\varphi|\nabla_b\varphi|^2 \\
&\geq -4\left|\varphi_{11}\right|^2 - \tfrac{16}{9}|\varphi_{\bar{1}}|^4 - \tfrac{4}{3}\Delta_b\varphi|\nabla_b\varphi|^2 \\
&= -4\left|\varphi_{11}\right|^2 - \tfrac{4}{9}|\nabla_b\varphi|^4 - \tfrac{4}{3}\Delta_b\varphi|\nabla_b\varphi|^2.
\end{aligned}$$

Here we have used the basic inequality $2\mathrm{Re}(zw) \leq \epsilon|z|^2 + \epsilon^{-1}|w|^2$ for all $\epsilon > 0$. All these imply

$$\begin{aligned}
\left(\Delta_b - \tfrac{\partial}{\partial t}\right)F \quad &\geq \quad -\tfrac{1}{t}F - \tfrac{2}{3}\langle\nabla_b\varphi, \nabla_b F\rangle + t[(\Delta_b\varphi)^2 + \tfrac{8}{3}\Delta_b\varphi|\nabla_b\varphi|^2 \\
&\quad\quad +\tfrac{32}{9}|\nabla_b\varphi|^4 - k_0\left|\nabla_b\varphi\right|^2 - 8u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*}] \\
&\geq \quad -\tfrac{2}{3}\langle\nabla_b\varphi, \nabla_b F\rangle + \tfrac{1}{9t}F(F-9) \\
&\quad\quad -k_0 t\left|\nabla_b\varphi\right|^2 - 8u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*}.
\end{aligned}$$

This completes the proof of Lemma 3.3. □

THEOREM 3.4. *Let (M, J, θ) be a closed pseudohermitian 3-manifold of zero torsion and nonnegative Tanaka-Webster scalar curvature. If $u(x,t)$ is the positive solution of (1.6) on $M \times [0,\infty)$ such that*

$$P_1 u = 0$$

at $t = 0$. Then u satisfies the estimate

$$\frac{|\nabla_b u|^2}{u^2} + 3\frac{u_t}{u} \leq \frac{9}{t} \tag{3.8}$$

on $M \times [0, \infty)$.

Proof. Applying Lemma 3.3 to φ by setting $A_{11} = 0,\ k_0 = 0$ and

$$\langle Pu + \bar{P}u, d_b u \rangle = 0.$$

Then we have

$$\left(\Delta_b - \frac{\partial}{\partial t}\right) F \geq -\frac{2}{3}\langle \nabla_b \varphi, \nabla_b F\rangle + \frac{1}{9t}F(F-9). \tag{3.9}$$

The theorem claims that F is at most 9. If not, at the maximum point (x_0, t_0) of F on $M \times [0, T]$ for some $T > 0$,

$$F(x_0, t_0) > 9.$$

Clearly, $t_0 > 0$, because $F(x, 0) = 0$. By the fact that (x_0, t_0) is a maximum point of F on $M \times [0, T]$, we have

$$\Delta_b F(x_0, t_0) \leq 0,$$
$$\nabla_b F(x_0, t_0) = 0,$$

and

$$F_t(x_0, t_0) \geq 0.$$

Combining with (3.9), this implies

$$0 \geq \frac{1}{9t_0} F(x_0, t_0)(F(x_0, t_0) - 9),$$

which is a contradiction. Hence $F \leq 9$ and the theorem follows. □

Then by combining Proposition 3.1 and Theorem 3.4, the subgradient estimate Theorem 1.3 follows easily for $n = 1$.

4. Subgradient estimates in the Heisenberg group H^1. In this section, we first establish Liouville-type theorems for the CR heat equation on a 3-dimensional Heisenberg group H^1. Secondly, we derive the subgradient estimate for CR Heat Kernel on H^1.

From [PP], we recall the following result.

Proposition 4.1. *If $u(x, t)$ be a positive smooth solution of (1.6) on $H^n \times [0, T)$, then u satisfies the estimate*

$$\frac{|\nabla_b u|^2}{u^2} - \frac{u_t}{u} \leq \frac{n}{t}$$

on $H^n \times [0, T)$.

THEOREM 4.2. *If $u(x,t)$ be a positive smooth solution of (1.6)*

$$(\Delta_b - \frac{\partial}{\partial t})u(x,t) = 0$$

on $H^1 \times [0,T)$ with

$$P_1 u = 0$$

at $t=0$, then u satisfies the subgradient estimate

$$\frac{|\nabla_b u|^2}{u^2} + 3\frac{u_t}{u} \leq \frac{9+\epsilon}{t}$$

on $H^1 \times [0,T)$ for any $\epsilon > 0$.

Proof. Let B_{2R} be a ball of radius $2R$ center at $O \in H^1$. Let $\varphi = \log u$ and $F = t(|\nabla_b \varphi|^2 + 3\varphi_t)$, then

$$\sup_{B_R}\left(\frac{|\nabla_b u|^2}{u^2} + 3\frac{u_t}{u}\right) = \sup_{B_R}\frac{F}{t}.$$

Let $\psi \in C_0^\infty(R)$ be a cut-off function ([DT]) such that $0 \leq \psi \leq 1$, $\psi(t) \equiv 1$ for $t \in [0,1]$, $\psi(t) \equiv 0$ for $t \geq 2$. We also require

$$\psi' \leq 0, \quad \psi'' \geq -C_1, \quad \text{and} \quad \frac{|\psi'|^2}{\psi} \leq C_2, \tag{4.1}$$

where C_1 and C_2 are positive constants. Denote by $d_c(x)$ be the Carnot-Carathéodory distance from O to x in H^1. Then we define $\eta(x) = \psi\left(\frac{d_c(x)}{R}\right)$. It is clear that $\text{supp}\eta \subset B_{2R}$ and $\eta|_{B_R} \equiv 1$.

We want to apply the maximum principle to ηF. The function η may not be smooth at the cut locus of $O \in H^1$. However, when applying the maximum principle, we can assume η is differentiable as in [LY].

If ηF attains its maximum at $(x_0,t_0) \in B_{2R} \times [0,T']$ with $0 < T' < T$, clearly we may assume $(\eta F)(x_0,t_0) > 0$ (otherwise $F \leq 0$, and the theorem is true). So $x_0 \in B_{2R}$, $t_0 > 0$, and by the maximum principle, at (x_0,t_0)

$$\nabla_b(\eta F) = F\nabla_b\eta + \eta\nabla_b F = 0, \tag{4.2}$$

$$\Delta_b(\eta F) \leq 0, \tag{4.3}$$

and

$$\frac{\partial}{\partial t}(\eta F) = \eta F_t \geq 0. \tag{4.4}$$

In the sequel, all computations will be at the point (x_0,t_0). By (4.2), $\nabla_b F = -F\nabla_b\eta/\eta$, and by (4.3)

$$\begin{aligned} 0 \geq \Delta_b(\eta F) &= F\Delta_b\eta + \eta\Delta_b F + 2\langle\nabla_b\eta, \nabla_b F\rangle \\ &= F\Delta_b\eta + \eta\Delta_b F - 2F\frac{|\nabla_b\eta|^2}{\eta}. \end{aligned} \tag{4.5}$$

By (4.1), we have

$$\frac{|\nabla_b \eta|^2}{\eta} = \frac{|\psi'|^2 |\nabla_b d_c|^2}{R^2 \psi} = \frac{|\psi'|^2}{R^2 \psi} \leq \frac{C_2}{R^2}, \tag{4.6}$$

and

$$\Delta_b \eta = \frac{\psi'' |\nabla_b d_c|^2}{R^2} + \frac{\psi' \Delta_b d_c}{R} = \frac{\psi''}{R^2} + \frac{\psi'}{R} \Delta_b d_c \geq -\frac{C_1}{R^2} - \frac{\sqrt{C_2}}{R} \Delta_b d_c.$$

Since in H^1, we have the sub-Laplacian comparison $(*)$ (see the proof in next section)

$$\Delta_b d_c \leq \frac{C}{d_c}, \tag{$*$}$$

for some constant C. Then

$$\Delta_b \eta \geq -\frac{C_3}{R^2}.$$

Substituting this into (4.5) and applying Lemma 2.3 and Lemma 3.3 with $A_{11} = 0$, $k_0 = 0$, all these imply

$$\begin{aligned} 0 \geq \Delta_b(\eta F) &\geq -\frac{C_3}{R^2} F - 2F \frac{|\nabla_b \eta|^2}{\eta} + \eta \Delta_b F \\ &\geq -\frac{C_3}{R^2} F - 2F \frac{|\nabla_b \eta|^2}{\eta} + \eta [F_t + 2\langle \nabla_b \varphi, \nabla_b F \rangle + \frac{1}{9t} F(F - 9)]. \end{aligned}$$

Since $\eta F_t = (\eta F)_t \geq 0$, $2\eta \langle \nabla_b \varphi, \nabla_b F \rangle = \frac{2}{3} F \langle \nabla_b \varphi, \nabla_b \eta \rangle$, the above inequality can be reduced as

$$0 \geq -\frac{C_3}{R^2} F - 2F \frac{|\nabla_b \eta|^2}{\eta} + \frac{2}{3} F \langle \nabla_b \varphi, \nabla_b \eta \rangle + \frac{1}{9t} \eta F (F - 9),$$

and multiplying by η, we get

$$\begin{aligned} 0 &\geq -\frac{C_3}{R^2} \eta F - 2F |\nabla_b \eta|^2 + \frac{2}{3} F \eta \langle \nabla_b \varphi, \nabla_b \eta \rangle + \frac{1}{9t} \eta^2 F (F - 9) \\ &= (\eta F) \left(-\frac{C_3}{R^2} - 2 \frac{|\nabla_b \eta|^2}{\eta} - \frac{\eta}{t} \right) + \frac{2}{3} \eta F \langle \nabla_b \varphi, \nabla_b \eta \rangle + \frac{1}{9t} (\eta F)^2 \\ &\geq (\eta F) \left(-\frac{C_3}{R^2} - 2 \frac{|\nabla_b \eta|^2}{\eta} - \frac{\eta}{t} \right) - 2\eta F |\nabla_b \varphi| |\nabla_b \eta| + \frac{1}{9t} (\eta F)^2 \end{aligned}$$

Using $0 \leq \eta \leq 1$, and (4.6), we get

$$\begin{aligned} 0 &\geq (\eta F) \left(-\frac{C_3}{R^2} - 2 \frac{C_2}{R^2} - \frac{1}{t} \right) - 2\eta^{3/2} F \frac{\sqrt{C_2}}{R} |\nabla_b \varphi| + \frac{1}{9t} (\eta F)^2 \\ &= (\eta F) \left(-\frac{1}{t} - \frac{C_4}{R^2} \right) - 2\eta^{3/2} F \frac{\sqrt{C_2}}{R} |\nabla_b \varphi| + \frac{1}{9t} (\eta F)^2, \end{aligned}$$

where $C_4 = C_3 + 2C_2$. Multiplying by t to the above inequality, this leads to

$$\begin{aligned} 0 &\geq (\eta F) \left(\frac{1}{9} \eta F - 1 - \frac{C_4}{R^2} t \right) - 2t \eta^{3/2} F \frac{\sqrt{C_2}}{R} |\nabla_b \varphi| \\ &= (\eta F) \left(\frac{1}{9} \eta F - 1 - \frac{C_4}{R^2} t - \frac{2\sqrt{C_2}}{R} \eta^{1/2} |\nabla_b \varphi| \, t \right). \end{aligned}$$

Therefore, we get

$$\eta F \leq 9 + \frac{9C_4}{R^2}t + \frac{18\sqrt{C_2}}{R}\eta^{1/2}\left|\nabla_b\varphi\right| t.$$

(i) If $\varphi_t(x_0, t_0) < 0$, then, by the Proposition 4.1, $|\nabla_b\varphi|^2 \leq |\nabla_b\varphi|^2 - \varphi_t \leq 1/t$ and using $0 \leq \eta \leq 1$, we have

$$\eta F \leq 9 + \frac{C_4}{R^2}t + \frac{18\sqrt{C_2}}{R}t^{1/2}.$$

Recall that all the computations are at (x_0, t_0) and (x_0, t_0) is the maximum point, $t_0 \leq T'$, so we have

$$(\eta F)(x, T') \leq (\eta F)(x_0, t_0) \leq 9 + \frac{C_4}{R^2}T' + \frac{18\sqrt{C_2}}{R}\sqrt{T'}.$$

But $\eta \equiv 1$ on B_R, hence

$$\sup_{x\in B_R}\left(\left|\nabla_b\varphi\right|^2 + 3\varphi_t\right)(x, T') \leq \frac{C_4}{R^2} + \frac{18\sqrt{C_2}}{R}\frac{1}{\sqrt{T'}} + \frac{9}{T'}. \tag{4.7}$$

Now for any fixed time $t \in (0, \infty)$, by letting $R \to \infty$, one obtains

$$\frac{\left|\nabla_b u\right|^2}{u^2} + 3\frac{u_t}{u} \leq \frac{9}{t}$$

on $H^1 \times [0, T)$.

(ii) If $\varphi_t(x_0, t_0) \geq 0$, then $t^{1/2}\left|\nabla_b\varphi\right| \leq F^{1/2}$. The above inequality leads to

$$\eta F - \frac{18\sqrt{C_2}}{R}t^{1/2}(\eta F)^{1/2} - \left(9 + \frac{C_4}{R^2}t\right) \leq 0.$$

Hence

$$\eta F \leq 9 + \frac{C_4}{R^2}t + \frac{18\sqrt{C_2}}{R}t^{1/2}(\eta F)^{1/2}.$$

If $(\eta F) \leq 1$, then

$$\eta F \leq 9 + \frac{C_4}{R^2}t + \frac{18\sqrt{C_2}}{R}t^{1/2}.$$

Otherwise,

$$\eta F \leq 9 + \frac{C_4}{R^2}t + \frac{18\sqrt{C_2}}{R}t^{1/2}(\eta F).$$

For fix t, we can choose R such that $\frac{18\sqrt{C_2}}{R}t^{1/2} \leq \frac{1}{2}$, thus

$$\eta F \leq 18 + \frac{C_4}{R^2}t$$

and similar argument as before

$$\sup_{x\in B_R}\left(\left|\nabla_b\varphi\right|^2 + 3\varphi_t\right)(x, T') \leq \frac{C_4}{R^2} + \frac{18}{T'}. \tag{4.8}$$

Now for any fixed time $t \in (0, \infty)$, by letting $R \to \infty$ such that $\frac{18\sqrt{C_2}}{R} t^{1/2} \to 0$, one obtains

$$\frac{|\nabla_b u|^2}{u^2} + 3\frac{u_t}{u} \leq \frac{9+\epsilon}{t}$$

on $H^1 \times [0, T)$ for any $\epsilon > 0$. □

Then, by combining Theorem 4.2 and Proposition 4.1, Theorem 1.4 follows for $n = 1$ easily.

Now we will apply the subgradient estimates in Theorem 4.2 and Proposition 4.1 to obtain the following Harnack inequality for positive solutions of the CR heat equation (1.6) on $H^1 \times [0, T)$.

THEOREM 4.3. *If $u(x, t)$ be a positive smooth solution of (1.6)*

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

on $H^1 \times [0, T)$ with

$$P_1 u = 0$$

at $t = 0$, then for all points x_1, x_2 in H^1 and times $0 < t_1 < t_2 < T$, we have the inequality

$$\frac{t_1}{t_2} \exp\left(-\frac{d_c^2(x_1, x_2)}{4(t_2 - t_1)}\right) \leq \frac{u(x_2, t_2)}{u(x_1, t_1)} \leq \left(\frac{t_2}{t_1}\right)^{(3+\epsilon)} \exp\left(\frac{3d_c^2(x_1, x_2)}{4(t_2 - t_1)}\right)$$

for any $\epsilon > 0$.

Proof. Let γ be a horizontal curve with $\gamma(t_1) = x_1$ and $\gamma(t_2) = x_2$. We define $\eta : [t_1, t_2] \to M \times [t_1, t_2]$ by

$$\eta(t) = (\gamma(t), t).$$

Clearly $\eta(t_1) = (x_1, t_1)$ and $\eta(t_2) = (x_2, t_2)$. Let $\varphi = \log u(x, t)$, integrate $\frac{d}{dt}\varphi$ along η, we get

$$\begin{aligned} \varphi(x_2, t_2) - \varphi(x_1, t_1) &= \int_{t_1}^{t_2} \frac{d}{dt}\varphi dt \\ &= \int_{t_1}^{t_2} \left\{\langle \dot{\gamma}, \nabla_b \varphi\rangle + \varphi_t\right\} dt. \end{aligned}$$

Applying Theorem 4.2 to φ_t, this yields

$$\begin{aligned} \varphi(x_2, t_2) - \varphi(x_1, t_1) &\leq \int_{t_1}^{t_2} \left\{|\dot{\gamma}|\, |\nabla_b \varphi| + \varphi_t\right\} dt \\ &\leq \int_{t_1}^{t_2} \left\{\frac{3}{4}|\dot{\gamma}|^2 + \frac{3+\epsilon}{t}\right\} dt \\ &= \int_{t_1}^{t_2} \frac{3}{4}|\dot{\gamma}|^2 dt + (3+\epsilon) \log\left(\frac{t_2}{t_1}\right). \end{aligned}$$

Then the right-hand side inequality in theorem 4.3 follows by taking exponentials of the above inequality. Similarly, we can also get the left-hand side inequality. □

As a consequence of Theorem 4.3 and [CY], we have

Corollary 4.4. *Let $H(x,y,t)$ be a L^2-heat kernel of (1.6) on $H^1 \times [0,T)$. Then for some constant δ and $0 < \epsilon < 1$, we have the inequality*

$$H(x,y,t) \leq \frac{C(\epsilon)^\delta}{V(B_x(\sqrt{t}))} \exp\left(-\frac{d_c^2(x,y)}{(4+\epsilon)t}\right) \leq \frac{C(\epsilon)^\delta}{t^2} \exp\left(-\frac{d_c^2(x,y)}{(4+\epsilon)t}\right)$$

with $C(\epsilon) \to \infty$ as $\epsilon \to 0$.

Remark 4.1. *Here we use the volume $V(B_x(R)) \leq CR^{(2n+2)}$ in an $(2n+1)$-dimensional Heisenberg group H^n ([DT]). One should compare this result with [BGG].*

Then Corollary 1.6 follows easily from Theorem 1.4 and Corollary 4.4.

5. Sub-Laplacian of Carnot-Caratheodory distance on Heisenberg groups H^n. In this section, we prove the sub-Laplacian comparison $(*)$ as in previous section. We consider the following two vector fields defined on $\mathbf{R}^3$ with coordinates $(x,t) = (x_1, x_2, t)$:

$$X_1 = \frac{\partial}{\partial x_1} + 2ax_2\frac{\partial}{\partial t} \quad \text{and} \quad X_2 = \frac{\partial}{\partial x_2} - 2ax_1\frac{\partial}{\partial t}$$

with $a > 0$. It is easy to check that

$$[X_1, X_2] = -4a\frac{\partial}{\partial t}.$$

Now we consider the following operator

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

The vector fields X_1, X_2 and $T = \frac{\partial}{\partial t}$ and the operator Δ_H are left-invariant with respect to the "Heisenberg translation": for $(x,t) = (x_1, x_2, t)$ and $(y,s) = (y_1, y_2, s) \in \mathbf{R}^3$,

$$(x,t) \circ (y,s) = (x_1 + y_1, x_2 + y_2, t + s + 2a[x_2 y_1 - x_1 y_2]).$$

Actually, the above multiplicative law defines a group structure on $\mathbf{R}^3$ which we call the 1-dimensional Heisenberg group with $(x,t)^{-1} = (-x, -t)$.

Remark 5.1. *By comparing the previous notations, we first put some conventions as followings: for $a = \frac{1}{2}$*

$$Z_1 = \frac{1}{2}(X_1 - iX_2) \text{ and } Z_{\bar{1}} = \frac{1}{2}(X_1 + iX_2)$$

and

$$J(X_1) = X_2 \text{ and } J(X_2) = -X_1$$

and

$$\Delta_b = -\Delta_H.$$

The symbol of Δ_H is

$$H(x,\xi,\theta) = \frac{1}{2}(\xi_1 + 2ax_2\theta)^2 + \frac{1}{2}(\xi_2 - 2ax_1\theta)^2 = \frac{1}{2}(\zeta_1^2 + \zeta_2^2),$$

where $\zeta_1 = \xi_1 + 2ax_2\theta$ and $\zeta_2 = \xi_2 - 2ax_1\theta$.

In this notation, Hamilton-Jacobi equations for the bicharacteristic curve $(x_1(s), x_2(s), t(s), \xi_1(s), \xi_2(s), \theta(s))$ take the form:

(5.1)

$$\begin{aligned}
\dot{x}_1(s) &= \tfrac{\partial H}{\partial \xi_1} = \xi_1 + 2ax_2\theta = \zeta_1(s),\\
\dot{x}_2(s) &= \tfrac{\partial H}{\partial \xi_2} = \xi_2 - 2ax_1\theta = \zeta_2(s),\\
\dot{t}(s) &= \tfrac{\partial H}{\partial \theta} = (\xi_1 + 2ax_2\theta)(2ax_2) - (\xi_2 - 2ax_1\theta)(2ax_1) = 2a(\zeta_1 x_1 - \zeta_2 x_2),\\
\dot{\xi}_1(s) &= -\tfrac{\partial H}{\partial x_1} = (2a\theta)(\xi_2 - 2ax_1\theta) = (2a\theta)\zeta_2,\\
\dot{\xi}_2(s) &= -\tfrac{\partial H}{\partial x_2} = -(2a\theta)(\xi_1 + 2ax_2\theta) = -(2a\theta)\zeta_1,\\
\dot{\theta}(s) &= -\tfrac{\partial H}{\partial t} = 0,
\end{aligned}$$

where the dot denotes $\frac{d}{ds}$. We let s run along the ray from 0 to a point $\tau \in \mathbf{C}$. Because of group invariance we need to consider paths relative to the origin and a point $(x,t) = (x_1, x_2, t)$ only, and assume boundary conditions

$$x_1(0) = 0, \quad x_2(0) = 0, \quad x_1(\tau) = x_1, \quad x_2(\tau) = x_2, \quad t(\tau) = t. \tag{5.2}$$

Then it is easy to see that the Hamiltonian,

$$\frac{1}{2}\dot{x}_1^2(s) + \frac{1}{2}\dot{x}_2^2(s) = H(x,\xi,\theta) = H_0 \equiv \frac{1}{2}(\zeta_1(0)\zeta_1(0) + \zeta_2(0)\zeta_2(0)).$$

is constant along a given bicharacteristic. The projection of the bicharacteristic curve onto the base is a subRiemannian geodesic connecting the point (x,t) to the origin.

From (5.1), we know that $\theta(s) = \theta(0) = \theta$ and we may take it to be the free parameter. Equations (5.1) imply that

$$\begin{aligned}
\dot{\zeta}_1 &= \dot{\xi}_1 + 2a\theta\dot{x}_2 = 2a\theta\zeta_2 + 2a\theta\zeta_2 = 4a\theta\zeta_2,\\
\dot{\zeta}_2 &= \dot{\xi}_2 - 2a\theta\dot{x}_1 = -2a\theta\zeta_1 - 2a\theta\zeta_1 = -4a\theta\zeta_1.
\end{aligned}$$

Hence,

$$\begin{aligned}
\zeta_1(s) &= \cos(4a\theta s)\zeta_1(0) + \sin(4a\theta s)\zeta_2(0),\\
\zeta_2(s) &= -\sin(4a\theta s)\zeta_1(0) + \cos(4a\theta s)\zeta_2(0).
\end{aligned}$$

Therefore, we may solve for $x(s)$ as a function of x, τ and θ, and then solve for $t(s)$ as a function of x, t, τ and θ. Here are the calculations.

$$\begin{aligned}
x_1(s) &= \int_0^s \zeta_1(\rho)d\rho = -\frac{1}{4a\theta}\{\zeta_2(s) - \zeta_2(0)\}\\
&= -\frac{1}{4a\theta}\left\{-\sin(4a\theta s)\zeta_1(0) + [\cos(4a\theta s) - 1]\zeta_2(0)\right\}\\
&= \frac{\sin(2a\theta s)}{2a\theta}\left\{\cos(2a\theta s)\zeta_1(0) + \sin(2a\theta s)\right\}
\end{aligned}$$

and

$$\begin{aligned}
x_2(s) &= \frac{1}{4a\theta}\{\zeta_1(s) - \zeta_1(0)\}\\
&= \frac{1}{4a\theta}\left\{[\cos(4a\theta s) - 1]\zeta_1(0) + \sin(4a\theta s)\zeta_2(0)\right\}\\
&= \frac{\sin(2a\theta s)}{2a\theta}\left\{-\cos(2a\theta s)\zeta_1(0) + \sin(2a\theta s)\right\}.
\end{aligned}$$

Therefore,

$$\begin{bmatrix} \zeta_1(0) \\ \zeta_2(0) \end{bmatrix} = \frac{2a\theta}{\sin(2a\theta\tau)} \begin{bmatrix} \cos(2a\theta\tau) & -\sin(2a\theta\tau) \\ \sin(2a\theta\tau) & \cos(2a\theta\tau) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}.$$

It follows that

$$H_0 = \frac{1}{2}\left(\zeta_1(0)\zeta_1(0) + \zeta_2(0)\zeta_2(0)\right) = \frac{(2a\theta)^2}{2\sin^2(2a\theta\tau)}(x_1^2 + x_2^2) = \frac{(2a\theta)^2}{2\sin^2(2a\theta\tau)}\|x\|^2.$$

When $\theta = 0$, we have $\zeta(s) = \zeta(0)$, $x(s) = \zeta(0)s$ and $t(s) = t(0)$. Substituting these calculations into (5.1), we have

$$\begin{aligned} t - t(s) &= 2a\int_s^\tau [\zeta_1(\rho)x_2(\rho) - \zeta_2(\rho)x_1(\rho)]\,d\rho \\ &= \tfrac{1}{2\theta}\int_s^\tau [1 - \cos(4a\theta\rho)]d\rho \cdot \left[\zeta_1^2(0) + \zeta_2^2(0)\right] \\ &= (\tau - s)\tfrac{2a^2\theta}{\sin^2(2a\theta\tau)}\|x\|^2 - \tfrac{a}{2}\cdot\tfrac{\sin(4a\theta\tau) - \sin(4a\theta s)}{\sin^2(2a\theta\tau)}\|x\|^2. \end{aligned}$$

THEOREM 5.1. *The solution of equations (5.1) with boundary conditions (5.2) is*

$$\begin{aligned} x_1(s) &= \tfrac{\sin(2a\theta s)}{\sin(2a\theta\tau)}\left\{\cos[2a\theta(s-\tau)]x_1 + \sin[2a\theta(s-\tau)]x_2\right\}, \\ &= \tfrac{\sin(2a\theta s)}{\sin(2a\theta\tau)}\left\{-\sin[2a\theta(s-\tau)]x_1 + \cos[2a\theta(s-\tau)]x_2\right\}, \\ &= \left[\tfrac{a}{2}\tfrac{\sin(4a\theta\tau) - \sin(4a\theta s)}{\sin^2(2a\theta\tau)} - (\tau - s)\tfrac{2a^2\theta}{\sin^2(2a\theta\tau)}\right](x_1^2 + x_2^2) - t. \end{aligned} \tag{5.3}$$

The value of the Hamiltonian H on this path is

$$H_0 = \frac{2a^2\theta^2}{\sin^2(2a\theta\tau)}(x_1^2 + x_2^2).$$

Next (5.3) yields

$$t - t(0) = a\mu(2a\theta\tau)\|x\|^2,$$

where we set

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

The action integral associated to the Hamiltonian curve is

$$S(x, t, \tau; \theta) = \int_0^\tau \left\{ \sum_{j=1}^2 \xi_j(s)\dot{x}_j(s) + \theta\dot{t}(s) - H(x(s), \xi(s), \theta) \right\} ds.$$

H is homogeneous of degree 2 with respect to (ξ_1, ξ_2, θ), so

$$S = \int_0^\tau \left\{ \sum_{j=1}^2 \xi_j \frac{\partial H}{\partial \xi_j} + \theta\frac{\partial H}{\partial \theta} - H \right\} ds = \int_0^\tau (2H - H)ds = \tau H_0. \tag{5.4}$$

From formulas (5.3), we have the following theorem:

THEOREM 5.2. *The action integral $S(x,t,\tau,\theta)$ is given by*

$$S(x,t,\tau,\theta) = \frac{\tau(2a\theta)^2}{2\sin^2(2a\theta\tau)}\|x\|^2, \\ = [t - t(0)]\theta + a\theta\cot(2a\theta\tau)(x_1^2 + x_2^2), \quad \theta \in \left[0, \frac{\pi}{a}\right).$$

It is convenient to fix τ, $\tau = 1$. Then the Hamiltonian paths are determined entirely by the parameter θ. We may take the end points to be $(\mathbf{0}, 0)$ and (x,t). Then θ must satisfy

$$t = a\mu(2a\theta)(x_1^2 + x_2^2) = a\mu(2a\theta)\|x\|^2.$$

It can be shown that μ is a monotone increasing diffeomorphism of the interval $(-\pi,\pi)$ onto $\mathbf{R}$. On each interval $(m\pi,(m+1)\pi)$, $m = 1,2,\ldots$, μ has a unique critical point z_m. On this interval μ decreases strictly from $+\infty$ to $\mu(z_m)$ and then increases strictly from $\mu(z_m)$ to $+\infty$. Now the complete picture of the geodesics is given in the following two theorems.

THEOREM 5.3. *There are finitely many geodesics that join the origin to (x,t) if and only if $x \neq \mathbf{0}$. These geodesics are parametrized by the solutions θ of*

$$a\mu(2a\theta)\|x\|^2 = |t|, \tag{5.5}$$

and their lengths increase strictly with θ. There is exactly one such geodesic if and only if

$$|t| < a\mu(z_1)\|x\|^2,$$

and the number of geodesics increases without bound as $\frac{|t|}{a\|x\|^2} \to \infty$.

The square of the length of the geodesic associated to a solution θ of (5.5) is

$$\begin{aligned} 2S(x,|t|,1,\theta) &= \tfrac{(2a\theta)^2}{\sin^2(2a\theta)}(x_1^2+x_2^2) \\ &= \tfrac{(2a\theta)^2}{\sin^2(2a\theta)}\tfrac{(x_1^2+x_2^2)}{(x_1^2+x_2^2)+|t|/a}\left[\tfrac{|t|}{a} + (x_1^2+x_2^2)\right] \\ &= \tfrac{(2a\theta)^2}{\sin^2(2a\theta)}\tfrac{1}{1+\mu(2a\theta)}\left[\tfrac{|t|}{a} + (x_1^2+x_2^2)\right] \\ &= \nu(2a\theta)\left(\tfrac{|t|}{a} + \|x\|^2\right), \end{aligned} \tag{5.6}$$

where $\nu(0) = 2$ and otherwise

$$\nu(z) = \frac{z^2}{\sin^2 z}\frac{1}{1+\mu(z)} = \frac{z^2}{z + \sin^2 z - \sin z\cos z}.$$

Consequently, if $2a\theta \in (m\pi,(m+1)\pi)$ the length d_θ of the geodesic satisfies

$$\frac{m^2\pi^2}{(m+1)\pi+2}\left(\frac{|t|}{a} + \|x\|^2\right) < (d_\theta)^2 < \frac{(m+1)^2\pi^2}{m\pi}\left(\frac{|t|}{a} + \|x\|^2\right).$$

When $x = \mathbf{0}$, we need to find the Hamiltonian paths connecting the origin to $(0,t)$, *i.e.*, $x_1(1) = 0$, $x_2(1) = 0$, $t(1) = t$. This implies that $\zeta_1(1) = \zeta_1(0)$ and $\zeta_2(1) = \zeta_2(0)$. It follows that

$$\zeta_1(1) = \cos(4a\theta)\zeta_1(0) + \sin(4a\theta)\zeta_2(0) = \zeta_1(0), \\ \zeta_2(1) = -\sin(4a\theta)\zeta_1(0) + \cos(4a\theta)\zeta_2(0) = \zeta_2(0).$$

This implies that

$$\sin(4a\theta) = 0, \quad \text{and} \quad \cos(4a\theta) = 1$$

i.e.,

$$2a\theta = m\pi, \qquad \text{with} \quad m = 1, 2, 3, \ldots.$$

In this case,

$$t = \frac{1}{2\theta}(\zeta_1^2(0) + \zeta_2^2(0)),$$

therefore, $\theta \neq 0$ and $m \neq 0$ in (5.4). We also know that

$$d_m^2 = \frac{m\pi|t|}{a}.$$

Summarizing, we have the following theorem.

THEOREM 5.4. *The geodesics that join the origin to a point* $(0, 0, t)$ *have lengths* d_1, d_2, d_3,..., *where*

$$d_m^2 = \frac{m\pi|t|}{a}.$$

Since $x_1(1) = x_2(1) = 0$, we may use $(\zeta_1(0), \zeta_2(0))$ to obtain the geodesics as follows:

$$\begin{aligned} x_1^{(m)}(s) &= -\frac{1}{2m\pi}\left\{-\sin(2m\pi s)\zeta_1(0) + [\cos(2m\pi s) - 1]\zeta_2(0)\right\} \\ &= \left(\frac{t}{4am\pi}\right)^{\frac{1}{2}}\left\{\sin(2m\pi s)\frac{\zeta_1(0)}{\|\zeta(0)\|} + [1 - \cos(2m\pi s)]\frac{\zeta_2(0)}{\|\zeta(0)\|}\right\}, \end{aligned}$$

where $\|\zeta(0)\| = \sqrt{\zeta_1^2(0) + \zeta_2^2(0)}$. Similarly, we have

$$\begin{aligned} x_2^{(m)}(s) &= \frac{1}{2m\pi}\left\{[\cos(2m\pi s) - 1]\zeta_1(0) + \sin(2m\pi s)\zeta_2(0)\right\} \\ &= \left(\frac{t}{4am\pi}\right)^{\frac{1}{2}}\left\{[\cos(2m\pi s) - 1]\frac{\zeta_1(0)}{\|\zeta(0)\|} + \sin(2m\pi s)\frac{\zeta_2(0)}{\|\zeta(0)\|}\right\}, \end{aligned}$$

and

$$t^{(m)}(s) = [2m\pi s - \sin(2m\pi s)]\,\frac{t}{2m\pi}.$$

This shows that for each fixed m, $m = 1, 2, \ldots$, the geodesics $(x_1^{(m)}(s), x_2^{(m)}(s), t^{(m)}(s))$ can be parametrized by a unit vector $\zeta(0)/\|\zeta(0)\|$ on the unit circle. These curves lie in a cylinder around the t-axis whose radius is $\mathcal{O}(1/\sqrt{m})$.

A special case of (5.6) is the square of the *Carnot-Caratheodory distance* $[d_c(x, t)]^2$:

$$[d_c(x, t)]^2 = 2S(x, |t|, 1; \theta_c) = \left[\frac{2a\theta_c}{\sin(2a\theta_c)}\right]^2 \|x\|^2 = \nu(2a\theta_c)\left(\frac{|t|}{a} + \|x\|^2\right),$$

where θ_c is the unique solution of $a\mu(2a\theta)\|x\|^2 = |t|$ in the interval $[0, \pi/2a)$. Introduce a new parameter $\phi = 2a\theta_c$. Then the Carnot-Caratheodory distance between the origin and point (x_1, x_2, t) can be expressed as

$$d_c(x,t) = \frac{\phi}{\sin\phi}\|x\| \quad \text{with} \quad a\mu(\phi)\|x\|^2 = |t| \quad \text{and} \quad \phi \in [0,\pi).$$

We will compute $\Delta_H d_c(x,t)$. In polar coordinates,

$$-\Delta_H = \frac{1}{2}(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial^2}{\partial r\partial\theta} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}) + 2a\frac{\partial^2}{\partial t\partial\theta} + 2a^2r^2\frac{\partial^2}{\partial t^2}.$$

Since $d_c(x,t)$ depends only on $r = \|x\| = \sqrt{x_1^2 + x_2^2}$, we have

$$-\Delta_H d_c(x,t) = (\frac{1}{2}\frac{\partial^2}{\partial r^2} + 2a^2r^2\frac{\partial^2}{\partial t^2})d_c(r,t).$$

Introduce a new variable $u = |t|/ar^2$, then

$$d_c(r,t) := f_c(r,u) = \frac{\phi}{\sin\phi}r \quad \text{where } u \text{ satisfies} \quad u = \mu(\phi) = \frac{\phi - \sin\phi\cos\phi}{\sin^2\phi}.$$

Hence

$$-\Delta_H d_c(r,t) = (\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{2}{r^2}\frac{\partial^2}{\partial u^2})f_c(r,u) = \frac{2}{r}\frac{\partial^2}{\partial u^2}(\frac{\phi}{\sin\phi}),$$

where u is given by $u = \mu(\phi)$. Let $g(\phi) = \frac{\phi}{\sin\phi}$. Then

$$\frac{dg}{du} = \frac{dg}{d\phi}\cdot\frac{d\phi}{du} \quad \text{and} \quad \frac{d^2g}{du^2} = \frac{d^2g}{d\phi^2}\cdot(\frac{d\phi}{du})^2 + \frac{dg}{d\phi}\cdot\frac{d^2\phi}{du^2}.$$

We next compute $\frac{dg}{d\phi}$, $\frac{d^2g}{d\phi^2}$, $\frac{d\phi}{du}$ and $\frac{d^2\phi}{du^2}$.

$$\frac{dg}{d\phi} = \frac{\sin\phi - \phi\cos\phi}{\sin^2\phi} \quad \text{and} \quad \frac{d^2g}{d\phi^2} = \frac{\phi(1+\cos^2\phi) - 2\sin\phi\cos\phi}{\sin^3\phi}.$$

Next $u = \mu(\phi)$ implies

$$1 = \mu'(\phi)\frac{d\phi}{du}, \quad \frac{d\phi}{du} = \frac{1}{\mu'(\phi)} \quad \text{and} \quad \frac{d^2\phi}{du^2} = -\frac{\mu''(\phi)}{(\mu'^3)}.$$

We now compute $\mu'(\phi)$ and $\mu''(\phi)$ from $\mu(\phi) = \phi\csc^2\phi - \cot\phi$.

$$\mu'^2\phi - 2\phi\csc^2\phi\cot\phi + \csc^2\phi = 2\csc^2\phi(1 - \phi\cot\phi).$$

and

$$\begin{aligned}&\mu''^2\phi\cot\phi(1-\phi\cot\phi) + 2\csc^2\phi(\phi\csc^2\phi - \cot\phi)\\ &= 2\csc^2\phi[\phi(3\cot^2\phi + 1) - 3\cot\phi].\end{aligned}$$

We finally compute $-\Delta_h f_c(r,u) = \frac{2}{r}\frac{d^2}{du^2}g(\phi)$.

$$\begin{aligned}-\Delta_H f_c(r,u) &= \frac{2}{r}\left[\frac{d^2g}{d\phi^2}\cdot(\frac{d\phi}{du})^2 + \frac{dg}{d\phi}\cdot\frac{d^2\phi}{du^2}\right]\\ &= \frac{2}{r}\left[\frac{d^2g}{d\phi^2}\cdot\frac{1}{(\mu'^2)} - \frac{dg}{d\phi}\frac{\mu''(\phi)}{(\mu'^3)}\right]\\ &= \frac{2}{r(\mu'^2)}\left[\frac{d^2g}{d\phi^2} - \frac{dg}{d\phi}\cdot\frac{\mu''(\phi)}{\mu'(\phi)}\right].\end{aligned}$$

We shall compute the term in $[\dots]$ in term of ϕ first.

$$\begin{aligned}
&\frac{d^2g}{d\phi^2}-\frac{dg}{d\phi}\cdot\frac{\mu''(\phi)}{\mu'(\phi)}\\
=&\frac{\phi(1+\cos^2\phi)-2\sin\phi\cos\phi}{\sin^3\phi}-\frac{\sin\phi-\phi\cos\phi}{\sin^2\phi}\cdot\frac{2\csc^2\phi[\phi(3\cot^2\phi+1)-3\cot\phi]}{2\csc^2\phi(1-\phi\cot\phi)}\\
=&\frac{\phi(1+\cos^2\phi)-2\sin\phi\cos\phi}{\sin^3\phi}-\frac{\phi(3\cot^2\phi+1)-3\cot\phi}{\sin\phi}\\
=&\frac{\phi(1+\cos^2\phi)-2\sin\phi\cos\phi-\phi(3\cos^2\phi+\sin^2\phi)+3\cos\phi\sin\phi}{\sin^3\phi}\\
=&\frac{\sin\phi\cos\phi-\phi\cos^2\phi}{\sin^3\phi}.
\end{aligned}$$

Hence we have

$$\begin{aligned}
-\Delta_H f_c(r,u)&=\frac{2}{r(\mu'^2}\left[\frac{d^2g}{d\phi^2}-\frac{dg}{d\phi}\cdot\frac{\mu''(\phi)}{\mu'(\phi)}\right]\\
&=\frac{\sin\phi\cos\phi-\phi\cos^2\phi}{\sin^3\phi}\cdot\frac{1}{2r\csc^4\phi(1-\phi\cot\phi)^2}\\
&=\frac{(1-\phi\cot\phi)\sin\phi\cos\phi}{2r\csc\phi(1-\phi\cot\phi)^2}\\
&=\frac{\sin^2\phi\cos\phi}{2r(1-\phi\cot\phi)}.
\end{aligned}$$

Since $d_c=\frac{\phi}{\sin\phi}r$,

$$-\Delta_H d_c=\frac{1}{2d_c}\cdot\frac{\phi\sin^2\phi\cos\phi}{\sin\phi-\phi\cos\phi}. \tag{5.7}$$

We next study the function $F(\phi)=\frac{\phi\sin^2\phi\cos\phi}{2(\sin\phi-\phi\cos\phi)}$ where ϕ is given by

$$ar^2\mu(\phi)=t\quad\text{with}\quad\mu(\phi)=\frac{\phi-\sin\phi\cos\phi}{\sin^2\phi}.$$

The function $F(\phi)$ is smooth on the interval $[0,\pi]$, decreasing from $[0,\phi_m]$ and increasing from $[\phi_m,\pi]$. ϕ_m is the unique critical point of $F(\phi)$ inside the interval $(0,\pi)$. $F(0)=3$, $F(\pi/2)=F(\pi)=0$.

As $r\to0$ with $t>0$ fixed, $\phi\to\pi^-$ and the equation $ar^2\mu(\phi)=t$ implies

$$\frac{ar^2}{t}\frac{\phi-\sin\phi\cos\phi}{\sin^2\phi}=1.$$

This shows that

$$\phi\to\pi\quad\text{and}\quad\sin\phi\sim(\frac{a\pi}{t})^{1/2}r\quad\text{as}\quad r\to0.$$

This implies (5.7) makes sense when $r=0$. This corresponds to $\phi=\pi$.

All these imply

$$\Delta_b d_c=-\Delta_H d_c\le\frac{3}{d_c}$$

and then the Sub-Laplacian comparison $(*)$ follows.

We now turn to the study of the $(2n+1)$-dimensional Heisenberg group H^n. The manifold is $\mathbf{R}^{2n}\times\mathbf{R}$ and the group law is given by

$$(\mathbf{x},t)\circ(\mathbf{y},s)=(\mathbf{x}+\mathbf{y},t+s+2\sum_{j=1}^{n}a_j[x_{2j}y_{2j-1}-x_{2j-1}y_{2j}])$$

for $a_1,\ a_2,\cdots,a_n$ are positive constants and numbered so that

$$0<a_1\le a_2\le\cdots\le a_n.$$

The vector fields

$$\begin{aligned}X_{2j-1}&=\frac{\partial}{\partial x_{2j-1}}+2a_jx_{2j}\frac{\partial}{\partial t}\\ X_{2j}&=\frac{\partial}{\partial x_{2j}}-2a_jx_{2j-1}\frac{\partial}{\partial t}\\ T&=\frac{\partial}{\partial t}\end{aligned}$$

are left-invariant and generate the Lie algebra. The associated Heisenberg sub-Laplacian is

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

The symbol of Δ_H is

$$H(\mathbf{x},\xi,\theta)=\frac{1}{2}\sum_{j=1}^{n}[(\xi_{2j-1}+2a_jx_{2j}\theta)^2+(\xi_{2j}-2a_jx_{2j-1}\theta)^2=\frac{1}{2}(\zeta_1^2+\zeta_2^2).$$

We can find the bicharacteristic curve connecting the point $(\mathbf{x},t)$ to the origin by solving the associated Hamilton's equations which take essentially the same form as (5.1). We will just list the formulae that we need and refer to [BGG] for details. The value of the Hamiltonian H on the bicharacteristic curve is the constant:

$$H_0=\sum_{j=1}^{n}\frac{2a_j^2\theta^2}{\sin^2(2a_j\tau\theta)}r_j^2$$

with $r_j^2=x_{2j-1}^2+x_{2j}^2$. The analogue of (5.5) is follows:

$$t=\sum_{j=1}^{n}a_j\mu(2a_j\tau\theta)r_j^2.$$

The action integral $S(\mathbf{x},t,\tau;\theta)$ takes a similar form:

$$S(\mathbf{x},t,\tau;\theta)=\sum_{j=1}^{n}\frac{4\tau a_j^2\theta^2}{\sin^2(2a_j\tau\theta)}r_j^2=t\theta+\sum_{j=1}^{n}a_j\theta\cot(2a_j\tau\theta)r_j^2.$$

When we study the classical action and Carnot-Caratheodory distance, we set $\tau = 1$. In the case of $\mathbf{x} \neq 0$, there are finitely many geodesics from the origin to $(\mathbf{x}, t)$. The geodesics are indexed by the solutions of

$$|t| = \sum_{j=1}^{n} a_j \mu(2a_j\theta) r_j^2 \tag{5.8}$$

and their lengths increase with θ. The Carnot-Caratheodory distance from the origin to $(\mathbf{x}, t)$ is

$$d^2(\mathbf{x}, t) = 2S(\mathbf{x}, |t|, 1; \theta_c)$$

where θ_c is the unique solution of (5.8) in the interval $[0, \pi/2a_n)$.

In the isotropic case $a_1 = a_2 = \cdots = a_n$, the results of the previous computations for $n = 1$ carry over with no change.

6. Subgradient estimate on higher dimensional pseudohermitian manifolds. Let (M, J, θ) be a closed pseudohermitian $(2n+1)$-manifold for $n \geq 2$. In this section, we derive the CR version of parabolic Li-Yau gradient estimate for the positive solution $u(x, t)$ of (1.6) on $M \times [0, \infty)$ for $n \geq 2$.

First, we derive the following inequalities which we need in the proof of Proposition 1.1.

LEMMA 6.1. *Let (M, J, θ) be a closed pseudohermitian $(2n+1)$-manifold. Let f be a smooth real-valued function on M. Then*

$$|(\nabla^H)^2 f|^2 \geq 2 \sum_{\alpha,\beta=1}^{n} |f_{\alpha\beta}|^2 + 2 \sum_{\substack{\alpha,\beta=1 \\ \alpha\neq\beta}}^{n} |f_{\alpha\overline{\beta}}|^2 + \frac{1}{2} \sum_{\alpha=1}^{n} |f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha}|^2.$$

Proof. Since

$$\begin{aligned} |(\nabla^H)^2 f|^2 &= 2\textstyle\sum_{\alpha,\beta=1}^{n} (f_{\alpha\beta} f_{\overline{\alpha}\overline{\beta}} + f_{\alpha\overline{\beta}} f_{\overline{\alpha}\beta}) \\ &= 2\textstyle\sum_{\alpha,\beta=1}^{n} (|f_{\alpha\beta}|^2 + |f_{\alpha\overline{\beta}}|^2) \\ &= 2(\textstyle\sum_{\alpha,\beta=1}^{n} |f_{\alpha\beta}|^2 + \sum_{\substack{\alpha,\beta=1 \\ \alpha\neq\beta}}^{n} |f_{\alpha\overline{\beta}}|^2 + \sum_{\alpha=1}^{n} |f_{\alpha\overline{\alpha}}|^2) \end{aligned}$$

and

$$\begin{aligned} \textstyle\sum_{\alpha=1}^{n} |f_{\alpha\overline{\alpha}}|^2 &= \tfrac{1}{4} \textstyle\sum_{\alpha=1}^{n} \left(|f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha}|^2 + f_0^2 \right) \\ &= \tfrac{1}{4} \textstyle\sum_{\alpha=1}^{n} |f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha}|^2 + \tfrac{n}{4} f_0^2. \end{aligned}$$

It follows that

$$\begin{aligned} |(\nabla^H)^2 f|^2 &= 2(\textstyle\sum_{\alpha,\beta=1}^{n} |f_{\alpha\beta}|^2 + \sum_{\substack{\alpha,\beta=1 \\ \alpha\neq\beta}}^{n} |f_{\alpha\overline{\beta}}|^2) + \tfrac{1}{2} \sum_{\alpha=1}^{n} |f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha}|^2 + \tfrac{n}{2} f_0^2 \\ &\geq 2(\textstyle\sum_{\alpha,\beta=1}^{n} |f_{\alpha\beta}|^2 + \sum_{\substack{\alpha,\beta=1 \\ \alpha\neq\beta}}^{n} |f_{\alpha\overline{\beta}}|^2) + \tfrac{1}{2} \sum_{\alpha=1}^{n} |f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha}|^2. \end{aligned}$$

□

LEMMA 6.2. *Let (M, J, θ) be a closed pseudohermitian $(2n+1)$-manifold for $n \geq 2$. Let f be a smooth real-valued function on M. Then*

$$\begin{aligned} \left\langle \nabla_b f, \nabla_b |\nabla_b f|^2 \right\rangle \leq (n+2) \sum_{\alpha,\beta=1}^{n} |f_{\alpha\beta}|^2 + (n+2) \sum_{\substack{\alpha,\beta=1 \\ \alpha\neq\beta}}^{n} |f_{\alpha\overline{\beta}}|^2 \\ + \left(\Delta_b f + |\nabla_b f|^2 \right) |\nabla_b f|^2 + \frac{(n+2)(n-1)}{4(n+1)} \sum_{\alpha=1}^{n} |f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha}|^2. \end{aligned}$$

Proof. We first derive

$$
\begin{aligned}
&\left\langle \nabla_b f, \nabla_b |\nabla_b f|^2\right\rangle \\
= \;& 4\sum_{\alpha,\beta=1}^n \mathrm{Re}(f_{\alpha\beta} f_{\overline{\alpha}} f_{\overline{\beta}} + f_{\alpha\overline{\beta}} f_{\overline{\alpha}} f_{\beta}) \\
= \;& 4\mathrm{Re}(\sum_{\alpha,\beta=1}^n f_{\alpha\beta} f_{\overline{\alpha}} f_{\overline{\beta}} + \sum_{\substack{\alpha,\beta=1\\ \alpha\neq\beta}}^n f_{\alpha\overline{\beta}} f_{\overline{\alpha}} f_{\beta}) + 2\sum_{\alpha=1}^n (f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha})|f_\alpha|^2 \\
\leq \;& (n+2)(\sum_{\alpha,\beta=1}^n |f_{\alpha\beta}|^2 + \sum_{\substack{\alpha,\beta=1\\ \alpha\neq\beta}}^n |f_{\alpha\overline{\beta}}|^2) + \tfrac{4}{n+2}\sum_{\alpha,\beta=1}^n |f_\alpha|^2|f_\beta|^2 \\
& + \tfrac{4}{n+2}\sum_{\substack{\alpha,\beta=1\\ \alpha\neq\beta}}^n |f_\alpha|^2|f_\beta|^2 + 2\sum_{\alpha=1}^n (f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha})|f_\alpha|^2 \\
= \;& (n+2)(\sum_{\alpha,\beta=1}^n |f_{\alpha\beta}|^2 + \sum_{\substack{\alpha,\beta=1\\ \alpha\neq\beta}}^n |f_{\alpha\overline{\beta}}|^2) + \tfrac{1}{n+2}|\nabla_b f|^4 \\
& + \tfrac{4}{n+2}\sum_{\substack{\alpha,\beta=1\\ \alpha\neq\beta}}^n |f_\alpha|^2|f_\beta|^2 + 2\sum_{\alpha=1}^n (f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha})|f_\alpha|^2.
\end{aligned} \tag{6.1}
$$

Here we used the identity $\sum_{\alpha,\beta=1}^n |f_\alpha|^2|f_\beta|^2 = (\sum_{\alpha=1}^n |f_\alpha|^2)^2 = \frac{1}{4}|\nabla_b f|^4$.

Now we compute the last term in the above inequality.

$$
\begin{aligned}
&\sum_{\alpha=1}^n (f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha})|f_\alpha|^2 \\
= \;& [\sum_{\alpha=1}^n (f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha})](\sum_{\beta=1}^n |f_\beta|^2) \\
& - \sum_{\alpha=1}^n (f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha})(\sum_{\substack{\beta=1\\ \beta\neq\alpha}}^n |f_\beta|^2) \\
\leq \;& \tfrac{1}{2}\Delta_b f |\nabla_b f|^2 + \sum_{\alpha=1}^n |f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha}|(\sum_{\substack{\beta=1\\ \beta\neq\alpha}}^n |f_\beta|^2) \\
\leq \;& \tfrac{1}{2}\Delta_b f |\nabla_b f|^2 + \tfrac{(n-1)(n+2)}{8(n+1)}\sum_{\alpha=1}^n |f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha}|^2 \\
& + \tfrac{2(n+1)}{(n-1)(n+2)}\sum_{\alpha=1}^n (\sum_{\substack{\beta=1\\ \beta\neq\alpha}}^n |f_\beta|^2)^2.
\end{aligned}
$$

Substituting the above inequality into (6.1), one obtains

$$
\begin{aligned}
&\left\langle \nabla_b f, \nabla_b |\nabla_b f|^2\right\rangle \\
\leq \;& (n+2)(\sum_{\alpha,\beta=1}^n |f_{\alpha\beta}|^2 + \sum_{\substack{\alpha,\beta=1\\ \alpha\neq\beta}}^n |f_{\alpha\overline{\beta}}|^2) + \Delta_b f |\nabla_b f|^2 \\
& + \tfrac{(n-1)(n+2)}{4(n+1)}\sum_{\alpha=1}^n |f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha}|^2 + \tfrac{1}{n+2}|\nabla_b f|^4 \\
& + \tfrac{4(n+1)}{(n+2)(n-1)}\sum_{\alpha=1}^n (\sum_{\substack{\beta=1\\ \beta\neq\alpha}}^n |f_\beta|^2)^2 + \tfrac{4}{n+2}\sum_{\substack{\alpha,\beta=1\\ \alpha\neq\beta}}^n |f_\alpha|^2|f_\beta|^2 \\
\leq \;& (n+2)(\sum_{\alpha,\beta=1}^n |f_{\alpha\beta}|^2 + \sum_{\substack{\alpha,\beta=1\\ \alpha\neq\beta}}^n |f_{\alpha\overline{\beta}}|^2) + \Delta_b f |\nabla_b f|^2 \\
& + \tfrac{(n+2)(n-1)}{4(n+1)}\sum_{\alpha=1}^n |f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha}|^2 + \tfrac{1}{n+2}|\nabla_b f|^4 \\
& + \tfrac{4(n+1)}{(n+2)(n-1)}\left(\sum_{\alpha=1}^n (\sum_{\substack{\beta=1\\ \beta\neq\alpha}}^n |f_\beta|^2)^2 + \sum_{\substack{\alpha,\beta=1\\ \alpha\neq\beta}}^n |f_\alpha|^2|f_\beta|^2\right) \\
= \;& (n+2)(\sum_{\alpha,\beta=1}^n |f_{\alpha\beta}|^2 + \sum_{\substack{\alpha,\beta=1\\ \alpha\neq\beta}}^n |f_{\alpha\overline{\beta}}|^2) + \Delta_b f |\nabla_b f|^2 \\
& + \tfrac{(n+2)(n-1)}{4(n+1)}\sum_{\alpha=1}^n |f_{\alpha\overline{\alpha}} + f_{\overline{\alpha}\alpha}|^2 + |\nabla_b f|^4.
\end{aligned}
$$

Here we have used the identity

$$
\sum_{\alpha=1}^n \left(\sum_{\substack{\beta=1\\ \beta\neq\alpha}}^n |f_\beta|^2\right)^2 + \sum_{\substack{\alpha,\beta=1\\ \alpha\neq\beta}}^n |f_\alpha|^2|f_\beta|^2 = (n-1)\left(\sum_{\alpha=1}^n |f_\alpha|^2\right)^2 = \tfrac{n-1}{4}|\nabla_b f|^4.
$$

This completes the proof of the Lemma. □

Now we can derive the following Proposition 1.1 which is exact form of Lemma 3.3 for $n \geq 2$.

Proof of Proposition 1.1. First differentiating (1.7) w.r.t. the t-variable, we have

$$\begin{aligned} G_t &= \frac{1}{t}G + t[|\nabla_b\varphi|^2 + (1+\frac{2}{n})\varphi_t]_t \\ &= \frac{1}{t}G + t[2(1+\frac{1}{n})\,|\nabla_b\varphi|^2 + (1+\frac{2}{n})\Delta_b\varphi]_t \\ &= \frac{1}{t}G + t[4(1+\frac{1}{n})\langle\nabla_b\varphi, \nabla_b\varphi_t\rangle + (1+\frac{2}{n})\Delta_b\varphi_t]. \end{aligned} \tag{6.2}$$

By using the CR version of Bochner formula (2.1) and Lemma 3.2, one obtains

$$\begin{aligned} \Delta_b G &= t\left(\Delta_b\,|\nabla_b\varphi|^2 + (1+\frac{2}{n})\Delta_b\varphi_t\right) \\ &= t[2|(\nabla^H)^2\varphi|^2 + 2(1+\frac{2}{n})\,\langle\nabla_b\varphi, \nabla_b\Delta_b\varphi\rangle \\ &\quad +2[2Ric-(n+2)Tor]((\nabla_b\varphi)_{\mathbf{C}}, (\nabla_b\varphi)_{\mathbf{C}}) \\ &\quad -\frac{8}{n}\langle P\varphi+\bar{P}\varphi, d_b\varphi\rangle_{L_\theta^*} + (1+\frac{2}{n})\Delta_b\varphi_t] \\ &\geq t[2|(\nabla^H)^2\varphi|^2 + 2(1+\frac{2}{n})\,\langle\nabla_b\varphi, \nabla_b\Delta_b\varphi\rangle - l_0\,|\nabla_b\varphi|^2 \\ &\quad -\frac{8}{n}\langle P\varphi+\bar{P}\varphi, d_b\varphi\rangle_{L_\theta^*} + (1+\frac{2}{n})\Delta_b\varphi_t] \\ &= t[2|(\nabla^H)^2\varphi|^2 + 2(1+\frac{2}{n})\,\langle\nabla_b\varphi, \nabla_b\Delta_b\varphi\rangle - l_0\,|\nabla_b\varphi|^2 \\ &\quad -\frac{8}{n}u^{-2}\left\langle Pu+\bar{P}u, d_bu\right\rangle_{L_\theta^*} + \frac{4}{n}\varphi_t|\nabla_b\varphi|^2 \\ &\quad +\frac{4}{n}\left\langle\nabla_b\varphi, \nabla_b|\nabla_b\varphi|^2\right\rangle + (1+\frac{2}{n})\Delta_b\varphi_t]. \end{aligned} \tag{6.3}$$

Here we have used the inequalities

$$[2Ric-(n+2)Tor]((\nabla_b\varphi)_C, (\nabla_b\varphi)_C) \geq -l_0\,|(\nabla_b\varphi)_C|^2 = -\frac{l_0}{2}\,|\nabla_b\varphi|^2$$

and

$$\varphi_t = \frac{u_t}{u} = \frac{\Delta_b u}{u}.$$

Applying the formula

$$\Delta_b\varphi = \varphi_t - |\nabla_b\varphi|^2 = \frac{n}{(n+2)t}G - \frac{2(n+1)}{n+2}\,|\nabla_b\varphi|^2 \tag{6.4}$$

and combining (6.2), (6.3), we conclude

$$\begin{aligned} &\left(\Delta_b - \frac{\partial}{\partial t}\right)G \\ &\geq -\frac{1}{t}G + t[2|(\nabla^H)^2\varphi|^2 + 2(1+\frac{2}{n})\,\langle\nabla_b\varphi, \nabla_b\Delta_b\varphi\rangle + \frac{4}{n}\left\langle\nabla_b\varphi, \nabla_b|\nabla_b\varphi|^2\right\rangle \\ &\quad -4(1+\frac{1}{n})\langle\nabla_b\varphi, \nabla_b\varphi_t\rangle - l_0\,|\nabla_b\varphi|^2 + \frac{4}{n}\varphi_t|\nabla_b\varphi|^2 - \frac{8}{n}u^{-2}\left\langle Pu+\bar{P}u, d_bu\right\rangle_{L_\theta^*}] \\ &= -\frac{1}{t}G - \frac{2n}{(n+2)}\langle\nabla_b\varphi, \nabla_b G\rangle + t[2|(\nabla^H)^2\varphi|^2 - \frac{4}{n+2}\left\langle\nabla_b\varphi, \nabla_b|\nabla_b\varphi|^2\right\rangle \\ &\quad -l_0\,|\nabla_b\varphi|^2 + \frac{4}{n}\varphi_t|\nabla_b\varphi|^2 - \frac{8}{n}u^{-2}\left\langle Pu+\bar{P}u, d_bu\right\rangle_{L_\theta^*}]. \end{aligned}$$

Now, by Lemma 6.1, Lemma 6.2, Cauchy-Schwarz inequality and applying the formula (6.4), we final have

$$
\begin{aligned}
&\left(\Delta_b - \frac{\partial}{\partial t}\right) G \\
\geq &-\frac{2n}{(n+2)}\langle \nabla_b \varphi, \nabla_b G\rangle + t[\frac{2}{n+1}\sum_{\alpha=1}^{n} |\varphi_{\alpha\overline{\alpha}} + \varphi_{\overline{\alpha}\alpha}|^2 + \frac{8}{n(n+2)}\varphi_t |\nabla_b \varphi|^2 \\
&-l_0 \left|\nabla_b \varphi\right|^2 - \frac{8}{n} u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*}] - \frac{1}{t}G \\
\geq &-\frac{2n}{(n+2)}\langle \nabla_b \varphi, \nabla_b G\rangle + t[\frac{2}{n(n+1)}(\Delta_b \varphi)^2 + \frac{8}{n(n+2)}\varphi_t |\nabla_b \varphi|^2 \\
&-l_0 \left|\nabla_b \varphi\right|^2 - \frac{8}{n} u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*}] - \frac{1}{t}G \\
= &-\frac{2n}{(n+2)}\langle \nabla_b \varphi, \nabla_b G\rangle + t[\frac{2n}{(n+1)(n+2)^2 t^2}G^2 + \frac{8}{n(n+2)^2}|\nabla_b \varphi|^4 \\
&-l_0 \left|\nabla_b \varphi\right|^2 - \frac{8}{n} u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*}] - \frac{1}{t}G.
\end{aligned}
$$

This completes the proof of Proposition 1.1. □

Following the same proof as in Theorem 3.4. We have the following result.

THEOREM 6.3. *Let (M, J, θ) be a closed pseudohermitian $(2n+1)$-manifold of zero torsion and nonnegative pseudohermitian Ricci tensors for $n \geq 2$. If $u(x,t)$ is the positive solution of (1.6) on $M \times [0, \infty)$ such that*

$$P_\beta u = 0$$

at $t = 0$. Then u satisfies the estimate

$$\frac{|\nabla_b u|^2}{u^2} + \frac{n+2}{n}\frac{u_t}{u} \leq \frac{(n+1)(n+2)^2}{2n}\frac{1}{t}$$

on $M \times [0, \infty)$.

Following the same proof as in Theorem 4.2. We have the following result.

THEOREM 6.4. *If $u(x,t)$ be a positive smooth solution of (1.6)*

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

on $H^n \times [0, T)$ with

$$P_\beta u = 0$$

at $t = 0$, then u satisfies the subgradient estimate

$$\frac{|\nabla_b u|^2}{u^2} + \frac{n+2}{n}\frac{u_t}{u} \leq [\frac{(n+1)(n+2)^2}{2n} + \epsilon]\frac{1}{t}$$

on $H^n \times [0, T)$ for any $\epsilon > 0$.

Then by combining Theorem 6.4 and Proposition 4.1, Theorem 1.4 follows easily for all n.

REFERENCES

[BCT] C. Berenstein, D. C. Chang and J. Tie, *Laguerre Calculus and Its Applications in the Heisenberg Group*, AMS/IP series in advanced mathematics #22, International Press, Cambridge, Massachusetts, 2001.

[BGG] R. Beals, B. Gaveau and P. C. Greiner, *Hamiltonian-Jacobi theory and the heat kernel on Heisenberg groups*, J. Math. Pures Appl., 79 (2000), pp. 633–689.

[CC] S.-C. Chang and H.-L. Chiu, *On the estimate of first eigenvalue of a sublaplacian on a pseudohermitian* 3*-manifold*, Pacific J. Math., 232:2 (2007), pp. 269–282.

[CC1] S.-C. Chang and H.-L. Chiu, *Nonnegativity of CR Paneitz operator and its Application to the CR Obata's Theorem in a Pseudohermitian* $(2n+1)$*-Manifold*, Journal of Geometric Analysis, 19 (2009), pp. 261–287.

[CC2] S.-C. Chang and H.-L. Chiu, *On the CR Analogue of Obata's Theorem in a Pseudohermitian* 3*-Manifold*, Math. Ann., 345:1 (2009), pp. 33–51.

[CCC] S.-C., Chang, J.-H. Cheng and H.-L. Chiu, *The Fourth-order Q-curvature flow on a CR 3-manifold*, Indiana Univ. Math. J., 56:4 (2007), pp. 1793–1826.

[CCW] S.-C. Chang, H.-L. Chiu and C.-T. Wu, *The Li-Yau-Hamilton inequality for Yamabe flow on a closed CR* 3*-manifold*, Trans. AMS., 362 (2010), pp. 1681–1698.

[CCh] S.-C., Chang and J.-H. Cheng, *The Harnack Estimate for the Yamabe Flow on CR Manifolds of Dimension* 3, Annals of Global Analysis and Geometry, 21:2 (2002), pp. 111–121.

[Chi] H.-L. Chiu, *The sharp lower bound for the first positive eigenvalue of the sublaplacian on a Pseudohermitian 3-manifold*, Ann. Glob. Anal. Geom., 30 (2006), pp. 81–96.

[Cho] W.-L. Chow, *Uber System Von Lineaaren Partiellen Differentialgleichungen erster Orduung*, Math. Ann., 117 (1939), pp. 98–105.

[CY] H.-D. Cao and S.-T. Yau, *Gradient Estimates, Harnack Inequalities and Estimates for Heat Kernels of the Sum of Squares of Vector Fields*, Math. Z., 211 (1992), pp. 485–504.

[DT] S. Dragomir and G. Tomassini, *Differential Geometry and Analysis on CR Manifolds*, Kirkhauser, Boston-Basel-Berlin, 2006.

[FH] C. Fefferman and K. Hirachi, *Ambient Metric Construction of Q-Curvature in Conformal and CR Geometries*, Math. Res. Lett., 10:5-6 (2003), pp. 819-831.

[GG] A. R. Gover and C. R. Graham, *CR Invariant Powers of the Sub-Laplacian*, J. Reine Angew. Math., 583 (2005), pp. 1–27.

[GL] C. R. Graham and J. M. Lee, *Smooth Solutions of Degenerate Laplacians on Strictly Pseudoconvex Domains*, Duke Math. J., 57 (1988), pp. 697–720.

[Gr] A. Greenleaf, *The first eigenvalue of a Sublaplacian on a Pseudohermitian manifold*, Comm. Part. Diff. Equ., 10(2):3 (1985), pp. 191–217.

[H] K. Hirachi, *Scalar Pseudo-hermitian Invariants and the Szegö Kernel on* 3*-dimensional CR Manifolds*, Lecture Notes in Pure and Appl. Math. 143, pp. 67–76, Dekker, 1992.

[Ha] R. S. Hamilton, *A Matrix Harnack Estimate for the Heat Equation*, CAG, 1 (1993), pp. 113–126.

[KS] A. Koranyi and N. Stanton, *Liouville Type Theorems for Some Complex Hypoelliptic Operators*, J. Funct. Anal., 60 (1985), pp. 370–377.

[JSC] D. Jerison and A. Sánchez-Calle, *Estimates for the Heat Kernel for A Sum of Squares of Vector Fields*, IUMJ, 35:4 (1986), pp. 835–854.

[LY] P. Li and S.-T. Yau, *On the Parabolic Kernel of the Schrődinger Operator*, Acta Math., 156 (1985), pp. 153–201.

[L1] J. M. Lee, *Pseudo-Einstein Structure on CR Manifolds*, Amer. J. Math., 110 (1988), pp. 157–178.

[P] S. Paneitz, *A Quartic Conformally Covariant Differential Operator for Arbitrary Pseudo-Riemannian Manifolds*, preprint, 1983.

[PP] A. Pascucci and S. Polidoro, *On the Harnack Inequality for a Class of Hypoelliptic Evolution Equations*, Trans. AMS, 356 (2004), pp. 4383–4394.

[SC] A. Sánchez-Calle, *Fundamental Solutions and Geometry of the Sum of Squares of Vector Fields*, Invent. Math., 78 (1984), pp. 143–160.

[SY] R. Schoen and S.-T. Yau, *Lectures on Differential Geometry*, International Press, 1994.

[T] N. Tanaka, *A differential Geometric Study on Strongly Pseudo-Convex Manifolds*, Kinokuniya Book Store Co., Ltd, Kyoto, 1975.

[W] J.-P. Wang, *Lecture Note in Geometric Analysis*, NCTS, Hsinchu, Taiwan, 2005 .

[We] S. M. Webster, *Pseudohermitian Structures on a Real Hypersurface*, J. Diff. Geom., 13 (1978), pp. 25–41.

[Y] S. -T. Yau, *Harmonic functions on complete Riemannian manifolds*, Comm. Pure Appl. Math., 28 (1975), pp. 201–228.