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Matrix Li–Yau–Hamilton inequality for the CR heat equation in pseudohermitian $(2n+1)$-manifolds

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Abstract In this paper, we first derive the CR analogue of matrix Li–Yau–Hamilton inequality for the positive solution to the CR heat equation in a closed pseudohermitian $(2n+1)$-manifold with nonnegative bisectional curvature and bitorsional tensor. We then obtain the CR Li–Yau gradient estimate in the Heisenberg group. We apply this CR gradient estimate and extend the CR matrix Li–Yau–Hamilton inequality to the case of the Heisenberg group. As a consequence, we derive the Hessian comparison property for the Heisenberg group.

1 Introduction

In the seminal paper, Li and Yau [34] established the parabolic Li–Yau Harnack estimate for the positive solution $u(x,t)$ of the time-independent heat equation

$$\frac{\partial}{\partial t}u\left(x,t\right)=\Delta u\left(x,t\right)$$

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in a complete Riemannian l-manifold with nonnegative Ricci curvature. Here Δ is the Laplace–Beltrami operator. Then Hamilton [24] extended the Li–Yau estimate to the full matrix version of the Hessian estimate of the positive solution u under the stronger assumptions that M is Ricci parallel and with nonnegative sectional curvature. Furthermore, Hamilton [23] proved the matrix Harnack inequality for solutions to the Ricci flow when the curvature operator is nonnegative. This inequality is called the "Li–Yau–Hamilton" type estimates. Since then, there were many additional works in this direction which cover various different geometric evolution equations such as the mean curvature flow [24], the Kähler–Ricci flow [6], the Yamabe flow [16], etc.

Along this line with method of Li–Yau gradient estimate, Cao and Yau [8] studied the heat equation

$$\frac{\partial}{\partial t}u\,(x,t)=Lu(x,t) \tag{1.1}$$

in a closed l-manifold with a positive measure and the subelliptic operator with respect to the sum of squares of vector fields $L=\sum_{i=1}^{h}X_i^2-Y,\ h\leq l,$ with $Y=\sum_{i=1}^{h}c_iX_i$ where $X_1,X_2,\ldots,X_h$ are smooth vector fields satisfying Hörmander's bracket generating condition: the vector fields together with their commutators of finite order span the tangent space at every point of M. Suppose that $[X_i,[X_j,X_k]]$ can be expressed as linear combinations of $X_1,X_2,\ldots,X_h$ and their brackets $[X_1,X_2],\ldots,[X_{l-1},X_h]$. They showed that the gradient estimate for the positive solution $u(x,t)$ of (1.1) on $M\times[0,\infty)$.

Recently, we [10] obtained the CR Cao–Yau type gradient estimate for the positive solution $u(x,t)$ of the CR heat equation

$$\frac{\partial}{\partial t}u\,(x,t)=\Delta_b u\,(x,t) \tag{1.2}$$

in a closed pseudohermitian $(2n+1)$-manifold (M,J,θ) with nonnegative Tanaka–Webster curvature and vanishing torsion. Here Δ_b is the time-independent sub-Laplacian operator.

In this paper, we first derive the following CR analogue of Kähler version of the matrix Li–Yau–Hamilton inequality [7] for any positive solution u to (1.2).

Theorem 1 *Let M be a closed pseudohermitian $(2n+1)$-manifold with nonnegative bisectional curvature and nonnegative bi-torsional tensor. Let u be the positive solution of the CR heat equation (1.2). In addition if the positive solution u satisfies the purely holomorphic Hessian operator $P_{\alpha\bar{\beta}}u=0$. Then*

$$(u_{\alpha\bar{\beta}}+u_{\bar{\beta}\alpha})+\frac{1}{2}\left[(u_\alpha V_{\bar{\beta}}+u_{\bar{\beta}}V_\alpha)+uV_\alpha V_{\bar{\beta}}\right]-\frac{t}{12}\frac{|u_0|^2}{u}h_{\alpha\bar{\beta}}+\frac{4}{t}uh_{\alpha\bar{\beta}}\geq 0 \tag{1.3}$$

for $t>0$ and any vector field $V=V^\alpha Z_\alpha$ of type $(1,0)$ on M. Here $P_{\alpha\bar{\beta}}$ is the purely holomorphic Hessian operator (Definition 1).

Then we derived the Li–Yau–Hamilton inequality as a corollary of the above theorem.

Corollary 1 *The CR matrix Li–Yau–Hamilton inequality (1.3) holds in a closed pseudohermitian* $(2n+1)$*-manifold with nonnegative bisectional curvature and vanishing torsion.*

Remark 1 If we choose the optimal $V = -\nabla_b u/u$ and take the trace of (1.3), we recapture the following CR Li-Yau gradient estimate derived by Chang et al. in [10] and [11]:

$$\frac{\partial}{\partial t}u - \frac{1}{4}\frac{\|\nabla_b u\|^2}{u} - \frac{nt}{12}\frac{|u_0|^2}{u} + \frac{4n}{t}u \geq 0. \tag{1.4}$$

When the manifold is complete and noncompact, we will need to use the CR Li–Yau Harnack inequality (4.14) and the Li–Tam mean value inequality (4.17) in the proof of the CR matrix Li–Yau–Hamilton inequality (1.3). However, the proofs of both inequalities rely on the CR Li-Yau gradient estimate (1.5). We refer to [7] for more details.

As shown in the Sect. 4, the proof of the CR Li–Yau gradient estimate (1.5) relies on the CR sub-Laplacian comparison property (4.12) and the extra u_0-growth property (6.20) with $|u_0| \leq \frac{C}{t}u$ that has no analogue in the Riemannian case. In particular, both properties holds in the Heisenberg group $\mathbf{H}^n$ which is flat and with vanishing torsion. However, both properties are wild open for a general complete and noncompact pseudohermitian $(2n+1)$-manifold.

Then we are able to derive the CR Li–Yau gradient estimate on $\mathbf{H}^n$.

Theorem 2 *Let* $(\boldsymbol{H}^n, J, \theta)$ *be the* $(2n+1)$*-dimensional Heisenberg group. If* $u(x,t)$ *is the positive solution of the CR heat equation (1.2) on* $\boldsymbol{H}^n \times [0,\infty)$*. Let* $\varphi = \ln u$*, and* $\alpha < -1$*. Then there exists a positive constant* C *depending on* α *such that*

$$|\nabla_b \varphi|^2 + \alpha\varphi_t + t\varphi_0^2 \leq \frac{C}{t}. \tag{1.5}$$

By applying Theorem 2, we have the following CR Liouville-type theorem for any positive pseudoharmonic function u on $(\mathbf{H}^n, J, \theta)$ which recaptured the Liouville theorem due to Chang et al. [12] and Koranyi and Stanton [28] by the method of Kevin transform.

Corollary 2 *Let* $(\boldsymbol{H}^n, J, \theta)$ *be the* $(2n+1)$*-dimensional Heisenberg group. If* $u(x,t)$ *is any positive smooth function with* $\Delta_b u = 0$*, then* $u(x,t)$ *is constant. That is, there does not exist any positive nonconstant pseudoharmonic function in* $\boldsymbol{H}^n$*.*

From the previous discuss and Theorem 1, we have the CR matrix Li–Yau–Hamilton inequality in $(\boldsymbol{H}^n, J, \theta)$ (see Sect. 5. for details).

Theorem 3 *Let* $(\boldsymbol{H}^n, J, \theta)$ *be the* $(2n+1)$*-dimensional Heisenberg group. If* $u(x,t)$ *is the positive solution of the CR heat equation (1.2) on* $\boldsymbol{H}^n \times [0,\infty)$*. Then the CR matrix Li–Yau–Hamilton inequality (1.3) holds.*

Remark 2 From the proof of Theorem 3 we observe that the CR matrix Li–Yau–Hamilton inequality (1.3) still holds in a complete noncompact pseudohermitian manifold whenever both the CR sub-Laplacian comparison property (4.12) and the u_0-growth property (6.20) hold. We should point out that the extra u_0-growth property (6.20) is equivalent to (5.2) that has no analogue in Kähler manifolds.

By applying Theorem 3 to the heat kernel $H(x, y, t)$ with $V = -\frac{\nabla_b H}{H}$, we obtain the well-known asymptotic of $H(x, o, t)$ ([1,2,19,31,43,44], etc)

$$-t \log H(x, o, t) \to \frac{1}{4} r^2(x), \quad \text{as } t \to 0.$$

Here $r(x)$ be the Carnot–Carathéodory distance between x and the origin $o \in \boldsymbol{H}^n$. We have the following complex Hessian comparison theorem for r on $\mathbf{H}^n$. This Hessian comparison property seems to be new even for the $(2n+1)$-dimensional Heisenberg group $\boldsymbol{H}^n$.

Corollary 3 *Let $(\boldsymbol{H}^n, J, \theta)$ be the standard $(2n+1)$-dimensional Heisenberg group. Then in the sense of distribution, we have*

$$\left[(r^2(x))_{\alpha\overline{\beta}} + (r^2(x))_{\overline{\beta}\alpha} \right] \leq (16 + C_0) h_{\alpha\overline{\beta}}(x)$$

for some constant C_0. In particular, we recapture the sub-Laplacian comparison property

$$\Delta_b r^2(x) \leq (16 + C_0) n$$

in the Heisenberg group.

The rest of the paper is organized as follows. In Sect. 2, we introduce the pseudohermitian manifolds and some basic notations. In Sect. 3, we prove the CR matrix Li–Yau–Hamilton inequality for the CR heat equation via methods developed in [10,34] and [7]. In Sect. 4, we prove the CR Li–Yau gradient estimate in the $(2n+1)$-dimensional Heisenberg group. Combining this with Theorem 1, we obtain the CR matrix Li–Yau–Hamilton inequality and the Hessian comparison property in the $(2n+1)$-dimensional Heisenberg group $\boldsymbol{H}^n$ in Sect. 5. Finally, we give the proof of u_0-growth property (6.20) in the Heisenberg group in Sect. 6.

2 Preliminary

First we introduce the basic concepts of the pseudohermitian $(2n+1)$-manifold (see [29,30] for more details). Let (M, ξ) be a $(2n+1)$-dimensional, orientable, contact manifold with contact structure ξ. 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 integrability condition: If X and Y are in ξ, then so are $[JX, Y] + [X, JY]$ and $J([JX, Y] + [X, JY]) = [JX, JY] - [X, Y]$.

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 $\left\{\theta, \theta^\alpha, \theta^{\bar\alpha}\right\}$, the coframe dual to $\{T, Z_\alpha, Z_{\bar\alpha}\}$, satisfies

$$d\theta = i h_{\alpha\bar\beta}\theta^\alpha \wedge \theta^{\bar\beta} \tag{2.1}$$

for some positive definite hermitian matrix of functions $(h_{\alpha\bar\beta})$, if we have this contact structure, we also call such M a strictly pseudoconvex CR $(2n+1)$-manifold.

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 $d\mu = \theta \wedge (d\theta)^n$, we get an inner product on the space of sections of each tensor bundle.

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

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

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

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

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

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

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

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

Here $R_\gamma{}^\delta{}_{\alpha\bar\beta}$ is the pseudohermitian curvature tensor, $R_{\alpha\bar\beta} = R_\gamma{}^\gamma{}_{\alpha\bar\beta}$ is the pseudohermitian Ricci curvature tensor and $A_{\alpha\beta}$ is the pseudohermitian torsion. Furthermore, we define the bi-sectional curvature

$$R_{\alpha\bar{\alpha}\beta\overline{\beta}}(X,Y)=R_{\alpha\bar{\alpha}\beta\overline{\beta}}X_\alpha X_{\overline{\alpha}}Y_\beta Y_{\bar{\beta}}$$

and the bi-torsion tensor

$$T_{\alpha\overline{\beta}}(X,Y):=i(A_{\bar{\beta}\bar{\rho}}X^{\overline{\rho}}Y_\alpha-A_{\alpha\rho}X^\rho Y_{\bar{\beta}})$$

and the torsion tensor

$$Tor(X,Y):=h^{\alpha\bar{\beta}}T_{\alpha\overline{\beta}}(X,Y)=i(A_{\overline{\alpha}\bar{\rho}}X^{\overline{\rho}}Y^{\overline{\alpha}}-A_{\alpha\rho}X^\rho Y^\alpha)$$

for any $X=X^\alpha Z_\alpha,\ Y=Y^\alpha Z_\alpha$ in $T_{1,0}$.

We will denote the components of the 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, $u_\alpha=Z_\alpha u,\ u_{\alpha\bar{\beta}}=Z_{\bar{\beta}}Z_\alpha u-\omega_\alpha{}^\gamma(Z_{\bar{\beta}})Z_\gamma u.$

For any smooth real-valued function u, the subgradient ∇_b is defined by $\nabla_b u\in\xi$ and $\langle Z,\nabla_b u\rangle_{L_\theta}=du(Z)$ for all vector fields Z tangent to the contact plane. Locally $\nabla_b u=\sum_\alpha u_{\bar{\alpha}}Z_\alpha+u_\alpha Z_{\bar{\alpha}}$. We also denote $u_0=Tu$.

We can use the connection to define the subhessian as the complex linear map

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

by

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

In particular,

$$|\nabla_b u|^2=2\sum_\alpha u_\alpha u_{\overline{\alpha}},\quad |\nabla_b^2 u|^2=2\sum_{\alpha,\beta}(u_{\alpha\beta}u_{\overline{\alpha}\overline{\beta}}+u_{\alpha\overline{\beta}}u_{\overline{\alpha}\beta}).$$

Also

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

The Kohn–Rossi Laplacian $\Box_b$ on functions is defined by

$$\Box_b\varphi=2\overline{\partial}_b^*\overline{\partial}_b\varphi=(\Delta_b+inT)\varphi=-2\varphi_{\overline{\alpha}}{}^{\overline{\alpha}}$$

and on (p,q)-forms is defined by

$$\Box_b=2(\overline{\partial}_b^*\overline{\partial}_b+\overline{\partial}_b\overline{\partial}_b^*).$$

Next we recall the following commutation relations [29]. Let φ be a scalar function and $\sigma = \sigma_\alpha \theta^\alpha$ be a $(1,0)$ form, then we have

$$\begin{aligned}
\varphi_{\alpha\beta} &= \varphi_{\beta\alpha},\\
\varphi_{\alpha\bar\beta} - \varphi_{\bar\beta\alpha} &= i h_{\alpha\bar\beta}\varphi_0,\\
\varphi_{0\alpha} - \varphi_{\alpha 0} &= A_{\alpha\beta}\varphi^{\beta},\\
\sigma_{\alpha,0\beta} - \sigma_{\alpha,\beta 0} &= \sigma_{\alpha,\bar\gamma} A^{\bar\gamma}{}_{\beta} - \sigma^{\bar\gamma} A_{\alpha\beta,\bar\gamma},\\
\sigma_{\alpha,0\bar\beta} - \sigma_{\alpha,\bar\beta 0} &= \sigma_{\alpha,\gamma} A^{\gamma}{}_{\bar\beta} + \sigma^{\bar\gamma} A_{\bar\gamma\bar\beta,\alpha},
\end{aligned}$$

and

$$\begin{aligned}
\sigma_{\alpha,\beta\gamma} - \sigma_{\alpha,\gamma\beta} &= i A_{\alpha\gamma}\sigma_\beta - i A_{\alpha\beta}\sigma_\gamma,\\
\sigma_{\alpha,\bar\beta\bar\gamma} - \sigma_{\alpha,\bar\gamma\bar\beta} &= i h_{\alpha\bar\beta} A_{\bar\gamma\bar\rho}\sigma^{\bar\rho} - i h_{\alpha\bar\gamma} A_{\bar\beta\bar\rho}\sigma^{\bar\rho},\\
\sigma_{\alpha,\beta\bar\gamma} - \sigma_{\alpha,\bar\gamma\beta} &= i h_{\beta\bar\gamma}\sigma_{\alpha,0} + R_{\alpha\bar\rho\beta\bar\gamma}\sigma^{\bar\rho}.
\end{aligned}$$

Moreover for multi-index $I = (\alpha_1, \ldots, \alpha_p)$, $\bar J = (\bar\beta_1, \ldots, \bar\beta_q)$, we denote $I(\alpha_k = \mu) = (\alpha_1, \ldots, \alpha_{k-1}, \mu, \alpha_{k+1}, \ldots, \alpha_p)$. Then

$$\begin{aligned}
\eta_{I\bar J,\mu\lambda} - \eta_{I\bar J,\lambda\mu} = {}& i\sum_{k=1}^{p}\left(\eta_{I(\alpha_k=\mu)\bar J} A_{\alpha_k\lambda} - \eta_{I(\alpha_k=\lambda)\bar J} A_{\alpha_k\mu}\right)\\
&- \; i\sum_{k=1}^{q}\left(\eta_{I\bar J(\bar\beta_k=\bar\gamma)} h_{\bar\beta_k\mu} A^{\bar\gamma}_{\lambda} - \eta_{I\bar J(\bar\beta_k=\bar\gamma)} h_{\bar\beta_k\lambda} A^{\bar\gamma}_{\mu}\right),
\end{aligned}$$

and

$$\begin{aligned}
\eta_{I\bar J,\lambda\bar\mu} - \eta_{I\bar J,\bar\mu\lambda} &= i h_{\lambda\bar\mu}\eta_{I\bar J,0} + \sum_{k=1}^{p}\eta_{I(\alpha_k=\gamma)\bar J} R_{\alpha_k}{}^{\gamma}{}_{\lambda\bar\mu} + \sum_{k=1}^{q}\eta_{I\bar J(\bar\beta_k=\bar\gamma)} R_{\bar\beta_k}{}^{\bar\gamma}{}_{\lambda\bar\mu}\\
\eta_{I\bar J,0\mu} - \eta_{I\bar J,\mu 0} &= A^{\bar\rho}_{\mu}\eta_{I\bar J,\bar\rho} - \sum_{k=1}^{p} A_{\alpha_k\mu,\bar\rho}\eta_{I(\alpha_k=\rho)\bar J} + \sum_{k=1}^{q} A_{\mu\rho,\bar\beta_k}\eta_{I\bar J(\bar\beta_k=\bar\rho)}.
\end{aligned}$$

3 CR matrix Li–Yau–Hamilton inequality

Let $u(x,t)$ be the positive solution of the CR heat equation (1.2). For the CR Li–Yau gradient estimate as in the paper [10], we observe that one of difficulties is to deal with CR Bochner formula (4.1) which involving a term $\langle J\nabla_b\varphi, \nabla_b\varphi_0\rangle$ that has no analogue in the Riemannian case. In order to overcome this difficulty, we introduce a new scalar Harnack quantity $G = t[|\nabla_b\varphi|^2 + \alpha\varphi_t + t\varphi_0^2]$ with $\varphi = \ln u$ by adding an extra term $t\varphi_0^2$ to $|\nabla_b\varphi|^2 + \alpha\varphi_t$ which was appeared in Li–Yau estimate ([34]). We refer to Sect. 4 for more details.

Now we want to find the right quantity for the CR matrix Li–Yau–Hamilton inequality. By comparing the Harnack quantity in [7] in case of Kä hler manifolds, we define the matrix Harnack quantity

$$N_{\alpha\bar{\beta}} = \frac{1}{2}(u_{\alpha\bar{\beta}} + u_{\bar{\beta}\alpha}) + 2\frac{u}{t}h_{\alpha\bar{\beta}} - b\frac{u_\alpha u_{\bar{\beta}}}{u} - at\frac{|u_0|^2}{u}h_{\alpha\bar{\beta}} \tag{3.1}$$

by adding an extra term $F := -at\frac{|u_0|^2}{u}h_{\alpha\bar{\beta}}$ in which the positive constants a and b to be determined later (say $a = \frac{1}{24}$ and $b = \frac{1}{4}$).

Definition 1 (i) [20] Define the purely holomorphic Hessian operator $P_{\alpha\bar{\beta}}$:

$$P_{\alpha\bar{\beta}}\varphi := -2i(A_{\alpha\gamma}\varphi^\gamma)_{\bar{\beta}}$$

and the purely holomorphic Poisson operator Q:

$$Q\varphi := h^{\alpha\bar{\beta}}(P_{\alpha\bar{\beta}}\varphi) = -2i(A_{\alpha\gamma}\varphi^\gamma)^\alpha$$

for any smooth function φ. Note that $P_{\alpha\bar{\beta}}\varphi = 0 = Q\varphi$ for any smooth function φ if $A_{\alpha\beta} = 0$ on M.

Lemma 1 *Let $u(x,t)$ be the positive solution of the CR heat equation (1.2). Then $\frac{1}{2}(u_{\alpha\bar{\beta}} + u_{\bar{\beta}\alpha})$ satisfies the following:*

$$\frac{1}{2}\left(\frac{\partial}{\partial t} - \Delta_b\right)\left(u_{\alpha\bar{\beta}} + u_{\bar{\beta}\alpha}\right) = 2R_{\alpha\bar{\gamma}\delta\bar{\beta}}u_{\gamma\bar{\delta}} - R_{\alpha\bar{\delta}}u_{\delta\bar{\beta}} - R_{\delta\bar{\beta}}u_{\alpha\bar{\delta}} + C_{\alpha\bar{\beta}},$$

where

$$\begin{aligned} C_{\alpha\bar{\beta}} &:= i\left(A_{\gamma\delta,\bar{\delta}}u_{\bar{\gamma}} - A_{\bar{\gamma}\bar{\delta},\delta}u_\gamma\right)h_{\alpha\bar{\beta}} + i\left(A_{\gamma\delta}u_{\bar{\gamma}\bar{\delta}} - A_{\bar{\gamma}\bar{\delta}}u_{\delta\gamma}\right)h_{\alpha\bar{\beta}} \\ &\quad + in\left(A_{\bar{\gamma}\bar{\beta}}u_{\alpha\gamma} - A_{\alpha\gamma}u_{\bar{\gamma}\bar{\beta}}\right) + in\left(A_{\bar{\gamma}\bar{\beta},\alpha}u_\gamma - A_{\gamma\alpha,\bar{\beta}}u_{\bar{\gamma}}\right) \\ &:= -(ReQu)h_{\alpha\bar{\beta}} + n(ReP_{\alpha\bar{\beta}}u). \end{aligned}$$

Note that $trC_{\alpha\bar{\beta}} = h^{\alpha\bar{\beta}}C_{\alpha\bar{\beta}} = 0$. In particular we have $C_{1\bar{1}} = 0$ for $n = 1$. In addition if the positive solution u satisfies $P_{\alpha\bar{\beta}}u = 0$ which is the case when the torsion is vanishing, then $u_{\alpha\bar{\beta}}$ satisfies the following CR Lichnerowicz–Laplacian heat equation [9]:

$$\left(\frac{\partial}{\partial t} - \Delta_b\right)u_{\alpha\bar{\beta}} = 2R_{\alpha\bar{\gamma}\delta\bar{\beta}}u_{\gamma\bar{\delta}} - R_{\alpha\bar{\delta}}u_{\delta\bar{\beta}} - R_{\delta\bar{\beta}}u_{\alpha\bar{\delta}}.$$

Proof Note that

$$\begin{aligned}
&\left(\frac{\partial}{\partial t}-\Delta_b\right)\left(u_{\mu\bar\lambda}+u_{\bar\lambda\mu}\right)\\
&=\frac{\partial}{\partial t}\left(u_{\mu\bar\lambda}+u_{\bar\lambda\mu}\right)-\Delta_b\left(u_{\mu\bar\lambda}+u_{\bar\lambda\mu}\right)\\
&=[(\Delta_b u)_{\mu\bar\lambda}-\Delta_b u_{\mu\bar\lambda}]+[(\Delta_b u)_{\bar\lambda\mu}-\Delta_b u_{\bar\lambda\mu}].
\end{aligned}$$

(i) We first compute $[(\Delta_b u)_{\mu\bar\lambda}-\Delta_b u_{\mu\bar\lambda}]$: By definition, we have

$$(\Delta_b u)_{\mu\bar\lambda}=(u_{\alpha\bar\alpha}+u_{\bar\alpha\alpha})_{\mu\bar\lambda}=u_{\alpha\bar\alpha\mu\bar\lambda}+u_{\bar\alpha\alpha\mu\bar\lambda}. \tag{3.2}$$

Compute

$$\begin{aligned}
u_{\alpha\bar\alpha\mu\bar\lambda}&=\left(u_{\alpha\mu\bar\alpha}-ih_{\mu\bar\alpha}u_{\alpha 0}-R_{\alpha\bar\rho\mu\bar\alpha}u_\rho\right)_{\bar\lambda}\\
&=u_{\alpha\mu\bar\alpha\bar\lambda}-ih_{\mu\bar\alpha}u_{\alpha 0\bar\lambda}-R_{\alpha\bar\rho\mu\bar\alpha,\bar\lambda}u_\rho-R_{\alpha\bar\rho\mu\bar\alpha}u_{\rho\bar\lambda}\\
&=u_{\mu\alpha\bar\alpha\bar\lambda}-ih_{\mu\bar\alpha}u_{\alpha 0\bar\lambda}-R_{\alpha\bar\rho\mu\bar\alpha,\bar\lambda}u_\rho-R_{\alpha\bar\rho\mu\bar\alpha}u_{\rho\bar\lambda}\\
&=u_{\mu\alpha\bar\lambda\bar\alpha}+i\left(u_{\sigma\alpha}h_{\mu\bar\alpha}A_{\bar\sigma\bar\lambda}-u_{\sigma\alpha}h_{\mu\bar\lambda}A_{\bar\sigma\bar\alpha}\right)\\
&\quad+i\left(nu_{\mu\sigma}A_{\bar\sigma\bar\lambda}-u_{\mu\sigma}h_{\alpha\bar\lambda}A_{\bar\sigma\bar\alpha}\right)\\
&\quad-ih_{\mu\bar\alpha}u_{\alpha 0\bar\lambda}-R_{\alpha\bar\rho\mu\bar\alpha,\bar\lambda}u_\rho-R_{\alpha\bar\rho\mu\bar\alpha}u_{\rho\bar\lambda}\\
&=\left(u_{\mu\bar\lambda\alpha}+ih_{\alpha\bar\lambda}u_{\mu 0}+R_{\mu\bar\rho\alpha\bar\lambda}u_\rho\right)_{\bar\alpha}\\
&\quad+i\left(u_{\sigma\alpha}h_{\mu\bar\alpha}A_{\bar\sigma\bar\lambda}-u_{\sigma\alpha}h_{\mu\bar\lambda}A_{\bar\sigma\bar\alpha}\right)\\
&\quad+i\left(nu_{\mu\sigma}A_{\bar\sigma\bar\lambda}-u_{\mu\sigma}h_{\alpha\bar\lambda}A_{\bar\sigma\bar\alpha}\right)\\
&\quad-ih_{\mu\bar\alpha}u_{\alpha 0\bar\lambda}-R_{\alpha\bar\rho\mu\bar\alpha,\bar\lambda}u_\rho-R_{\alpha\bar\rho\mu\bar\alpha}u_{\rho\bar\lambda}\\
&=u_{\mu\bar\lambda\alpha\bar\alpha}+ih_{\alpha\bar\lambda}u_{\mu 0\bar\alpha}-ih_{\mu\bar\alpha}u_{\alpha 0\bar\lambda}\\
&\quad-R_{\alpha\bar\rho\mu\bar\alpha,\bar\lambda}u_\rho-R_{\alpha\bar\rho\mu\bar\alpha}u_{\rho\bar\lambda}+R_{\mu\bar\rho\alpha\bar\lambda,\bar\alpha}u_\rho+R_{\mu\bar\rho\alpha\bar\lambda}u_{\rho\bar\alpha}\\
&\quad+i\left(u_{\sigma\alpha}h_{\mu\bar\alpha}A_{\bar\sigma\bar\lambda}-u_{\sigma\alpha}h_{\mu\bar\lambda}A_{\bar\sigma\bar\alpha}\right)+i\left(nu_{\mu\sigma}A_{\bar\sigma\bar\lambda}-u_{\mu\sigma}h_{\alpha\bar\lambda}A_{\bar\sigma\bar\alpha}\right).
\end{aligned} \tag{3.3}$$

Here we have use commutation relations

$$\begin{aligned}
u_{\mu\alpha\bar\alpha\bar\lambda}=u_{\mu\alpha\bar\lambda\bar\alpha}&+i\left(u_{\sigma\alpha}h_{\mu\bar\alpha}A_{\bar\sigma\bar\lambda}-u_{\sigma\alpha}h_{\mu\bar\lambda}A_{\bar\sigma\bar\alpha}\right)\\
&+i\left(nu_{\mu\sigma}A_{\bar\sigma\bar\lambda}-u_{\mu\sigma}h_{\alpha\bar\lambda}A_{\bar\sigma\bar\alpha}\right)
\end{aligned}$$

and

$$\begin{aligned}
u_{\mu\alpha\bar\lambda\bar\alpha}&=\left(u_{\mu\bar\lambda\alpha}+ih_{\alpha\bar\lambda}u_{\mu 0}+R_{\mu\bar\rho\alpha\bar\lambda}u_\rho\right)_{\bar\alpha}\\
&=u_{\mu\bar\lambda\alpha\bar\alpha}+ih_{\alpha\bar\lambda}u_{\mu 0\bar\alpha}+R_{\mu\bar\rho\alpha\bar\lambda,\bar\alpha}u_\rho+R_{\mu\bar\rho\alpha\bar\lambda}u_{\rho\bar\alpha}.
\end{aligned}$$

Similar, we have

$$
\begin{aligned}
u_{\bar{\alpha}\alpha\mu\bar{\lambda}} = u_{\mu\bar{\lambda}\bar{\alpha}\alpha} &+ ih_{\mu\bar{\alpha}}A_{\bar{\lambda}\bar{\rho},\alpha}u_{\rho} + ih_{\mu\bar{\alpha}}A_{\bar{\lambda}\bar{\rho},\alpha}u_{\rho\alpha} \\
&- ih_{\mu\bar{\lambda}}A_{\bar{\alpha}\bar{\rho},\alpha}u_{\rho} - ih_{\mu\bar{\lambda}}A_{\bar{\alpha}\bar{\rho}}u_{\rho\alpha} - i\left(nA_{\mu\rho}u_{\bar{\rho}}\right)_{\bar{\lambda}} + i\left(h_{\bar{\alpha}\mu}A_{\alpha\rho}u_{\bar{\rho}}\right)_{\bar{\lambda}} \\
&+ R_{\mu\bar{\rho}\alpha\bar{\lambda}}u_{\rho\bar{\alpha}} + R_{\bar{\alpha}\rho\alpha\bar{\lambda}}u_{\mu\bar{\rho}} - ih_{\mu\bar{\alpha}}u_{0\alpha\bar{\lambda}} + ih_{\alpha\bar{\lambda}}u_{\mu\bar{\alpha}0}
\end{aligned}
\tag{3.4}
$$

It follow from (3.2), (3.3) and (3.4) that

$$
\begin{aligned}
&(\Delta_b u)_{\mu\bar{\lambda}} - \Delta_b u_{\mu\bar{\lambda}} \\
&= 2R_{\mu\bar{\rho}\alpha\bar{\lambda}}u_{\rho\bar{\alpha}} - R_{\rho\bar{\lambda}}u_{\mu\bar{\rho}} - R_{\bar{\rho}\mu}u_{\rho\bar{\lambda}} + \left(R_{\mu\bar{\rho}\alpha\bar{\lambda},\bar{\alpha}} - R_{\alpha\bar{\rho}\mu\bar{\alpha},\bar{\lambda}}\right)u_{\rho} \\
&\quad + ih_{\alpha\bar{\lambda}}u_{\mu0\bar{\alpha}} - ih_{\mu\bar{\alpha}}u_{\alpha0\bar{\lambda}} - ih_{\mu\bar{\alpha}}u_{0\alpha\bar{\lambda}} + ih_{\alpha\bar{\lambda}}u_{\mu\bar{\alpha}0} \\
&\quad + i\left(u_{\sigma\alpha}h_{\mu\bar{\alpha}}A_{\bar{\sigma}\bar{\lambda}} - u_{\sigma\alpha}h_{\mu\bar{\lambda}}A_{\bar{\sigma}\bar{\alpha}}\right) + i\left(nu_{\mu\sigma}A_{\bar{\sigma}\bar{\lambda}} - u_{\mu\sigma}h_{\alpha\bar{\lambda}}A_{\bar{\sigma}\bar{\alpha}}\right) \\
&\quad + ih_{\mu\bar{\alpha}}A_{\bar{\lambda}\bar{\rho},\alpha}u_{\rho} + ih_{\mu\bar{\alpha}}A_{\bar{\lambda}\bar{\rho},\alpha}u_{\rho\alpha} - ih_{\mu\bar{\lambda}}A_{\bar{\alpha}\bar{\rho},\alpha}u_{\rho} \\
&\quad - ih_{\mu\bar{\lambda}}A_{\bar{\alpha}\bar{\rho}}u_{\rho\alpha} - i\left(nA_{\mu\rho}u_{\bar{\rho}}\right)_{\bar{\lambda}} + i\left(h_{\bar{\alpha}\mu}A_{\alpha\rho}u_{\bar{\rho}}\right)_{\bar{\lambda}}
\end{aligned}
\tag{3.5}
$$

By the CR Bianchi identity [29] and the commutation relation, the third line of RHS in (3.5) reduces to

$$
\begin{aligned}
&R_{\mu\bar{\rho}\alpha\bar{\lambda},\bar{\alpha}} - R_{\alpha\bar{\rho}\mu\bar{\alpha},\bar{\lambda}} \\
&\quad = R_{\alpha\bar{\rho}\mu\bar{\lambda},\bar{\alpha}} - R_{\alpha\bar{\rho}\mu\bar{\alpha},\bar{\lambda}} \\
&\quad = R_{\bar{\rho}\alpha\bar{\lambda}\mu,\bar{\alpha}} - R_{\bar{\rho}\alpha\bar{\alpha}\mu,\bar{\lambda}} \\
&\quad = -iA_{\bar{\rho}\bar{\alpha},\alpha}h_{\mu\bar{\lambda}} - iA_{\bar{\rho}\bar{\alpha},\mu}h_{\alpha\bar{\lambda}} + iA_{\bar{\rho}\bar{\lambda},\alpha}h_{\mu\bar{\alpha}} + iA_{\bar{\rho}\bar{\lambda},\mu}h_{\alpha\bar{\alpha}} \\
&\quad = -iA_{\bar{\rho}\bar{\alpha},\alpha}h_{\mu\bar{\lambda}} - iA_{\bar{\rho}\bar{\alpha},\mu}h_{\alpha\bar{\lambda}} + iA_{\bar{\rho}\bar{\lambda},\alpha}h_{\mu\bar{\alpha}} + inA_{\bar{\rho}\bar{\lambda},\mu}
\end{aligned}
$$

and the fourth line reduces to

$$
\begin{aligned}
&ih_{\alpha\bar{\lambda}}u_{\mu0\bar{\alpha}} - ih_{\mu\bar{\alpha}}u_{\alpha0\bar{\lambda}} - ih_{\mu\bar{\alpha}}u_{0\alpha\bar{\lambda}} + ih_{\alpha\bar{\lambda}}u_{\mu\bar{\alpha}0} \\
&\quad = iu_{\mu0\bar{\lambda}} - iu_{\mu0\bar{\lambda}} - iu_{0\mu\bar{\lambda}} + iu_{\mu\bar{\lambda}0} \\
&\quad = iu_{\mu\bar{\lambda}0} - iu_{0\mu\bar{\lambda}} \\
&\quad = -iA_{\mu\rho,\bar{\lambda}}u_{\bar{\rho}} - iA_{\mu\rho}u_{\bar{\rho}\bar{\lambda}} - iA_{\bar{\rho}\bar{\lambda}}u_{\mu\rho} - iA_{\bar{\rho}\bar{\lambda},\mu}u_{\rho}
\end{aligned}
$$

(ii) We compute $[(\Delta_b u)_{\bar{\lambda}\mu} - \Delta_b u_{\bar{\lambda}\mu}]$ by take the conjugate of $[(\Delta_b u)_{\mu\bar{\lambda}} - \Delta_b u_{\mu\bar{\lambda}}]$ and then switch index λ and μ.

Now we finish the proof of the lemma by arranging all the torsion terms together in (i) and (ii). □

Note that it follows from commutation relation [10] that

$$
\Delta_b u_0 = (\Delta_b u)_0 + 2\left[\left(A_{\alpha\beta}u^{\alpha}\right)^{\beta} + (A_{\overline{\alpha}\overline{\beta}}u^{\overline{\alpha}})^{\overline{\beta}}\right].
$$

Hence

$$[\Delta_b, T]\, u = -2\mathrm{Im} Q u.$$

Proof of Theorem 1 As in [24], it suffices to prove that the Hermitian symmetric (1, 1)-tensor

$$N_{\alpha\bar{\beta}} = \frac{1}{2}\left(u_{\alpha\bar{\beta}} + u_{\bar{\beta}\alpha}\right) + 2\frac{u}{t} h_{\alpha\bar{\beta}} - b\frac{u_\alpha u_{\bar{\beta}}}{u} - F h_{\alpha\bar{\beta}} \geq 0$$

for $t > 0$ and some constants a and b to be determined. Here

$$F := at\frac{|u_0|^2}{u}.$$

Now we first compute

$$\begin{aligned}
\left(\frac{\partial}{\partial t} - \Delta_b\right)\frac{u_\alpha u_{\bar{\beta}}}{u} &= \frac{\partial}{\partial t}\left(\frac{u_\alpha u_{\bar{\beta}}}{u}\right) - \Delta_b\left(\frac{u_\alpha u_{\bar{\beta}}}{u}\right) \\
&= \frac{-1}{u^2}\Delta_b u \cdot u_\alpha u_{\bar{\beta}} + \frac{1}{u}\left(\Delta_b u\right)_\alpha u_{\bar{\beta}} \\
&\quad + \frac{1}{u} u_\alpha \left(\Delta_b u\right)_{\bar{\beta}} - \Delta_b\left(\frac{1}{u} u_\alpha u_{\bar{\beta}}\right)
\end{aligned}$$

and

$$\begin{aligned}
\Delta_b\left(\frac{1}{u} u_\alpha u_{\bar{\beta}}\right) &= \left(\frac{-\Delta_b u}{u^2} + \frac{4}{u^3} u_{\bar{\gamma}} u_\gamma\right) u_\alpha u_{\bar{\beta}} + \frac{1}{u}\Delta_b\left(u_\alpha u_{\bar{\beta}}\right) \\
&\quad - \frac{2}{u^2} u_\gamma \left(u_\alpha u_{\bar{\beta}}\right)_{\bar{\gamma}} - \frac{2}{u^2} u_{\bar{\gamma}}\left(u_\alpha u_{\bar{\beta}}\right)_\gamma .
\end{aligned}$$

Hence

$$\begin{aligned}
\left(\frac{\partial}{\partial t} - \Delta_b\right)\frac{u_\alpha u_{\bar{\beta}}}{u} &= -\frac{2}{u} u_{\alpha\gamma} u_{\bar{\beta}\bar{\gamma}} - \frac{2}{u} u_{\alpha\bar{\gamma}} u_{\bar{\beta}\gamma} - \frac{2}{u^3}\left|\nabla_b u\right|^2 u_\alpha u_{\bar{\beta}} \\
&\quad + \frac{2}{u^2} u_\gamma \left(u_\alpha u_{\bar{\beta}}\right)_{\bar{\gamma}} + \frac{2}{u^2} u_{\bar{\gamma}}\left(u_\alpha u_{\bar{\beta}}\right)_\gamma \\
&\quad + \frac{1}{u}\left(\left(\Delta_b u\right)_\alpha - \Delta_b\left(u_\alpha\right)\right) u_{\bar{\beta}} + \frac{1}{u}\left(\left(\Delta_b u\right)_{\bar{\beta}} - \Delta_b\left(u_{\bar{\beta}}\right)\right) u_\alpha .
\end{aligned}$$

Then we apply Lemma 1 and obtain

$$\begin{aligned}
&\left(\frac{\partial}{\partial t}-\Delta_b\right)N_{\alpha\bar\beta}\\
&\quad = 2R_{\alpha\bar\gamma\delta\bar\beta}u_{\gamma\bar\delta}-R_{\alpha\bar\sigma}u_{\sigma\bar\beta}-R_{\sigma\bar\beta}u_{\alpha\bar\sigma}+C_{\alpha\bar\beta}\\
&\qquad +b\left(\frac{2}{u}u_{\alpha\gamma}u_{\bar\beta\bar\gamma}+\frac{2}{u}u_{\alpha\bar\gamma}u_{\bar\beta\gamma}+\frac{2}{u^3}\left|\nabla_b u\right|^2u_\alpha u_{\bar\beta}-\frac{2}{u^2}u_\gamma\left(u_{\alpha\bar\gamma}u_{\bar\beta}+u_\alpha u_{\bar\beta\bar\gamma}\right)\right)\\
&\qquad -b\frac{2}{u^2}u_{\bar\gamma}\left(u_{\alpha\gamma}u_{\bar\beta}+u_\alpha u_{\bar\beta\gamma}\right)-2\frac{u}{t^2}h_{\alpha\bar\beta}-b\frac{1}{u}\left((\Delta_b u)_\alpha-\Delta_b\left(u_\alpha\right)\right)u_{\bar\beta}\\
&\qquad -b\frac{1}{u}\left((\Delta_b u)_{\bar\beta}-\Delta_b\left(u_{\bar\beta}\right)\right)u_\alpha-\left(\frac{\partial}{\partial t}-\Delta_b\right)Fh_{\alpha\bar\beta}.
\end{aligned}$$

Next we observe that

$$\begin{aligned}
&\frac{1}{u}\left((\Delta_b u)_\alpha-\Delta_b\left(u_\alpha\right)\right)u_{\bar\beta}\\
&\quad =\frac{1}{u}\left(u_{\gamma\bar\gamma\alpha}+u_{\bar\gamma\gamma\alpha}-u_{\alpha\gamma\bar\gamma}-u_{\alpha\bar\gamma\gamma}\right)u_{\bar\beta}\\
&\quad =\frac{1}{u}\left(u_{\gamma\alpha\bar\gamma}-ih_{\alpha\bar\gamma}u_{\gamma0}-R_{\bar\gamma\alpha}u_\gamma+u_{\alpha\bar\gamma\gamma}-ih_{\alpha\bar\gamma}u_{0\gamma}-inA_{\alpha\gamma}u_{\bar\gamma}\right.\\
&\qquad \left.+ih_{\bar\gamma\alpha}A_{\gamma\sigma}u_{\bar\sigma}-u_{\alpha\gamma\bar\gamma}-u_{\alpha\bar\gamma\gamma}\right)u_{\bar\beta}\\
&\quad =\frac{1}{u}\left(-iu_{\alpha0}u_{\bar\beta}-R_{\bar\gamma\alpha}u_\gamma u_{\bar\beta}-iu_{0\alpha}u_{\bar\beta}-inA_{\alpha\gamma}u_{\bar\gamma}u_{\bar\beta}+iA_{\alpha\sigma}u_{\bar\sigma}u_{\bar\beta}\right)\\
&\quad =-\frac{1}{u}R_{\bar\gamma\alpha}u_\gamma u_{\bar\beta}-2i\frac{u_{0\alpha}u_{\bar\beta}}{u}-(n-2)\,i\frac{1}{u}A_{\alpha\rho}u_{\bar\rho}u_{\bar\beta}. \qquad (3.6)
\end{aligned}$$

Thus

$$\begin{aligned}
&\left(\frac{\partial}{\partial t}-\Delta_b\right)N_{\alpha\bar\beta}\\
&\quad =2R_{\alpha\bar\gamma\delta\bar\beta}N_{\gamma\bar\delta}-R_{\alpha\bar\sigma}N_{\sigma\bar\beta}-R_{\sigma\bar\beta}N_{\alpha\bar\sigma}+C_{\alpha\bar\beta}\\
&\qquad +2bR_{\alpha\bar\gamma\delta\bar\beta}\frac{u_\gamma u_{\bar\delta}}{u}+b(n-2)\,i\frac{1}{u}A_{\alpha\rho}u_{\bar\rho}u_{\bar\beta}-b(n-2)\,i\frac{1}{u}A_{\bar\beta\bar\rho}u_\rho u_\alpha\\
&\qquad +\frac{2b}{u}\left(u_{\alpha\gamma}-\frac{u_\alpha u_\gamma}{u}\right)\left(u_{\bar\beta\bar\gamma}-\frac{u_{\bar\gamma}u_{\bar\beta}}{u}\right)\\
&\qquad +2b\left(\frac{1}{u}u_{\alpha\bar\gamma}u_{\gamma\bar\beta}-\frac{1}{u^2}u_\gamma u_{\alpha\bar\gamma}u_{\bar\beta}-\frac{1}{u^2}u_{\bar\gamma}u_\alpha u_{\gamma\bar\beta}\right)\\
&\qquad +2bi\frac{u_0}{u^2}u_\alpha u_{\bar\beta}-2bi\frac{u_0}{u}u_{\alpha\bar\beta}-\left(\frac{\partial}{\partial t}-\Delta_b\right)Fh_{\alpha\bar\beta}\\
&\qquad +b\left|\nabla_b u\right|^2\frac{u_\alpha u_{\bar\beta}}{u^3}-\frac{2u}{t^2}h_{\alpha\bar\beta}+2bi\frac{u_{0\alpha}u_{\bar\beta}}{u}-2bi\frac{u_{0\bar\beta}u_\alpha}{u}.
\end{aligned}$$

We can rewrite $N_{\alpha\bar{\beta}}$ as following:

$$N_{\alpha\bar{\beta}} = u_{\alpha\bar{\beta}} - \frac{1}{2} i u_0 h_{\alpha\bar{\beta}} + 2\frac{u}{t} h_{\alpha\bar{\beta}} - b\frac{u_\alpha u_{\bar{\beta}}}{u} - F h_{\alpha\bar{\beta}}.$$

Then we replace $u_{\alpha\bar{\gamma}} = N_{\alpha\bar{\gamma}} + \frac{i u_0 h_{\alpha\bar{\gamma}}}{2} - 2\frac{u}{t} h_{\alpha\bar{\gamma}} + b\frac{u_\alpha u_{\bar{\gamma}}}{u} + F h_{\alpha\bar{\beta}}$ into third and forth line of RHS as above, and this yields

$$\begin{aligned}
&2b\left(\frac{1}{u} u_{\alpha\bar{\gamma}} u_{\gamma\bar{\beta}} - \frac{1}{u^2} u_\gamma u_{\alpha\bar{\gamma}} u_{\bar{\beta}} - \frac{1}{u^2} u_{\bar{\gamma}} u_\alpha u_{\gamma\bar{\beta}}\right) \\
&\quad + ib\frac{2u_0}{u^2} u_\alpha u_{\bar{\beta}} - ib\frac{2u_0}{u} u_{\alpha\bar{\beta}} - \left(\frac{\partial}{\partial t} - \Delta_b\right) F h_{\alpha\bar{\beta}} \\
&= \frac{2b}{u} N_{\alpha\bar{\gamma}} N_{\beta\bar{\gamma}} - \frac{8b}{t} N_{\alpha\bar{\beta}} + 8b\frac{u}{t^2} h_{\alpha\bar{\beta}} + \left(b^3 - 2b^2\right) |\nabla_b u|^2 \frac{u_\alpha u_\beta}{u^3} \\
&\quad + \left(8b - 8b^2\right) \frac{1}{t} \frac{u_\alpha u_{\bar{\beta}}}{u} + b\frac{u_0^2}{2u} h_{\alpha\bar{\beta}} + b^2 \frac{2u_\beta u_{\bar{\gamma}}}{u^2} N_{\alpha\bar{\gamma}} + b^2 \frac{2u_\alpha u_{\bar{\gamma}}}{u^2} N_{\gamma\bar{\beta}} \\
&\quad - b\frac{2}{u^2} u_\gamma u_{\bar{\beta}} N_{\alpha\bar{\gamma}} - b\frac{2}{u^2} u_{\bar{\gamma}} u_\alpha N_{\gamma\bar{\beta}} + \frac{4b}{u} F N_{\alpha\bar{\beta}} + \frac{2b}{u} F^2 h_{\alpha\bar{\beta}} \\
&\quad + 4\left(b^2 - b\right) \frac{F u_\alpha u_{\bar{\beta}}}{u^2} - 2b\frac{4}{t} F h_{\alpha\bar{\beta}} - \left(\frac{\partial}{\partial t} - \Delta_b\right) F h_{\alpha\bar{\beta}}.
\end{aligned}$$

Finally one obtains

$$\begin{aligned}
&\left(\frac{\partial}{\partial t} - \Delta_b\right) N_{\alpha\bar{\beta}} \\
&= 2R_{\alpha\bar{\gamma}\delta\bar{\beta}} N_{\gamma\bar{\delta}} - R_{\alpha\bar{\sigma}} N_{\sigma\bar{\beta}} - R_{\sigma\bar{\beta}} N_{\alpha\bar{\sigma}} + C_{\alpha\bar{\beta}} \\
&\quad + 2bR_{\alpha\bar{\gamma}\delta\bar{\beta}} \frac{u_\gamma u_{\bar{\delta}}}{u} + b(n-2)\, i\frac{1}{u} A_{\alpha\rho} u_{\bar{\rho}} u_{\bar{\beta}} - b(n-2)\, i\frac{1}{u} A_{\bar{\beta}\bar{\rho}} u_\rho u_\alpha \\
&\quad + \frac{2b}{u}\left(u_{\alpha\gamma} - \frac{u_\alpha u_\gamma}{u}\right)\left(u_{\bar{\beta}\bar{\gamma}} - \frac{u_{\bar{\gamma}} u_{\bar{\beta}}}{u}\right) + \frac{2b}{u} N_{\alpha\bar{\gamma}} N_{\beta\bar{\gamma}} - \frac{8b}{t} N_{\alpha\bar{\beta}} \\
&\quad + b^2 \frac{2u_{\bar{\beta}} u_\gamma}{u^2} N_{\alpha\bar{\gamma}} + b^2 \frac{2u_\alpha u_{\bar{\gamma}}}{u^2} N_{\gamma\bar{\beta}} - \frac{2b}{u^2} u_\gamma u_{\bar{\beta}} N_{\alpha\bar{\gamma}} - \frac{2b}{u^2} u_{\bar{\gamma}} u_\alpha N_{\gamma\bar{\beta}} \\
&\quad + \frac{4b}{u} F N_{\alpha\bar{\beta}} - \left(\frac{\partial}{\partial t} - \Delta_b\right) F h_{\alpha\bar{\beta}} + \frac{2b}{u} F^2 h_{\alpha\bar{\beta}} + 4\left(b^2 - b\right) \frac{F u_\alpha u_{\bar{\beta}}}{u^2} \\
&\quad + (8b - 2)\frac{u}{t^2} h_{\alpha\bar{\beta}} + b\frac{u_0^2}{2u} h_{\alpha\bar{\beta}} + \left(8b - 8b^2\right)\frac{1}{t}\frac{u_\alpha u_{\bar{\beta}}}{u} \\
&\quad + \left(b^3 - 2b^2 + b\right) |\nabla_b u|^2 \frac{u_\alpha u_\beta}{u^3} - \frac{8b}{t} F h_{\alpha\bar{\beta}} + 2bi\frac{u_{0\alpha} u_{\bar{\beta}}}{u} - 2bi\frac{u_{0\bar{\beta}} u_\alpha}{u}
\end{aligned} \tag{3.7}$$

Note the first and second line of RHS are positive by curvature assumption. The third and fourth line are nonnegative while we apply on null vector of $N_{\alpha\bar{\beta}}$.

In the rest of the proof we will determine F so the rest terms are nonnegative. First we observe that

$$\left(\frac{\partial}{\partial t}-\Delta_b\right)\frac{u_0^2}{u}=\frac{2u_0}{u}[T,\Delta_b]u-\frac{2\left\|\nabla_b u_0\right\|^2}{u}+\frac{4u_0\left\langle\nabla_b u_0,\nabla_b u\right\rangle}{u^2}-2u_0^2\frac{\left\|\nabla_b u\right\|^2}{u^3}$$
$$=-2\left\|u^{-\frac{1}{2}}\nabla_b u_0-u^{-\frac{3}{2}}u_0\nabla_b u\right\|^2,$$

here we have used the fact that $[T,\Delta_b]u=2\mathrm{Im}Qu=0$ if $P_{\alpha\bar{\beta}}u=0$. The last four lines of (3.7) is reduced to

$$\begin{aligned}&\left(\frac{b}{2}-a\left(1+8b\right)\right)\frac{u_0^2}{u}h_{\alpha\bar{\beta}}+2at\left\|u^{-\frac{1}{2}}\nabla_b u_0-u^{-\frac{3}{2}}u_0\nabla_b u\right\|^2h_{\alpha\bar{\beta}}\\&+2\left(a^2t^2b\frac{u_0^4}{u^3}h_{\alpha\bar{\beta}}+2\frac{\left(b^2-b\right)}{\sqrt{b}}at\sqrt{b}\frac{u_0^2u_\alpha u_{\bar{\beta}}}{u^3}+\frac{\left(b^2-b\right)^2}{b}\frac{\left|\nabla_b u\right|^2}{2}\frac{u_\alpha u_{\bar{\beta}}}{u^3}\right)\\&+\left(8b-2\right)\frac{u}{t^2}h_{\alpha\bar{\beta}}+2bi\frac{u_{0\alpha}u_{\bar{\beta}}}{u}-2bi\frac{u_{0\bar{\beta}}u_\alpha}{u}+8b\left(1-b\right)\frac{u_\alpha u_{\bar{\beta}}}{tu}.\end{aligned}\tag{3.8}$$

Note that the second line above is a complete square. To handle the last term, we have the following calculation

$$\begin{aligned}&2bi\frac{u_{0\alpha}u_{\bar{\beta}}}{u}-2bi\frac{u_{0\bar{\beta}}u_\alpha}{u}+8b\left(1-b\right)\frac{u_\alpha u_{\bar{\beta}}}{tu}\\&=2bi\frac{u_{0\alpha}-\frac{u_0u_\alpha}{u}}{\sqrt{u}}\frac{u_{\bar{\beta}}}{\sqrt{u}}-2bi\frac{u_{0\bar{\beta}}-\frac{u_0u_{\bar{\beta}}}{u}}{\sqrt{u}}\frac{u_\alpha}{\sqrt{u}}+8b\left(1-b\right)\frac{u_\alpha u_{\bar{\beta}}}{tu}\\&=b\left(\varepsilon\frac{u_{0\alpha}-\frac{u_0u_\alpha}{u}}{\sqrt{u}}-\frac{2}{\varepsilon}i\frac{u_\alpha}{\sqrt{u}}\right)\left(\varepsilon\frac{u_{0\bar{\beta}}-\frac{u_0u_{\bar{\beta}}}{u}}{\sqrt{u}}+\frac{2}{\varepsilon}i\frac{u_{\bar{\beta}}}{\sqrt{u}}\right)\\&\quad-b\varepsilon^2\frac{u_{0\alpha}-\frac{u_0u_\alpha}{u}}{\sqrt{u}}\frac{u_{0\bar{\beta}}-\frac{u_0u_{\bar{\beta}}}{u}}{\sqrt{u}}-\frac{4b}{\varepsilon^2}\frac{u_\alpha u_{\bar{\beta}}}{u}+8b\left(1-b\right)\frac{u_\alpha u_{\bar{\beta}}}{tu}.\end{aligned}\tag{3.9}$$

By choosing $\varepsilon^2=\frac{4at}{b}$, we have

$$\begin{aligned}&2at\left\|u^{-\frac{1}{2}}\nabla_b u_0-u^{-\frac{3}{2}}u_0\nabla_b u\right\|^2h_{\alpha\bar{\beta}}-b\varepsilon^2\frac{u_{0\alpha}-\frac{u_0u_\alpha}{u}}{\sqrt{u}}\frac{u_{0\bar{\beta}}-\frac{u_0u_{\bar{\beta}}}{u}}{\sqrt{u}}\\&=2at\left\|u^{-\frac{1}{2}}\nabla_b u_0-u^{-\frac{3}{2}}u_0\nabla_b u\right\|^2h_{\alpha\bar{\beta}}-4at\frac{u_{0\alpha}-\frac{u_0u_\alpha}{u}}{\sqrt{u}}\frac{u_{0\bar{\beta}}-\frac{u_0u_{\bar{\beta}}}{u}}{\sqrt{u}}\\&\geq 0.\end{aligned}$$

Next we combine (3.8) and (3.9), and this yields

$$\begin{aligned}
&\left(\frac{b}{2}-a\left(1+8b\right)\right)\frac{u_0^2}{u}h_{\alpha\bar\beta}+2at\left\|u^{-\frac{1}{2}}\nabla_b u_0-u^{-\frac{3}{2}}u_0\nabla_b u\right\|^2 h_{\alpha\bar\beta}\\
&\quad+2\left(a^2t^2b\frac{u_0^4}{u^3}h_{\alpha\bar\beta}+2\frac{\left(b^2-b\right)}{\sqrt{b}}at\sqrt{b}\frac{u_0^2u_\alpha u_{\bar\beta}}{u^3}+\frac{\left(b^2-b\right)^2}{b}\frac{|\nabla_b u|^2}{2}\frac{u_\alpha u_{\bar\beta}}{u^3}\right)\\
&\quad+\left(8b-2\right)\frac{u}{t^2}h_{\alpha\bar\beta}+2bi\frac{u_{0\alpha}u_{\bar\beta}}{u}-2bi\frac{u_{0\bar\beta}u_\alpha}{u}+8b\left(1-b\right)\frac{u_\alpha u_{\bar\beta}}{tu}\\
&\geq\left(\frac{b}{2}-a\left(1+8b\right)\right)\frac{u_0^2}{u}h_{\alpha\bar\beta}+\left(8b-2\right)\frac{u}{t^2}h_{\alpha\bar\beta}+\left(8b\left(1-b\right)-\frac{b^2}{a}\right)\frac{u_\alpha u_{\bar\beta}}{tu}\\
&=0
\end{aligned}$$

when we choose a and b so that

$$\begin{aligned}
\frac{b}{2}-a\left(1+8b\right)&=0,\\
8b-2&=0,\\
8b\left(1-b\right)-\frac{b^2}{a}&=0.
\end{aligned}$$

This implies

$$a=\frac{1}{24}\quad\text{and}\quad b=\frac{1}{4}.$$

Hence (3.7) yields

$$\begin{aligned}
&\left(\frac{\partial}{\partial t}-\Delta_b\right)N_{\alpha\bar\beta}\\
&\geq 2R_{\alpha\bar\gamma\delta\bar\beta}N_{\gamma\bar\delta}-R_{\alpha\bar\sigma}N_{\sigma\bar\beta}-R_{\sigma\bar\beta}N_{\alpha\bar\sigma}+\frac{1}{2u}R_{\alpha\bar\gamma\delta\bar\beta}u_\gamma u_{\bar\delta}\\
&\quad+\frac{1}{2u}\left(u_{\alpha\gamma}-\frac{u_\alpha u_\gamma}{u}\right)\left(u_{\bar\beta\bar\gamma}-\frac{u_{\bar\gamma}u_{\bar\beta}}{u}\right)+\frac{1}{2u}N_{\alpha\bar\gamma}N_{\beta\bar\gamma}-\frac{2}{t}N_{\alpha\bar\beta}\\
&\quad+\frac{1}{8}\frac{u_{\bar\beta}u_\gamma}{u^2}N_{\alpha\bar\gamma}+\frac{1}{8}\frac{u_\alpha u_{\bar\gamma}}{u^2}N_{\gamma\bar\beta}-\frac{1}{2u^2}u_\gamma u_{\bar\beta}N_{\alpha\bar\gamma}-\frac{1}{2u^2}u_{\bar\gamma}u_\alpha N_{\gamma\bar\beta}+\frac{1}{u}FN_{\alpha\bar\beta}\\
&\quad+C_{\alpha\bar\beta}+\frac{1}{4u}\left(n-2\right)i\left[A_{\alpha\rho}u_{\bar\rho}u_{\bar\beta}-A_{\bar\beta\bar\rho}u_\rho u_\alpha\right].
\end{aligned}\tag{3.10}$$

which is nonnegative after applying on the null vectors of $N_{\alpha\bar\beta}$ if we assume that the bisectional curvature, bi-torsion tensor and $C_{\alpha\bar\beta}$ are nonnegative. □

4 The CR gradient estimate and Harnack inequality in Heisenberg groups

In this section, we will apply the method of the CR Li–Yau gradient estimate [10,34] and the CR Bochner formula (4.1) to derive the CR gradient estimate and the CR Harnack inequality for the positive solution of the CR heat equation (1.2) in the $(2n+1)$-dimensional Heisenberg group.

We first recall the following CR version of the Bochner formula in a complete pseudohermitian $(2n+1)$-manifold.

Lemma 2 ([21]) *For any smooth real-valued function φ,*

$$\frac{1}{2}\Delta_b \left|\nabla_b\varphi\right|^2 = \left|(\nabla^H)^2\varphi\right|^2 + \langle\nabla_b\varphi, \nabla_b\Delta_b\varphi\rangle + 2\left\langle J\nabla_b\varphi, \nabla_b\varphi_0\right\rangle + [2Ric - (n-2)Tor]\left((\nabla_b\varphi)_{\mathbb{C}}, (\nabla_b\varphi)_{\mathbb{C}}\right). \tag{4.1}$$

Here $(\nabla_b\varphi)_{\mathbb{C}} = \varphi^\alpha Z_\alpha$ is the corresponding complex $(1,0)$-vector of $\nabla_b\varphi$.

Since

$$\left|(\nabla^H)^2\varphi\right|^2 = 2\sum_{\alpha,\beta}(|\varphi_{\alpha\beta}|^2 + |\varphi_{\alpha\overline{\beta}}|^2) \geq 2\sum_{\alpha}|\varphi_{\alpha\overline{\alpha}}|^2 \geq \frac{1}{2n}\left(\Delta_b\varphi\right)^2 + \frac{n}{2}\varphi_0^2$$

and for any $v > 0$,

$$2\left\langle J\nabla_b\varphi, \nabla_b\varphi_0\right\rangle \leq 2\left|\nabla_b\varphi\right|\left|\nabla_b\varphi_0\right| \leq v^{-1}\left|\nabla_b\varphi\right|^2 + v\left|\nabla_b\varphi_0\right|^2.$$

Therefore, for any real-valued function φ and any $v > 0$, we have the Bochner inequality

$$\frac{1}{2}\Delta_b\left|\nabla_b\varphi\right|^2 \geq \frac{1}{2n}\left(\Delta_b\varphi\right)^2 + \frac{n}{2}\varphi_0^2 + \langle\nabla_b\varphi, \nabla_b\Delta_b\varphi\rangle - v\left|\nabla_b\varphi_0\right|^2 + [2Ric - (n-2)Tor - 2v^{-1}]\left((\nabla_b\varphi)_{\mathbb{C}}, (\nabla_b\varphi)_{\mathbb{C}}\right). \tag{4.2}$$

Now let $u(x,t)$ be a positive solution of the CR heat equation (1.2) and

$$\varphi(x,t) = \ln u(x,t).$$

Then $\varphi(x,t)$ satisfies

$$\left(\Delta_b - \frac{\partial}{\partial t}\right)\varphi = -\left|\nabla_b\varphi\right|^2 \tag{4.3}$$

and from Lemma 3.5 in [10]

$$\left(\Delta_b - \frac{\partial}{\partial t}\right)\varphi_0 = -2\left\langle\nabla_b\varphi, \nabla_b\varphi_0\right\rangle + 2V(\varphi), \tag{4.4}$$

where the operator V is defined by

$$V(\varphi) = (A_{\alpha\beta}\varphi^{\beta}),^{\alpha} + (A_{\overline{\alpha}\overline{\beta}}\varphi^{\overline{\beta}}),^{\overline{\alpha}} + A_{\alpha\beta}\varphi^{\alpha}\varphi^{\beta} + A_{\overline{\alpha}\overline{\beta}}\varphi^{\overline{\alpha}}\varphi^{\overline{\beta}}.$$

Therefore, if $A_{\alpha\beta} = 0$ then one obtains $V(\varphi) = 0$.

Lemma 3 *Let $(\boldsymbol{H}^n, J, \theta)$ be the $(2n+1)$-dimensional Heisenberg group. If $u(x,t)$ is a positive solution of (1.2) on $\boldsymbol{H}^n \times [0,\infty)$. Let $\varphi(x,t) = \ln u(x,t)$, then for any given $\alpha \leq -1$, the function*

$$G(x,t) := t\left[|\nabla_b\varphi|^2(x,t) + \alpha\varphi_t(x,t) + t\varphi_0^2(x,t)\right]$$

satisfies the inequality

$$\begin{aligned}\left(\Delta_b - \frac{\partial}{\partial t}\right)G \geq& -2\langle\nabla_b\varphi, \nabla_b G\rangle - t^{-1}G + \alpha^{-2}n^{-1}t^{-1}G^2 + \alpha^{-2}n^{-1}(\alpha+1)^2 t|\nabla_b\varphi|^4 \\ &- 2n^{-1}\alpha^{-2}[(\alpha+1)|\nabla_b\varphi|^2 + t\varphi_0^2]G + 2[\alpha^{-2}n^{-1}(\alpha+1)t^2\varphi_0^2 - 1]|\nabla_b\varphi|^2.\end{aligned} \tag{4.5}$$

Proof We first rewrite G as

$$G = t\left[|\nabla_b\varphi|^2 + \alpha\varphi_t + t\varphi_0^2\right] = t[(\alpha+1)|\nabla_b\varphi|^2 + \alpha\Delta_b\varphi + t\varphi_0^2].$$

By taking $v = t$ into the inequality (4.2), we compute

$$\begin{aligned}\Delta_b G &= t[\Delta_b|\nabla_b\varphi|^2 + \alpha\Delta_b\varphi_t + t\Delta_b\varphi_0^2] \\ &\geq t\left[\frac{1}{n}(\Delta_b\varphi)^2 + n\varphi_0^2 + 2\langle\nabla_b\varphi, \nabla_b\Delta_b\varphi\rangle\right. \\ &\qquad \left. + \alpha\Delta_b\varphi_t + 2t\varphi_0\Delta_b\varphi_0 - 2t^{-1}|\nabla_b\varphi|^2\right],\end{aligned}$$

and (4.4) yields that

$$\begin{aligned}\frac{\partial}{\partial t}G &= t^{-1}G + t\left[2(\alpha+1)\langle\nabla_b\varphi, \nabla_b\varphi_t\rangle + \alpha\Delta_b\varphi_t + \varphi_0^2 + 2t\varphi_0\varphi_{0t}\right] \\ &= t^{-1}G + t\left[2(\alpha+1)\langle\nabla_b\varphi, \nabla_b\varphi_t\rangle + \alpha\Delta_b\varphi_t + \varphi_0^2\right. \\ &\quad \left. + 2t\varphi_0\Delta_b\varphi_0 + 2t\left\langle\nabla_b\varphi, \nabla_b\varphi_0^2\right\rangle\right],\end{aligned}$$

Thus, we have

$$\left(\Delta_b - \frac{\partial}{\partial t}\right)G \geq -2\langle\nabla_b\varphi, \nabla_b G\rangle - t^{-1}G + t\left[n^{-1}(\Delta_b\varphi)^2 - 2t^{-1}|\nabla_b\varphi|^2\right], \tag{4.6}$$

where we have used

$$\langle \nabla_b \varphi, \nabla_b G\rangle = t[(\alpha+1)\langle \nabla_b \varphi, \nabla_b \varphi_t\rangle + t\langle \nabla_b \varphi, \nabla_b \varphi_0^2\rangle - \langle \nabla_b \varphi, \nabla_b \Delta_b \varphi\rangle].$$

However, since

$$\Delta_b \varphi = -|\nabla_b \varphi|^2 + \varphi_t = \alpha^{-1}\left[t^{-1}G - (\alpha+1)|\nabla_b \varphi|^2 - t\varphi_0^2\right],$$

This implies

$$\begin{aligned}(\Delta_b \varphi)^2 \geq{} & \alpha^{-2}t^{-2}G^2 - 2\alpha^{-2}t^{-1}G[(\alpha+1)|\nabla_b \varphi|^2 + t\varphi_0^2] \\ & + \alpha^{-2}[(\alpha+1)^2|\nabla_b \varphi|^4 + 2(\alpha+1)t\varphi_0^2|\nabla_b \varphi|^2].\end{aligned}$$

The Lemma is proved by substituting this inequality into (4.6). □

Next we apply the lemma to prove prove Theorem 2.

Proof Let B_{2R} be a ball of radius $2R$ center at $O \in \boldsymbol{H}^n$ with $R > 1$. Let $\psi \in C_0^\infty(R)$ be a cut-off function 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 that

$$\psi' \leq 0,\ \psi'' \geq -C_1, \ \text{and}\ \frac{|\psi'|^2}{\psi} \leq C_2, \tag{4.7}$$

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

$$G = t\left[|\nabla_b \varphi|^2 + \alpha\varphi_t + t\varphi_0^2\right]$$

we consider the function ηG with support on $B_{2R} \times (0, \mathrm{T}]$. Let $(x_0, t_0) \in B_{2R} \times (0, \mathrm{T}]$ be the point where ηG attains its maximum. Note that at (x_0, t_0) we have the following properties

$$\nabla_b(\eta G) = G\nabla_b \eta + \eta \nabla_b G = 0, \tag{4.8}$$
$$\Delta_b(\eta G) \leq 0, \tag{4.9}$$

and

$$\frac{\partial}{\partial t}(\eta G) = \eta G_t \geq 0. \tag{4.10}$$

In the sequel, all computations will be at the point (x_0, t_0) and we may assume that

$$(\eta G)(x_0, t_0) > 0,$$

otherwise $(\eta G)(x_0, t_0) \le 0$, and the theorem is obviously true. By (4.8), $\nabla_b G = -G\nabla_b \eta/\eta$, and from (4.9)

$$0 \ge \Delta_b(\eta G) = G\Delta_b \eta + \eta \Delta_b G + 2\langle \nabla_b \eta, \nabla_b G\rangle = G\Delta_b \eta + \eta \Delta_b G - 2\eta^{-1} G\,|\nabla_b \eta|^2 . \tag{4.11}$$

(4.7) implies

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

and

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

The CR sub-Laplacian comparison property in [14] yields

$$\Delta_b d_c \le \frac{C}{d_c}, \tag{4.12}$$

for some constant C, and hence

$$\Delta_b \eta \ge -\frac{C_3}{R}.$$

Substituting these into (4.11) and then applying the inequality (4.5), (6.20) yields the following estimate

$$t_0^2 \varphi_0^2 \le C_5,$$

for some constant $C_5 > 0$. Combining these estimates, we obtain

$$\begin{aligned} 0 &\ge \Delta_b(\eta G) \ge -C_3 R^{-1} G - 2C_2 R^{-1} G + \eta \Delta_b G \\ &\ge -C_4 R^{-1} G + \eta \left[G_t - 2\langle \nabla_b \varphi, \nabla_b G\rangle - t_0^{-1} G + n^{-1}\alpha^{-2} t_0^{-1} G^2 \right] \\ &\quad - 2\eta n^{-1}\alpha^{-2} \left[(\alpha+1)\,|\nabla_b \varphi|^2 + t_0 \varphi_0^2 \right] G + n^{-1}\alpha^{-2}(\alpha+1)^2 \eta t_0\,|\nabla_b \varphi|^4 \\ &\quad + 2\eta \left[n^{-1}\alpha^{-2}(\alpha+1) C_5 - 1 \right] |\nabla_b \varphi|^2 , \end{aligned}$$

where $C_4 = C_3 + 2C_2$.

Since $\eta G_t = (\eta G)_t \ge 0$, $\eta\langle \nabla_b \varphi, \nabla_b G\rangle = G\langle \nabla_b \varphi, \nabla_b \eta\rangle$, then by the following inequality

$$\begin{aligned} &n^{-1}\alpha^{-2}(\alpha+1)^2 t_0\,|\nabla_b \varphi|^4 + 2\left[n^{-1}\alpha^{-2}(\alpha+1) C_5 - 1 \right] |\nabla_b \varphi|^2 \\ &\quad \ge -2t_0^{-1} \left[n^{-1}\alpha^{-2} C_5^2 + n\alpha^2 (\alpha+1)^{-2} \right], \end{aligned}$$

the above inequality can be reduced to

$$\begin{aligned}0 \geq\ & n^{-1}\alpha^{-2}t_0^{-1}\eta G^2 - (C_4 R^{-1} + t_0^{-1}\eta)G - 2G\langle\nabla_b\varphi, \nabla_b\eta\rangle \\ & - 2n^{-1}\alpha^{-2}\left[(\alpha+1)\left|\nabla_b\varphi\right|^2 + t_0\varphi_0^2\right]\eta G \\ & - 2\eta t_0^{-1}\left[n^{-1}\alpha^{-2}C_5^2 + n\alpha^2(\alpha+1)^{-2}\right].\end{aligned}$$

Next we multiply the above inequality by ηt_0, since $0 \leq \eta \leq 1$ and $\langle\nabla_b\varphi, \nabla_b\eta\rangle \leq \left|\nabla_b\varphi\right|\left|\nabla_b\eta\right|$, we get

$$\begin{aligned}0 \geq\ & n^{-1}\alpha^{-2}(\eta G)^2 - (C_4 R^{-1} t_0 + 1)\eta G - 2t_0\left|\nabla_b\varphi\right|\left|\nabla_b\eta\right|\eta G \\ & - 2n^{-1}\alpha^{-2}\eta t_0\left[(\alpha+1)\left|\nabla_b\varphi\right|^2 + t_0\varphi_0^2\right]\eta G \\ & - 2\left[n^{-1}\alpha^{-2}C_5^2 + n\alpha^2(\alpha+1)^{-2}\right]. \end{aligned} \tag{4.13}$$

Observe that there exists a constant $C_6 > 0$ such that

$$-2n^{-1}\alpha^{-2}(\alpha+1)\eta\left|\nabla_b\varphi\right|^2 - 2\sqrt{C_2}R^{-1}\eta^{1/2}\left|\nabla_b\varphi\right| \geq C_6\alpha^2(\alpha+1)^{-1}R^{-2}.$$

Hence combining this with (4.13) and using $t_0^2\varphi_0^2 \leq C_5$ again, we can conclude that

$$\begin{aligned}0 \geq\ & n^{-1}\alpha^{-2}(\eta G)^2 + \left[C_7 t_0\alpha^2(\alpha+1)^{-1}R^{-1} - 1 - 2n^{-1}\alpha^{-2}C_5\right]\eta G \\ & - 2\left[n^{-1}\alpha^{-2}C_5^2 + n\alpha^2(\alpha+1)^{-2}\right]\end{aligned}$$

for some constant $C_7 > 0$. This implies that at the maximum point (x_0, t_0)

$$\eta G \leq C_8\alpha^2\left[C_5 - (\alpha+1)^{-1}(1 + \alpha^2 t_0 R^{-1})\right]$$

for some constant $C_8 > 0$. In particular since $t_0 \leq \mathrm{T}$, when restricted on $B_{2R} \times \{\mathrm{T}\}$ we have

$$\left|\nabla_b\varphi\right|^2 + \alpha\varphi_t + \mathrm{T}\varphi_0^2 \leq C_8\alpha^2\left[(C_5 - (\alpha+1)^{-1})\mathrm{T}^{-1} - \alpha^2(\alpha+1)^{-1}R^{-1}\right].$$

Theorem 2 follows by letting $t = \mathrm{T}$ and taking $R \to \infty$. □

The first application of the theorem is the Harnack inequality on the Heisenberg group.

Corollary 4 *Let $(\boldsymbol{H}^n, J, \theta)$ be the $(2n+1)$-dimensional Heisenberg group. If $u(x,t)$ is the positive solution of the CR heat equation (1.2) on $\boldsymbol{H}^n \times [0, \infty)$, we have the Harnack inequality*

$$\frac{u(x_1, t_1)}{u(x_2, t_2)} \leq \left(\frac{t_2}{t_1}\right)^{C_2} \exp\left(\frac{d_c(x_1, x_2)^2}{2(t_2 - t_1)}\right) \tag{4.14}$$

for any x_1, x_2 *in* $\boldsymbol{H}^n$ *and* $0 < t_1 < t_2 < \infty$, *where* $d_c(x_1, x_2)$ *is the Carnot–Carathéodory distance between* x_1 *and* x_2.

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

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

Clearly, $\eta(t_1) = (x_1, t_1)$ and $\eta(t_2) = (x_2, t_2)$. Integrating along η, we get

$$\begin{aligned} \ln u(x_1, t_1) - \ln u(x_2, t_2) &= -\int_{t_1}^{t_2} \frac{d}{dt} \ln u dt \\ &= \int_{t_1}^{t_2} \left[-\langle \dot{\gamma}, \nabla_b (\ln u) \rangle - (\ln u)_t \right] dt. \end{aligned} \tag{4.15}$$

On the other hand, Theorem 2 implies that

$$-(\ln u)_t \leq A t^{-1} + \alpha^{-1} \left| \nabla_b (\ln u) \right|^2$$

where $A = -C_1 \alpha [C_1 - (\alpha + 1)^{-1}]$ for some constant C_1 depending only on n. Hence (4.15) is reduced to

$$\ln \frac{u(x_1, t_1)}{u(x_2, t_2)} \leq \int_{t_1}^{t_2} \left[|\dot{\gamma}| \left| \nabla_b (\ln u) \right| + \alpha^{-1} \left| \nabla_b (\ln u) \right|^2 + A t^{-1} \right] dt.$$

Applying the inequality

$$\alpha^{-1} \left| \nabla_b (\ln u) \right|^2 + |\dot{\gamma}| \left| \nabla_b (\ln u) \right| \leq -\frac{\alpha}{4} |\dot{\gamma}|^2$$

and choosing

$$|\dot{\gamma}| = \frac{d_c(x_1, x_2)}{t_2 - t_1},$$

we conclude that

$$\ln \frac{u(x_1, t_1)}{u(x_2, t_2)} \leq -\frac{\alpha}{4} \frac{d_c(x_1, x_2)^2}{t_2 - t_1} + A \ln \frac{t_2}{t_1}.$$

By taking exponential of both sides, we have

$$\frac{u(x_1,t_1)}{u(x_2,t_2)} \le \left(\frac{t_2}{t_1}\right)^{-C_1\alpha[C_1-(\alpha+1)^{-1}]} \exp\left(-\frac{\alpha d_c(x_1,x_2)^2}{4(t_2-t_1)}\right).$$

The result follows by choosing $\alpha = -2$. □

As a consequence of Corollary 4 and [8], we have the following upper bound estimate for the heat kernel of (1.2).

Corollary 5 *Let* $(\boldsymbol{H}^n, J, \theta)$ *be the* $(2n+1)$*-dimensional Heisenberg group and* $H(x,y,t)$ *be the heat kernel of (1.2) on* $M \times [0,\infty)$*. Then for some constant* $\delta > 1$ *and* $0 < \epsilon < 1$*,* $H(x,y,t)$ *satisfies the estimate*

$$H(x,y,t) \le C(\epsilon)^{\delta} V^{-\frac{1}{2}}\left(B_x(\sqrt{t})\right) V^{-\frac{1}{2}}\left(B_y(\sqrt{t})\right) \exp\left(-\frac{d_c^2(x,y)}{(4+\epsilon)t}\right) \tag{4.16}$$

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

Once we have the upper bound estimate for the heat kernel and the sub-Laplacian comparison property (4.12), we can then apply the arguments of Li–Tam as in [33] or [32] and obtain the following mean value inequality.

Corollary 6 *Let* $(\boldsymbol{H}^n, J, \theta)$ *be the* $(2n+1)$*-dimensional Heisenberg group and* g *be subsolution of the CR heat equation such that*

$$\left(\frac{\partial}{\partial t} - \Delta_b\right) g(x,t) \le 0.$$

Then for some constant C *depend on* δ, τ, η*, such that* $0 < \delta < 1$, $0 < \tau < T$, $0 < \eta < \frac{1}{2}$*, the following inequality holds for any* $\rho > 2\sqrt{T}$,

$$\sup_{B_p((1-\delta)\rho)\times[\tau,T]} g \le C \int_{(1-\eta)\tau}^{T} \int_{B_p(\rho)} g(y,s)\, dy ds. \tag{4.17}$$

5 Complete noncompact case

In [7], Cao and Ni derived the matrix Harnack estimates for the positive solution of the heat equation on a complete noncompact Kähler manifold with nonnegative bisectional curvature by using the key estimate (5.1) which is derived from the result of the Li–Yau heat kernel estimate [34]. For a general complete noncompact pseudohermitian manifold, we do not have the Li–Yau type heat kernel estimates. However, we do have the CR corresponding result of the Li–Yau heat kernel on the Heisenberg group as in Corollary 5. Comparing the method of Cao–Ni, we should point out that we also need the extra u_0-growth property (5.2) that has no analogue in Kähler manifolds.

Lemma 4 *Let $(\boldsymbol{H}^n, J, \theta)$ be the $(2n+1)$-dimensional Heisenberg group. $u(x,t)$ is a positive solution of the CR heat equation (1.2) on $\boldsymbol{H}^n \times [0,\infty)$. Then for $0 < \delta \le t \le 2-\delta$, there exists a constant $b > 0$ (might depends on δ) such that*

$$u(x,t) \le \exp\left(b\left(r^2(x)+1\right)\right) \tag{5.1}$$

and

$$|u_0|(x,t) \le \exp\left(b\left(r^2(x)+1\right)\right). \tag{5.2}$$

Proof Let $o \in M$ be a fixed point. Since our focus here is to obtain an upper bound on u for positive time, we may assume that $u(x,t)$ is defined on $M \times [0,2]$. By Harnack inequality in Corollary 4, we have, for $0 < t < 2$

$$u(x,t) \le \frac{C}{t^{C_2}} u(o,2)\exp(ar^2(x)).$$

Here a is a constant and $r^2(x)$ is the Carnot–Carathé odory distance $d_c(o,x)$. In particular, for $0 < \delta \le t \le 2-\delta$, there exists a constant $b > 0$ such that

$$u(x,t) \le \exp\left(b(r^2(x)+1)\right).$$

But applying (6.20) in next section, we obtain

$$|u_0(x,t)| \le \frac{C}{t} u(x,t).$$

Hence this implies

$$|u_0|(x,t) \le \exp\left(b\left(r^2(x)+1\right)\right).$$

□

Lemma 5 *Let M be a complete pseudohermitian $(2n+1)$-manifold with nonnegative bisectional curvature and nonnegative bi-torsion tensor. Let u be any positive solution of the CR heat equation (1.2). Then*

$$\left(\frac{\partial}{\partial t} - \Delta_b\right)\|\nabla_b u\|^2 \le -2\left\|u_{\alpha\beta}\right\|^2 - \frac{1}{2}\left\|u_{\alpha\bar\beta} + u_{\bar\beta\alpha}\right\|^2 + 4\left\|\nabla_b(u_0)\right\|\left\|\nabla_b u\right\|.$$

Furthermore if we assume the positive solution u satisfies the purely holomorphic Hessian operator $P_{\alpha\bar\beta}u = 0$.

$$\left(\frac{\partial}{\partial t} - \Delta_b\right)\left\|u_{\alpha\bar\beta} + u_{\bar\beta\alpha}\right\|^2 \le 0.$$

Proof We calculate

$$
\begin{aligned}
&\left(\frac{\partial}{\partial t}-\Delta_b\right)\|\nabla_b u\|^2\\
&=\left(\frac{\partial}{\partial t}-\Delta_b\right)2u_\alpha u_{\bar\alpha}\\
&=2\left(\Delta_b u\right)_\alpha u_{\bar\alpha}+2\left(\Delta_b u\right)_{\bar\alpha}u_\alpha-\left(2u_\alpha u_{\bar\alpha}\right)_{\beta\bar\beta}-\left(2u_\alpha u_{\bar\alpha}\right)_{\bar\beta\beta}\\
&=2\left(2u_{\beta\bar\beta\alpha}-inu_{0\alpha}\right)u_{\bar\alpha}+conj.-\left(2u_\alpha u_{\bar\alpha}\right)_{\beta\bar\beta}-conj\\
&=4u_{\alpha\beta\bar\beta}u_{\bar\alpha}-4ih_{\alpha\bar\beta}u_{\beta 0}u_{\bar\alpha}-4R_{\bar\rho\alpha}u_\rho u_{\bar\alpha}-2inu_{0\alpha}u_{\bar\alpha}\\
&\quad+4u_{\bar\alpha\bar\beta\beta}u_\alpha+4ih_{\bar\alpha\beta}u_{\bar\beta 0}u_\alpha-4R_{\rho\bar\alpha}u_{\bar\rho}u_\alpha+2inu_{0\bar\alpha}u_\alpha\\
&\quad-\left(2u_{\alpha\beta\bar\beta}u_{\bar\alpha}+2u_{\alpha\beta}u_{\bar\alpha\bar\beta}+2u_{\alpha\bar\beta}u_{\bar\alpha\beta}+2u_\alpha u_{\bar\alpha\beta\bar\beta}\right)\\
&\quad-\left(2u_{\bar\alpha\bar\beta\beta}u_\alpha+2u_{\bar\alpha\bar\beta}u_{\alpha\beta}+2u_{\bar\alpha\beta}u_{\alpha\bar\beta}+2u_{\bar\alpha}u_{\alpha\bar\beta\beta}\right)\\
&=-4ih_{\alpha\bar\beta}u_{\beta 0}u_{\bar\alpha}-4R_{\bar\rho\alpha}u_\rho u_{\bar\alpha}-2inu_{0\alpha}u_{\bar\alpha}\\
&\quad+4ih_{\bar\alpha\beta}u_{\bar\beta 0}u_\alpha-4R_{\rho\bar\alpha}u_{\bar\rho}u_\alpha+2inu_{0\bar\alpha}u_\alpha-4u_{\alpha\beta}u_{\bar\alpha\bar\beta}-4u_{\alpha\bar\beta}u_{\bar\alpha\beta}\\
&\quad+2u_{\bar\alpha}\left(inu_{\alpha 0}+R_{\alpha\bar\rho}u_\rho\right)-2u_\alpha\left(inu_{\bar\alpha 0}-R_{\bar\alpha\rho}u_{\bar\rho}\right)\\
&=-4u_{\alpha\beta}u_{\bar\alpha\bar\beta}-4u_{\alpha\bar\beta}u_{\bar\alpha\beta}-4R_{\bar\rho\alpha}u_\rho u_{\bar\alpha}\\
&\quad-4iu_{0\alpha}u_{\bar\alpha}+4iu_{0\bar\alpha}u_\alpha+2i\left(n-2\right)A_{\bar\alpha\bar\beta}u_\beta u_\alpha-2i\left(n-2\right)A_{\alpha\beta}u_{\bar\beta}u_{\bar\alpha}.
\end{aligned}
$$

Then the curvature assumptions yield

$$
\left(\frac{\partial}{\partial t}-\Delta_b\right)\|\nabla_b u\|^2\le-2\left\|u_{\alpha\beta}\right\|^2-\frac{1}{2}\left\|u_{\alpha\bar\beta}+u_{\bar\beta\alpha}\right\|^2+4||\nabla_b\left(u_0\right)||\,\|\nabla_b u\|
$$

and this implies

$$
\begin{aligned}
&\left(\frac{\partial}{\partial t}-\Delta_b\right)\left\|u_{\alpha\bar\beta}+u_{\bar\beta\alpha}\right\|^2\\
&=2\left(\left(\frac{\partial}{\partial t}-\Delta_b\right)\left(u_{\alpha\bar\beta}+u_{\bar\beta\alpha}\right)\right)\left(u_{\bar\alpha\beta}+u_{\beta\bar\alpha}\right)+conj\\
&\quad-2\left(\left(u_{\alpha\bar\beta}+u_{\bar\beta\alpha}\right)_\gamma\left(u_{\bar\alpha\beta}+u_{\beta\bar\alpha}\right)_{\bar\gamma}\right)+conj\\
&\le 2\left(\left(\frac{\partial}{\partial t}-\Delta_b\right)\left(u_{\alpha\bar\beta}+u_{\bar\beta\alpha}\right)\right)\left(u_{\bar\alpha\beta}+u_{\beta\bar\alpha}\right)+conj\\
&=2\left(2R_{\alpha\bar\gamma\delta\bar\beta}u_{\gamma\bar\delta}-R_{\alpha\bar\delta}u_{\delta\bar\beta}-R_{\delta\bar\beta}u_{\alpha\bar\delta}+C_{\alpha\bar\beta}\right)\left(u_{\bar\alpha\beta}+u_{\beta\bar\alpha}\right)+conj\\
&=\left[2R_{\alpha\bar\gamma\delta\bar\beta}\left(u_{\gamma\bar\delta}+u_{\bar\delta\gamma}\right)-R_{\alpha\bar\delta}\left(u_{\delta\bar\beta}+u_{\bar\beta\delta}\right)-R_{\delta\bar\beta}\left(u_{\alpha\bar\delta}+u_{\bar\delta\alpha}\right)+C_{\alpha\bar\beta}\right]\cdot\\
&\quad\times\left(u_{\bar\alpha\beta}+u_{\beta\bar\alpha}\right)+conj\le 0.
\end{aligned}
$$

Here we have used $[\Delta_b, T]u = 0,\ C_{\alpha\bar{\beta}} = 0$ and the following inequality:

$$\begin{aligned}&\left(2R_{\alpha\bar{\gamma}\delta\bar{\beta}}\left(u_{\gamma\bar{\delta}} + u_{\bar{\delta}\gamma}\right) - R_{\alpha\bar{\delta}}\left(u_{\delta\bar{\beta}} + u_{\bar{\beta}\delta}\right) - R_{\delta\bar{\beta}}\left(u_{\alpha\bar{\delta}} + u_{\bar{\delta}\alpha}\right)\right)\left(u_{\bar{\alpha}\beta} + u_{\beta\bar{\alpha}}\right)\\ &= 2R_{\alpha\bar{\beta}\beta\bar{\alpha}}\lambda_\alpha\lambda_\beta - 2R_{\gamma\bar{\gamma}}\left(\lambda_\gamma\right)^2\\ &= -R_{\alpha\bar{\beta}\beta\bar{\alpha}}(\lambda_\alpha - \lambda_\beta)^2\\ &\leq 0.\end{aligned}$$

Here we denote $u_{\gamma\bar{\gamma}} + u_{\bar{\gamma}\gamma} = \lambda_\gamma$ (since $u_{\gamma\bar{\delta}} + u_{\bar{\delta}\gamma}$ is symmetric and then can be diagonalized). □

Combining Lemma 4 and Lemma 5, we are able to obtain the following integral estimate.

Lemma 6 *Let* $(\boldsymbol{H}^n, J, \theta)$ *be the standard* $(2n+1)$*-dimensional Heisenberg group. If* $u(x,t)$ *is the positive solution of the CR heat equation (1.2) on* $\boldsymbol{H}^n \times [0,\infty)$ *. There exists a constant* $\hat{b} > 0$, *depending only on b such that*

$$\int_{2\delta}^{T}\int_{M} e^{-\hat{b}r^2}\left(\|\nabla_b u_0\|^2 + \|\nabla_b u\|^2 + \left\|u_{\alpha\beta}\right\|^2 + \left\|u_{\alpha\bar{\beta}} + u_{\bar{\beta}\alpha}\right\|^2\right)d\mu dt < \infty.$$

Proof Let ϕ be a cut-off function such that $\phi = 0$ for $d_c(x,p) > 2R,\ t < \delta$, and $\phi = 1$ as $d_c(x,p) < R,\ t > 2\delta$ and $|\nabla_b\phi| \leq \frac{C}{R}$. We multiply ϕ^2 on both sides of the following equation

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

Then we integrate

$$\begin{aligned}\int_0^T\int_M \|\nabla_b u\|^2\phi^2 d\mu dt &\leq \int_0^T\int_M\left(\left(\Delta_b - \frac{\partial}{\partial t}\right)u^2\right)\phi^2 d\mu dt\\ &= \int_0^T\int_M\left(\Delta_b u^2\right)\phi^2 d\mu dt + \int_M u^2(x,0)\,\phi^2(x,0)\,d\mu\\ &\quad - \int_M u^2(x,T)\,\phi^2(x,T)\,d\mu + \int_0^T\int_M u^2(x,t)\left(\phi^2\right)_t d\mu dt\\ &\leq \int_0^T\int_M u^2(x,t)\left(\phi^2\right)_t d\mu dt - \int_0^T\int_M 2\phi\left\langle\nabla_b u^2, \nabla_b\phi\right\rangle d\mu dt. \qquad (5.3)\end{aligned}$$

Young's inequality yields

$$\int_0^T \int_M 2\phi \left\langle \nabla_b u^2, \nabla_b \phi \right\rangle d\mu dt$$
$$\leq \frac{1}{2} \int_0^T \int_M \|\nabla_b u\|^2 \phi^2 d\mu dt + 8 \int_0^T \int_M u^2 \|\nabla_b \phi\|^2 d\mu dt.$$

Then (5.3) is reduced to

$$\int_{2\delta}^T \int_M \|\nabla_b u\|^2 \phi^2 d\mu dt \leq 2 \int_{\delta}^T \int_M u^2 \left(8 \|\nabla_b \phi\|^2 + \left(\phi^2\right)_t \right) d\mu dt.$$

That is, there exists a positive constant C independent of R such that

$$\int_{2\delta}^T \int_{B_p(R)} \|\nabla_b u\|^2 d\mu dt \leq C \int_{\delta}^T \int_{B_p(2R)} u^2 d\mu dt.$$

By choosing $R = 2^n$ and $b_1 > 4b$, we obtain

$$\begin{aligned}
\int_{2\delta}^T \int_M e^{-b_1 r^2} \|\nabla_b u\|^2 d\mu dt &\leq \sum_{n=1}^{\infty} e^{-b_1 (2^n)^2} \int_{\delta}^T \int_{B_p(2^{n+1}) \setminus B_p(2^n)} \|\nabla_b u\|^2 d\mu dt \\
&\leq C \sum_{n=1}^{\infty} e^{-b_1 (2^n)^2} \int_{\delta}^T \int_{B_p(2^{n+1})} u^2 d\mu dt \\
&\leq C \sum_{n=1}^{\infty} e^{-b_1 (2^n)^2} e^{b 2^{2n+2}} \int_{\delta}^T \int_{B_p(2^{n+1})} e^{-br^2} u^2 d\mu dt \\
&\leq C \int_{\delta}^T \int_M e^{-br^2} u^2 d\mu dt \cdot \sum_{n=1}^{\infty} \left(\frac{e^{4b}}{e^{b_1}} \right)^{4^n} < \infty,
\end{aligned} \tag{5.4}$$

where in the last inequality we use the growth rate of u as in Lemma 4, i.e.,

$$\int_{2\delta}^T \int_M e^{-b_1 r^2} \|\nabla_b u\|^2 d\mu dt < \infty. \tag{5.5}$$

Again $[\Delta_b, T]u = 0$ implies

$$\left(\frac{\partial}{\partial t} - \Delta_b\right) u_0^2 \leq -2 \left\|\nabla_b u_0\right\|^2.$$

Applying Lemma 4, we have, for some positive constant $b_2 > 0$, the following equality holds

$$\int_\delta^T \int_M e^{-b_2 r^2} \left\|\nabla_b u_0\right\|^2 d\mu dt < \infty. \tag{5.6}$$

Lemma 5 and $[\Delta_b, T]u = 0$ imply

$$\left(\frac{\partial}{\partial t} - \Delta_b\right)\left(\|\nabla_b u\|^2 + u_0^2 + u^2\right) \leq -2\left\|u_{\alpha\beta}\right\|^2 - \frac{1}{2}\left\|u_{\alpha\bar{\beta}} + u_{\bar{\beta}\alpha}\right\|^2. \tag{5.7}$$

Next we multiply the test function ϕ^2 and integrate as in (5.3), and obtain

$$\begin{aligned}
&\int_0^T \int_M \left(2\left\|u_{\alpha\beta}\right\|^2 + \frac{1}{2}\left\|u_{\alpha\bar{\beta}} + u_{\bar{\beta}\alpha}\right\|^2\right)\phi^2 d\mu dt \\
&\quad \leq \int_0^T \int_M \left(\left(\Delta_b - \frac{\partial}{\partial t}\right)\left(\|\nabla_b u\|^2 + u_0^2 + u^2\right)\right)\phi^2 d\mu dt \\
&\quad \leq \int_0^T \int_M \left(\|\nabla_b u\|^2 + u_0^2 + u^2\right)(\phi^2)_t d\mu \\
&\qquad - \int_0^T \int_M 2\phi\left\langle \nabla_b(\|\nabla_b u\|^2 + u_0^2 + u^2), \nabla_b\phi\right\rangle d\mu dt.
\end{aligned}$$

Young's inequality again yields

$$\begin{aligned}
&\int_0^T \int_M \left(\left\|u_{\alpha\beta}\right\|^2 + \left\|u_{\alpha\bar{\beta}} + u_{\bar{\beta}\alpha}\right\|^2\right)\phi^2 d\mu dt \\
&\quad \leq C \int_M \left(\|\nabla_b u_0\|^2 + \|\nabla_b u\|^2 + u_0^2 + u^2\right)\left(\|\nabla_b\phi\|^2 + \left(\phi^2\right)_t\right) d\mu.
\end{aligned}$$

Now apply the same argument as in (5.4), for some positive constant $b_3 > 0$, we have

$$\int_{2\delta}^{T}\int_{M} \exp\left(-b_3 r^2\right)\left(\left\|u_{\alpha\beta}\right\|^2 + \left\|u_{\alpha\bar{\beta}} + u_{\bar{\beta}\alpha}\right\|^2\right) d\mu dt < \infty. \tag{5.8}$$

Finally Choose $\hat{b} = \max\{b_1, b_2, b_3\}$, and combine (5.6), (5.5) and (5.8), we have proved the estimate. □

The result of Lemma 6 can be improved to the following pointwise estimate by the mean valued inequality.

Lemma 7 *Let $(\boldsymbol{H}^n, J, \theta)$ be the $(2n+1)$-dimensional Heisenberg group. If $u(x,t)$ is the positive solution of the CR heat equation (1.2) on $\boldsymbol{H}^n \times [0,\infty)$. For $t > \delta$, there exists $\tilde{b} > 0$ such that*

$$\begin{aligned} \left\|\nabla_b u\right\|^2(x,t) &\leq \exp\left(\tilde{b}\left(r^2+1\right)\right) \\ \left\|u_{\alpha\bar{\beta}} + u_{\bar{\beta}\alpha}\right\|^2(x,t) &\leq \exp\left(\tilde{b}\left(r^2+1\right)\right). \end{aligned} \tag{5.9}$$

Proof We denote $\Phi = \|\nabla_b u\|^2 + u_0^2 + u^2$. It follows from (5.7) that Φ is a subsolution of the CR heat equation. We multiple factor $e^{-b(\rho^2+1)}$ on both sides of the mean value inequality (4.17), we have

$$\begin{aligned} & e^{-b(\rho^2+1)} \sup_{B_p((1-\delta)\rho)\times[\tau,T]} \Phi(x,t) \\ & \leq Ce^{-b(\rho^2+1)} \int_{(1-\eta)\tau}^{T}\int_{B_p(\rho)} \Phi(y,s)\,dyds \\ & \leq C\int_{(1-\eta)\tau}^{T}\int_{B_p(\rho)} e^{-b(r^2(y)+1)}\Phi(y,s)\,dyds \\ & < \infty, \end{aligned}$$

where $r(y)$ is the Carnot–Carathéodory distance between p and y. The last inequality is followed from Lemma 4 and Lemma 6. Now we substitute $\rho = \frac{1}{1-\delta}r(x)$, we have for any $x \in B_p\left(\frac{1}{1-\delta}r(x)\right)$, $\tau < t < T$,

$$\Phi(x,t) \leq C' e^{b\left(\frac{1}{1-\delta}\right)^2(r^2(x)+1)}.$$

The other inequality in (5.9) can be proved similarly. □

Lemma 8 *Let $(\boldsymbol{H}^n, J, \theta)$ be the standard $(2n+1)$-dimensional Heisenberg group and φ be a smooth function on $\boldsymbol{H}^n$ such that*

$$\exp\left(k_1\left(r^2+1\right)\right) \leq \varphi \leq \exp\left(k_2\left(r^2+1\right)\right)$$

for some constant $k_2 > k_1 > 0$, then there exists $T_m > 0$ depending only on k_2 such that the Cauchy problem

$$\begin{cases} \left(\frac{\partial}{\partial t} - \Delta_b\right) g = 0 \\ g\left(x, 0\right) = \varphi \end{cases}$$

has a solution g on $\boldsymbol{H}^n \times [0, T]$. Moreover, there exist constants $C_1, C_2 > 0$ such that

$$C_1 \exp\left(\frac{k_1}{4} r^2\right) \leq g\left(x, t\right) \leq C_2 \exp\left(3k_2 r^2\right)$$

on $\boldsymbol{H}^n \times [0, T_m]$.

Proof Similar argument as in Lemma 1.1 in [41], where the proof only using the heat kernel estimate (4.16) and the sub-Laplacian comparison property (4.12). □

Proof of Theorem 3 It follows from Lemma 8 with $\phi = e^{\frac{\kappa}{\delta}t} g$ for $t > \delta$, we have

$$\left(\frac{\partial}{\partial t} - \Delta_b\right)\phi = \frac{\kappa}{\delta}\phi$$

and

$$\phi\left(x, t\right) \geq C_1 \exp\left(2\tilde{b}\left(r^2+1\right)\right)$$

for a positive constant C_1 and a positive constant κ which needs to be determined later.

Let $N_{\alpha\bar{\beta}}$ be the matrix Harnack quantity in (3.1) We consider the following $(1, 1)$-tensor

$$\hat{N}_{\alpha\bar{\beta}} = t^2 N_{\alpha\bar{\beta}} + \varepsilon\phi h_{\alpha\bar{\beta}}. \tag{5.10}$$

We only need to prove that $\hat{N}_{\alpha\bar{\beta}} > 0$ for any $\varepsilon > 0$. We shall prove this by contradiction. Suppose it is not true, then by the growth rate of ϕ and the fact that $N_{\alpha\bar{\beta}} > 0$ at $t = 0$, there exists a first time t_0 and by Lemma 7, a point $x_0 \in \boldsymbol{H}^n$ and a unit vector v at x_0 such that $\hat{N}_{\alpha\bar{\beta}}\left(x_0, t_0\right) v^\alpha v^{\bar{\beta}} = 0$. Now we choose a normal coordinate around x_0 and extend v to a local unit vector field near x_0. Then at x_0

$$\Delta_b\left(\hat{N}_{\alpha\bar{\beta}} v^\alpha v^{\bar{\beta}}\right) = \Delta_b\left(\hat{N}_{\alpha\bar{\beta}}\right) v^\alpha v^{\bar{\beta}}.$$

Since $\hat{N}_{\alpha\bar{\beta}}v^{\alpha}v^{\bar{\beta}} \geq 0$ for all (x, t) with $t \leq t_0$ and x close to x_0, we see that at (x_0, t_0),

$$0 \geq \left(\frac{\partial}{\partial t} - \Delta_b\right)(\hat{N}_{\alpha\bar{\beta}}v^{\alpha}v^{\bar{\beta}}). \tag{5.11}$$

On the other hand, (3.10) implies, at (x_0, t_0)

$$\begin{aligned}
&\left(\frac{\partial}{\partial t} - \Delta_b\right)\hat{N}_{\alpha\bar{\beta}}v^{\alpha}v^{\bar{\beta}} \\
&\quad = \left(\left(\frac{\partial}{\partial t} - \Delta_b\right)\hat{N}_{\alpha\bar{\beta}}\right)v^{\alpha}v^{\bar{\beta}} \\
&\quad \geq t^2\left(2R_{\alpha\bar{\gamma}\delta\bar{\beta}}N_{\gamma\bar{\delta}} - R_{\alpha\bar{\sigma}}N_{\sigma\bar{\beta}} - R_{\sigma\bar{\beta}}N_{\alpha\bar{\sigma}} + C_{\alpha\bar{\beta}}\right)v^{\alpha}v^{\bar{\beta}} \\
&\qquad + t^2\,(Rm - Tor)\left(\frac{\nabla_b u}{\sqrt{u}}, v\right) + t^2\frac{1}{2u}N_{\alpha\bar{\gamma}}N_{\beta\bar{\gamma}}v^{\alpha}v^{\bar{\beta}} \\
&\qquad + t^2\left(\frac{u_{\bar{\beta}}u_{\gamma}}{8u^2}\hat{N}_{\alpha\bar{\gamma}} + \frac{u_{\alpha}u_{\bar{\gamma}}}{8u^2}\hat{N}_{\gamma\bar{\beta}} - \frac{1}{2u^2}u_{\gamma}u_{\bar{\beta}}\hat{N}_{\alpha\bar{\gamma}} - \frac{1}{2u^2}u_{\bar{\gamma}}u_{\alpha}\hat{N}_{\gamma\bar{\beta}}\right)v^{\alpha}v^{\bar{\beta}} \\
&\qquad + \frac{3}{4}\frac{\kappa}{\delta}t^2\varepsilon\phi\frac{u_{\bar{\beta}}u_{\gamma}v^{\gamma}v^{\bar{\beta}}}{u^2} + t^2\frac{F}{u}N_{\alpha\bar{\beta}}v^{\alpha}v^{\bar{\beta}} + \varepsilon\frac{\kappa}{\delta}\phi\,|v|^2.
\end{aligned} \tag{5.12}$$

Since $\hat{N}_{\alpha\bar{\beta}}\,(x_0, t_0)\,v^{\alpha}v^{\bar{\beta}} = 0$, it follows from (5.10) that at (x_0, t_0)

$$t^2\frac{1}{u}FN_{\alpha\bar{\beta}}v^{\alpha}v^{\bar{\beta}} = -\frac{F}{u}\varepsilon\phi\,|v|^2.$$

Now $\frac{F}{u} = \frac{t}{24}\frac{(u_0)^2}{u^2}$ and (6.20) yield

$$t^2\frac{1}{u}FN_{\alpha\bar{\beta}}v^{\alpha}v^{\bar{\beta}} \geq -\frac{C}{t}\varepsilon\phi\,|v|^2 \geq -\frac{C}{\delta}\varepsilon\phi\,|v|^2$$

for some constant C. Hence

$$t^2\frac{1}{u}FN_{\alpha\bar{\beta}}v^{\alpha}v^{\bar{\beta}} + \varepsilon\frac{\kappa}{\delta}\phi\,|v|^2 \geq \left(\kappa - \frac{C}{\delta}\right)\varepsilon\phi\,|v|^2 > 0$$

if we choose

$$\kappa > \frac{C}{\delta}.$$

That is $\left(\frac{\partial}{\partial t} - \Delta_b\right)\hat{N}_{\alpha\bar{\beta}}v^{\alpha}v^{\bar{\beta}} > 0$. This contradicts to (5.11).

This shows that $\hat{N}_{\alpha\bar{\beta}} \geq 0$ for all $0 < \delta \leq t \leq 2 - \delta$. Taking $\varepsilon \to 0$ and $\delta \to 0$ and repeating the argument to the later time, we prove the lemma. □

Proof of Corollary 3 Applying Theorem 3 to the heat kernel $H(x, y, t)$ with $V = -\frac{\nabla_b H}{H}$, we have

$$-t\left[(\log H(x,y,t))_{\alpha\overline{\beta}} + (\log H(x,y,t))_{\overline{\beta}\alpha}\right] - \frac{3}{2}t\left[(\log H(x,y,t))_{\alpha}(\log H(x,y,t))_{\overline{\beta}}\right] \leq 4h_{\alpha\overline{\beta}}.$$

But $-t\log H(x, o, t) \to \frac{1}{4}r^2(x)$ as $t \to 0$. Therefore

$$-t\left[(\log H(x,o,t))_{\alpha\overline{\beta}} + (\log H(x,o,t))_{\overline{\beta}\alpha}\right] \to \frac{1}{4}\left[(r^2(x))_{\alpha\overline{\beta}} + (r^2(x))_{\overline{\beta}\alpha}\right]$$

in the sense of distribution. On the other hand,

$$\frac{3}{2}t|\nabla_b(\log H(x,o,t)|^2 \leq C_0$$

for some constant C_0 in a Heisenberg group $\boldsymbol{H}^n$ due to the dilation δ_r in $\boldsymbol{H}^n$ as in [27, Theorem 1]. Therefore,

$$\left[(r^2(x))_{\alpha\overline{\beta}} + (r^2(x))_{\overline{\beta}\alpha}\right] \leq (16 + C_0)h_{\alpha\overline{\beta}}(x).$$

□

6 The T-derivative of heat kernel of the sub-Laplacian in Heisenberg groups

6.1 The Heisenberg group

We start with the most general definition of the Heisenberg group. In the end, what we need is the special case of $n = 1$. The non-isotropic Heisenberg group $\boldsymbol{H}^n$ is the Lie group with underlying manifold

$$\mathbb{C}^n \times \mathbb{R} = \{[\mathbf{z}, t] : \mathbf{z} \in \mathbb{C}^n,\ t \in \mathbb{R}\}$$

and multiplication law

$$[\mathbf{z}, t] \cdot [\mathbf{w}, s] = \left[\mathbf{z} + \mathbf{w}, t + s + 2\mathrm{Im}\sum_{j=1}^{n} a_j z_j \bar{w}_j\right], \tag{6.1}$$

where $\mathbf{a} = (a_1, a_2, \ldots, a_n) \in \mathbb{R}^n_+$.

It is easy to check that the multiplication (6.1) does indeed make $\mathbb{C}^n \times \mathbb{R}$ into a group whose identity is the origin $e = [\mathbf{0}, 0]$, and where the inverse is given by $[\mathbf{z}, t]^{-1} = [-\mathbf{z}, -t]$.

The Lie algebra of $\boldsymbol{H}^n$ is a vector space which, together with a Lie bracket operation defined on it, represents the infinitesimal action of $\boldsymbol{H}^n$. Let $\mathfrak{h}_n$ denote the vector space of left-invariant vector fields on $\boldsymbol{H}^n$. Note that this linear space is closed with respect to the bracket operation

$$[\mathbf{V}_1, \mathbf{V}_2] = \mathbf{V}_1\mathbf{V}_2 - \mathbf{V}_2\mathbf{V}_1.$$

The space $\mathfrak{h}_n$, equipped with this bracket, is referred to as the Lie algebra of $\boldsymbol{H}^n$. Lie algebra structure of $\mathfrak{h}_n$ is most readily understood by describing it in terms of the following basis:

$$\mathbf{X}_j = \frac{\partial}{\partial x_j} + 2a_j y_j \frac{\partial}{\partial t}, \quad \mathbf{Y}_j = \frac{\partial}{\partial y_j} - 2a_j x_j \frac{\partial}{\partial t} \quad \text{and} \quad \mathbf{T} = \frac{\partial}{\partial t}; \tag{6.2}$$

where $j = 1, 2, \ldots, n$, $\mathbf{z} = (z_1, z_2, \ldots, z_n) \in \mathbb{C}^n$ with $z_j = x_j + iy_j$; $t \in \mathbb{R}$.

Note that we have the commutation relations

$$[\mathbf{Y}_j, \mathbf{X}_k] = 4a_j\delta_{jk}\mathbf{T} \quad \text{for} \quad j,\ k = 1, 2, \ldots, n. \tag{6.3}$$

Next, we define the complex vector fields

$$\begin{aligned} \bar{\mathbf{Z}}_j &= \frac{1}{2}(\mathbf{X}_j + i\mathbf{Y}_j) = \frac{\partial}{\partial \bar{z}_j} - ia_j z_j \frac{\partial}{\partial t} \quad \text{and} \\ \mathbf{Z}_j &= \frac{1}{2}(\mathbf{X}_j - i\mathbf{Y}_j) = \frac{\partial}{\partial z_j} + ia_j \bar{z}_j \frac{\partial}{\partial t} \end{aligned} \tag{6.4}$$

for $j = 1, 2, \ldots, n$. Here, as usual,

$$\frac{\partial}{\partial z_j} = \frac{1}{2}\left(\frac{\partial}{\partial x_j} - i\frac{\partial}{\partial y_j}\right) \quad \text{and} \quad \frac{\partial}{\partial \bar{z}_j} = \frac{1}{2}\left(\frac{\partial}{\partial x_j} + i\frac{\partial}{\partial y_j}\right).$$

The commutation relations (6.3) then become

$$[\bar{\mathbf{Z}}_j, \mathbf{Z}_k] = 2ia_j\delta_{jk}\mathbf{T}$$

with all other commutators among the $\mathbf{Z}_j$, $\bar{\mathbf{Z}}_k$ and $\mathbf{T}$ vanishing.

The Heisenberg sub-Laplacian is the differential operator

$$\mathfrak{L}_{\mathbf{a},\lambda} = -\frac{1}{2}\sum_{j=1}^{n}(\mathbf{Z}_j\bar{\mathbf{Z}}_j + \bar{\mathbf{Z}}_j\mathbf{Z}_j) + i\lambda\mathbf{T} = -\frac{1}{4}\sum_{j=1}^{n}(\mathbf{X}_j^2 + \mathbf{Y}_j^2) + i\lambda\mathbf{T} \tag{6.5}$$

with $\mathbf{Z}_j$ and $\bar{\mathbf{Z}}_j$ given by (6.4). In the case of $a_j = 1$ for all j's, the operator $\mathfrak{L}_\lambda$ was first introduced by Folland‘ and Stein [18] in the study of $\bar{\partial}_b$ complex on a non-degenerate CR manifold. They found the fundamental solution of $\mathfrak{L}_\lambda$. Beals and Greiner [4] solved the case that a_j's may be different.

Let functions $f,\ g \in \mathcal{S}(\boldsymbol{H}^n)$, the Heisenberg convolution is given by

$$f * g(\mathbf{x}) = \int_{\boldsymbol{H}^n} f(\mathbf{y}) g(\mathbf{y}^{-1}\mathbf{x}) dV(\mathbf{y}); \tag{6.6}$$

here $dV(\mathbf{y})$ is the Haar measure on $\boldsymbol{H}^n$ and is exactly the Euclidean measure on $\mathbb{R}^{2n+1}$.

Twisted Convolution. We focus our attention on the phase space $\mathbb{R}^n \times \mathbb{R}^n$, which we identify with $\mathbb{C}^n$ via $\zeta \in \mathbb{C}^n,\ \zeta = u + iv \leftrightarrow (\mathbf{u}, \mathbf{v}) \in \mathbb{R}^n \times \mathbb{R}^n$.

On it, we consider the symplectic form $\langle \cdot, \cdot \rangle$ given by the Heisenberg group multiplication law (6.1) and defined by

$$\langle \mathbf{z}, \mathbf{w} \rangle = 2\mathrm{Im}(A\mathbf{z} \cdot \bar{\mathbf{w}}) = 2\mathrm{Im}\left(\sum_{j=1}^{n} a_j z_j \bar{w}_j \right),$$

where $\mathbf{z},\ \mathbf{w} \in \mathbb{C}^n$. With τ a fixed real constant, we can define the *twisted convolution* of two functions F and G by

$$(F *_\tau G)(\mathbf{z}) = \int_{\mathbb{C}^n} e^{-i\tau \langle \mathbf{z}, \mathbf{w} \rangle} F(\mathbf{z} - \mathbf{w}) G(\mathbf{w}) d\mathbf{w}; \tag{6.7}$$

here $d\mathbf{w}$ is the Euclidean measure on $\mathbb{C}^n$. Notice that, in view of the antisymmetry of $\langle \cdot, \cdot \rangle$, we have that $\langle \mathbf{z} - \mathbf{w}, \mathbf{w} \rangle = -\langle \mathbf{w}, \mathbf{z} \rangle$; thus

$$G *_\tau F = F *_{-\tau} G,$$

so the twisted convolution is not commutative.

The twisted convolution arises when we analyze the convolution of functions on the Heisenberg group in terms of the Fourier transform in the t-variable. To see this, let $f(\mathbf{z}, t)$ be a test function on $\boldsymbol{H}^n$. Define

$$\widetilde{f}_\tau(\mathbf{z}) = f(\mathbf{z}, \cdot)\hat{\ }(\tau) = \int_{\mathbb{R}} f(\mathbf{z}, t) e^{-i\tau t} dt. \tag{6.8}$$

Similarly define $\widetilde{g}_\tau$ when g is another test function on $\boldsymbol{H}^n$. Suppose $f * g$ is the convolution of f and g on $\boldsymbol{H}^n$. Then

$$\widetilde{(f * g)}_\tau = \widetilde{f}_\tau *_\tau \widetilde{g}_\tau. \tag{6.9}$$

Integration by parts also yields

$$\widetilde{\left(\frac{\partial f}{\partial t} \right)} = \int_{\mathbb{R}} e^{-it\cdot\tau} \frac{\partial f}{\partial t} dt = i\tau \widetilde{f} \tag{6.10}$$

We take the partial Fourier transform of the complex vector fields Z_j and $\bar{Z}_j$ with respect to t and obtain

$$\widetilde{Z}_j = \frac{\partial}{\partial z_j} - a_j \bar{z}_j \tau \quad \text{and} \quad \widetilde{\bar{Z}}_j = \frac{\partial}{\partial \bar{z}_j} + a_j z_j \tau.$$

The fundamental solution and heat kernel of $\mathfrak{L}_{\mathbf{a},\lambda}$ can be derived via the Laguerre calculus. Here we give the basic definitions of Laguerre functions.

Laguerre Functions. The generalized Laguerre polynomials $L_k^{(\alpha)}(x)$ are defined by their usual generating function formula:

$$\sum_{k=1}^{\infty} L_k^{(\alpha)}(x) w^k = \frac{1}{(1-w)^{\alpha+1}} \exp\left\{-\frac{xw}{1-w}\right\}, \tag{6.11}$$

for $\alpha = 0, 1, 2, \ldots,\ x \geq 0$, and $|w| < 1$.

Definition 2 Let $z = |z|e^{i\theta}$ and $k,\ p = 0, 1, 2, \ldots$. Then we define

$$\begin{aligned} &\widetilde{\mathcal{W}}_k^{(p)}(z, \tau) \\ &= \frac{2|\tau|}{\pi} \left[\frac{\Gamma(k+1)}{\Gamma(k+p+1)}\right]^{1/2} (2|\tau||z|^2)^{p/2} e^{ip\theta} e^{-|\tau||z|^2} L_k^{(p)}(2|\tau||z|^2) \end{aligned} \tag{6.12}$$

$$\begin{aligned} &\widetilde{\mathcal{W}}_k^{(-p)}(z, \tau) \\ &= \frac{2|\tau|}{\pi} (-1)^p \left[\frac{\Gamma(k+1)}{\Gamma(k+p+1)}\right]^{1/2} (2|\tau||z|^2)^{p/2} e^{-ip\theta} e^{-|\tau||z|^2} L_k^{(p)}(2|\tau||z|^2) \end{aligned} \tag{6.13}$$

We define the n-dimensional version of the exponential Laguerre functions on $\boldsymbol{H}^n$ by the n-fold product:

$$\widetilde{\mathcal{W}}_{\mathbf{k}}^{(\mathbf{p})}(\mathbf{z}, \tau) = \prod_{j=1}^{n} a_j \widetilde{\mathcal{W}}_{k_j}^{(p_j)}(\sqrt{a_j} z_j, \tau)$$

where $\widetilde{\mathcal{W}}_{k_j}^{(p_j)}(\sqrt{a_j} z_j, \tau)$'s are given by (6.12) and (6.13).

6.2 The fundamental solution of $\mathfrak{L}_{a,\lambda}$

Let $\mathbf{K}_\lambda(\mathbf{z}, t) \in C^\infty(\boldsymbol{H}^n \backslash \{0\})$ be the fundamental solution of $\mathfrak{L}_{\mathbf{a},\lambda}$, i.e.,

$$\mathfrak{L}_{\mathbf{a},\lambda}[f(\mathbf{z}, t) * \mathbf{K}_\lambda] = \mathfrak{L}_{\mathbf{a},\lambda} \left[\int_{\boldsymbol{H}^n} f(\mathbf{w}, s) \mathbf{K}_\lambda([\mathbf{w}, s]^{-1}[\mathbf{z}, t]) d\mathbf{w} ds\right] = f(\mathbf{z}, t)$$

for any $f \in \mathcal{S}(\boldsymbol{H}^n)$. The result from Laguerre calculus (see [5,21]) yields that

$$\widetilde{\mathbf{K}}_\lambda(\mathbf{z},\tau) = |\tau|^{-1}\sum_{|\mathbf{k}|=0}^{\infty}\left(\sum_{j=1}^{n}(2k_j+1)a_j - \lambda\,\mathrm{sgn}(\tau)\right)^{-1}\prod_{j=1}^{n} a_j\widetilde{\mathcal{W}}_{k_j}^{(0)}(\sqrt{a_j}z_j,\tau). \tag{6.14}$$

We can apply the generating formula of Laguerre function to compute the sum in the right hand side. First we introduce the following integral representation of A^{-1}:

$$\frac{1}{A} = \int_0^\infty e^{-As}ds \quad \text{for} \quad \mathrm{Re}(A) > 0.$$

Then we can write (6.14) in the following form:

$$\widetilde{\mathbf{K}}_\lambda(\mathbf{z},\tau) = \frac{1}{|\tau|}\sum_{|\mathbf{k}|=0}^{\infty}\int_0^\infty e^{-\left(\sum_{j=1}^{n}(2k_j+1)a_j-\lambda\mathrm{sgn}(\tau)\right)s}ds\prod_{j=1}^{n} a_j\widetilde{\mathcal{W}}_{k_j}^{(0)}(\sqrt{a_j}z_j,\tau).$$

Next we interchange the summation and integration, and use the definitions of $\widetilde{\mathcal{W}}_{k_j}^{(0)}$,

$$\begin{aligned}
\widetilde{\mathbf{K}}_\lambda(\mathbf{z},\tau) &= \int_0^\infty\sum_{|\mathbf{k}|=0}^{\infty} e^{-\left(\sum_{j=1}^{n}(2k_j+1)a_j-\lambda\mathrm{sgn}(\tau)\right)s}ds\prod_{j=1}^{n} a_j\widetilde{\mathcal{W}}_{k_j}^{(0)}(\sqrt{a_j}z_j,\tau)\\
&= \frac{1}{|\tau|}\int_0^\infty\sum_{|\mathbf{k}|=0}^{\infty} e^{-\left(\sum_{j=1}^{n}(2k_j+1)a_j-\lambda\mathrm{sgn}(\tau)\right)s}ds\prod_{j=1}^{n} 2a_je^{-a_j|\tau||z_j|^2}L_{k_j}^{(0)}(2a_j|\tau||z_j|^2)\\
&= \frac{|\tau|^{n-1}}{\pi^n}\int_0^\infty e^{\lambda\mathrm{sgn}(\tau)s}\prod_{j=1}^{n}2a_je^{-a_js-a_j|\tau||z_j|^2}\sum_{k_j=0}^{\infty}(e^{-2a_js})^{k_j}L_{k_j}^{(0)}(2a_j|\tau||z_j|^2)ds
\end{aligned}$$

Apply the generating formula for the Laguerre polynomials

$$\sum_{k=0}^{\infty}L_k^{(p)}(x)z^k = \frac{1}{(1-z)^{p+1}}\exp\left\{-\frac{xz}{1-z}\right\}$$

to the last formula for $\widetilde{\mathbf{K}}(\mathbf{z},\tau)$, we obtain

$$\widetilde{\mathbf{K}}_\lambda(\mathbf{z},\tau) = \frac{|\tau|^{n-1}}{\pi^n}\int_0^\infty e^{\lambda \mathrm{sgn}(\tau)s}\prod_{j=1}^n \frac{2a_j e^{-a_j s}}{1-e^{-2a_j s}}\exp\left\{-a_j|\tau||z_j|^2\left[1+\frac{2e^{-2a_j s}}{1-e^{-2a_j s}}\right]\right\} ds$$
$$= \frac{|\tau|^{n-1}}{\pi^n}\int_0^\infty e^{\lambda \mathrm{sgn}(\tau)s}\prod_{j=1}^n \frac{a_j}{\sinh(a_j s)}\exp\left\{-|\tau|\sum_{j=1}^n a_j|z_j|^2\coth(a_j s)\right\} ds$$

Then one can take the inverse Fourier transform and find the fundamental solution $\mathbf{K}_\lambda(\mathbf{z}, t)$ at the origin and other points by translation via the group law.

6.3 The Heat Kernel

In the isotropic case, the heat kernel was independently studied by Gaveau [19] via probability method and Hulanicki [26] using the Fourier transform on $\boldsymbol{H}^n$ and the basis of Laguerre functions. Later, Beals and Greiner [4] solved the general case by a different method. $h_s(\mathbf{z}, t)$ can be derived easily via the Laguerre calculus.

Taking the Fourier transform with respect to the t-variable, we can write the Fourier transform of the heat kernel $\widetilde{h}_s(\mathbf{z}, t)$ as

$$\begin{aligned}\widetilde{h}_s(\mathbf{z},\tau) &= \exp\left\{-s\widetilde{\mathfrak{L}}_{\mathbf{a},\lambda}\right\}\widetilde{\mathbf{I}} = \sum_{|\mathbf{k}|=0}^\infty \exp\{-s\widetilde{\mathfrak{L}}_{\mathbf{a},\lambda}\}\left[\prod_{j=1}^n a_j\widetilde{\mathcal{W}}^{(0)}_{k_j}(\sqrt{a_j}z_j,\tau)\right]\\ &= \sum_{|\mathbf{k}|=0}^\infty e^{-s\sum_{j=1}^n a_j|\tau|(2k_j+1)+s\lambda\tau}\prod_{j=1}^n a_j\widetilde{\mathcal{W}}^{(0)}_{k_j}(\sqrt{a_j}z_j,\tau).\end{aligned}$$

Next, a similar computation as in the computation of the fundamental solution leads to

$$\widetilde{h}_s(\mathbf{z},\tau) = \frac{e^{\lambda\tau s}}{\pi^n}\left[\prod_{j=1}^n\frac{a_j|\tau|}{\sinh(a_j|\tau|s)}\right]\exp\left\{-|\tau|\sum_{j=1}^n a_j|z_j|^2\coth(a_j|\tau|s)\right\}. \tag{6.15}$$

Since

$$\prod_{j=1}^n\frac{a_j|\tau|}{\sinh(a_j|\tau|s)} = \prod_{j=1}^n\frac{a_j\tau}{\sinh(a_j\tau s)} \quad \text{and} \quad |\tau|\coth(a_j|\tau|s) = \tau\coth(a_j\tau s),$$

we can simplify (6.15) by removing the absolute sign for τ and have

$$\widetilde{h}_s(\mathbf{z},\tau) = \frac{e^{\lambda\tau s}}{\pi^n}\left[\prod_{j=1}^n\frac{a_j\tau}{\sinh(a_j\tau s)}\right]\exp\left\{-\tau\sum_{j=1}^n a_j|z_j|^2\coth(a_j\tau s)\right\}. \tag{6.16}$$

Taking the inverse Fourier transform, we can get the heat kernel

$$h_s(\mathbf{z}, t) = \frac{1}{2\pi^{n+1}} \int_{-\infty}^{\infty} \left[\prod_{j=1}^{n} \frac{a_j \tau}{\sinh(a_j \tau s)} \right] e^{it\tau + \lambda\tau s - \sum_{j=1}^{n} \frac{a_j \tau}{\tanh(a_j \tau s)} |z_j|^2} d\tau.$$

We substitute the variable τ by τ/s in the integral and obtain

$$h_s(\mathbf{z}, t) = \frac{1}{2(\pi s)^{n+1}} \int_{-\infty}^{\infty} \left[\prod_{j=1}^{n} \frac{a_j \tau}{\sinh(a_j \tau)} \right] e^{\frac{it\tau}{s} + \lambda\tau - \frac{1}{s} \sum_{j=1}^{n} \frac{a_j \tau}{\tanh(a_j \tau)} |z_j|^2} d\tau. \tag{6.17}$$

We are interested in the case of $n = 1$ and $\lambda = 0$, and the estimates of the derivative of the heat kernel along the Reed vector field $\frac{\partial}{\partial t}$. In this case, we set $a_1 = a$, $n = 1$ and $\lambda = 1$ in (6.17) and the heat kernel have the form:

$$h_s(z, t) = \frac{1}{2(\pi s)^2} \int_{-\infty}^{\infty} \frac{a\tau}{\sinh(a\tau)} \exp\left\{ -\frac{\tau}{s} \left[\frac{a}{\tanh(a\tau)} |z|^2 - it \right] \right\} d\tau. \tag{6.18}$$

Take the derivative of the heat kernel with respect to t, we have

$$\left(\frac{\partial}{\partial t}\right)^m h_s(z, t) = \frac{i^m}{2\pi^2 s^{m+2}} \int_{-\infty}^{\infty} \frac{a\tau^{m+1}}{\sinh(a\tau)} \exp\left\{ -\frac{\tau}{s} \left[\frac{a}{\tanh(a\tau)} |z|^2 - it \right] \right\} d\tau.$$

First the following simple estimates:

$$1 \le \frac{\tau}{\tanh \tau} \le c(1 + |\tau|) \quad \text{and} \quad 0 \le \frac{\tau}{\sinh \tau} \le c(1 + |\tau|)e^{-|\tau|}$$

imply

$$\left| \left(\frac{\partial}{\partial t}\right)^m h_s(z, t) \right| \le \frac{c}{2\pi^2 s^{m+2}} \int_{-\infty}^{\infty} (1 + a|\tau|)|\tau|^m e^{-a|\tau|} \exp\left\{ -\frac{|z|^2}{s} \right\} d\tau$$
$$\le \frac{K_m}{2\pi^2 s^{m+2}} e^{-\frac{|z|^2}{s}}$$

for $K_m = \int_{-\infty}^{\infty} (1 + a|\tau|)|\tau|^m e^{-a|\tau|} d\tau$ when $z \neq 0$. Here c is a constant. This implies the integral is absolutely convergent when $z \neq 0$. In the case of $z = 0$, we need to change the contour of the integral.

In order to get some better estimates, we need to introduce the Carnot–Caratheodory distance. We first introduce two following function to simplify the notations:

$$f(z, t, \tau) = \frac{a\tau}{\tanh(a\tau)} |z|^2 - it\tau \quad \text{and} \quad v(\tau) = \frac{a\tau}{\sinh(a\tau)}.$$

Then the unique critical point of $f(z,t,\tau)$ as a function of τ in the strip $\{|\Im m\tau| < \pi/a\}$ is the point $\tau_c = i\theta_c(z,t)$, where θ_c is the solution of

$$t = a|z|^2\mu(a\theta), \quad \text{here} \quad \mu(\phi) = \frac{\phi}{\sin^2\phi} - \cot\phi.$$

The Carnot-Caratheodory distance $d(z,t)$ between $(0,0)$ and (z,t) and the value of $f(z,t,\tau_c)$ has the relation

$$f(z,t,\tau_c) = \frac{1}{2}d^2(z,t) = \nu(a\theta_c)\left(\frac{|t|}{a} + |z|^2\right) \quad \text{with} \quad \nu(\phi) = \frac{\phi^2}{\phi + \sin^2\phi - \sin\phi\cos\phi}.$$

Then the heat kernel satisfies the upper estimate [3]:

$$h_s(z,t) \le \frac{C}{s^2}e^{-d(z,t)^2/2s}\min\left\{1, \left(\frac{u}{|z|^2 d(z,t)}\right)^{\frac{1}{2}}\right\}, \quad (z,t,s) \in \boldsymbol{H}^1 \times \mathbb{R}_+ \tag{6.19}$$

The heat kernel also satisfies:

$$h_s(z,t) = C\frac{e^{-d(z,t)^2/2s}}{s^2}\left\{\left(\frac{2\pi s}{f''(i\theta_c)}\right)^{1/2} v(i\theta_c) + O(\sqrt{s}e^{-c/sqrts}) + O(s)\right\}$$

where $f''(i\theta_c) = \frac{\partial^2 f}{\partial\tau^2}|_{\tau=i\theta_c}$. Combine these two estimates, we have

$$\frac{C_1}{s^2}e^{-d(z,t)^2/2s} \le h_s(z,t) \le \frac{C_2}{s^2}e^{-d(z,t)^2/2s}$$

Then we can apply the same method to derive the upper estimate of the derivative of the heat kernel and get

$$\left|\left(\frac{\partial}{\partial t}\right)^m h_s(z,t)\right| \le \frac{C_3}{s^{m+2}}e^{-d(z,t)^2/2s}$$

We want to bound the derivative of the heat kernel by the heat kernel when s is large, i.e., we want to find $M > 0$ so that

$$\left|\left(\frac{\partial}{\partial t}\right)^m h_s(z,t)\right| \le M h_s(z,t).$$

It suffices that

$$\frac{C_3}{s^{m+2}}e^{-d(z,t)^2/2s} \le M\frac{C_1}{s^2}e^{-d(z,t)^2/2s} \quad \text{this implies} \quad M \ge \frac{C_3}{C_2 s^m}.$$

Hence, if we fix $s > 0$ and take $M \geq \frac{C_3}{C_2 s^m}$, then we will have

$$\left|\left(\frac{\partial}{\partial t}\right)^m h_s(z,t)\right| \leq M h_s(z,t) \tag{6.20}$$

In the case of $z = 0$, the integral in the heat kernel can be computed explicitly and has been done in [3]. In this case, we assume that $s > 0$ and

$$h_t(0,s) = \frac{1}{4at^2}\frac{e^{-\pi s/2at}}{(1+e^{-\pi s/2at})^2} = \frac{1}{4at^2}e^{-\pi s/2at}\{1 + O(e^{-\pi s/2at})\}.$$

In this case $d(0,s)^2 = \pi|s|/2$. So the upper estimate (6.19) also holds in this case.

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