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LI-YAU GRADIENT ESTIMATE AND ENTROPY FORMULAE FOR THE CR HEAT EQUATION IN A CLOSED PSEUDOHERMITIAN 3-MANIFOLD

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Abstract

In this paper, we derive two subgradient estimates of the CR heat equation in a closed pseudohermitian 3-manifold which are served as the CR version of the Li-Yau gradient estimate. With its applications, we first get a subgradient estimate of the logarithm of the positive solution of the CR heat equation. Secondly, we have the Harnack inequality and upper bound estimate for the heat kernel. Finally, we obtain Perelman-type entropy formulae for the CR heat equation.

1. Introduction

In the seminal paper of [**LY**], P. Li and S.-T. Yau established the parabolic Li-Yau gradient estimate and Harnack inequality for the positive solution of the heat equation in a complete Riemannian m-manifold with nonnegative Ricci curvature. Recently, G. Perelman ([**Pe1**]) derived the remarkable entropy formula, which is important in the study of Ricci flow. The derivation of the entropy formula resembles Li-Yau gradient estimate for the heat equation. All these eventually lead to the solution of Poincaré conjecture and Thurston geometrization conjecture in a 3-manifold by the Ricci flow due to R. S. Hamilton ([**H1**], [**H2**], [**H3**], [**H4**]) and G. Perelman ([**Pe1**], [**Pe2**], [**Pe3**]).

In this paper, we derive corresponding estimates in a closed pseudohermitian 3-manifold (M, J, θ) (see next section for definition). More precisely, there is a corresponding CR geometrization problem in a contact 3-manifold via the torsion flow (1.7). Then it is important for us to derive the CR Li-Yau type gradient estimate as well as the CR Perelman-type entropy formula for the CR heat equation (1.1)

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

on $M \times [0,\ \infty)$. Here Δ_b is the sub-Laplacian in a closed pseudohermitian 3-manifold (M, J, θ).

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Along this line with the method of gradient estimate, it is the very first paper of H.-D. Cao and S.-T. Yau ([**CY**]) to consider the heat equation

$$(L-\frac{\partial}{\partial t})u\,(x,t)=0 \tag{1.2}$$

in a closed m-manifold with a positive measure and an operator with respect to the sum of squares of vector fields

$$L=\sum_{i=1}^{l}X_i^2,\quad l\leq m,$$

where $X_1,\ X_2,\ldots,X_l$ are smooth vector fields that satisfy Hörmander's condition: the vector fields together with their commutators up to 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 $X_1,\ X_2,\ldots,X_l$ and their brackets $[X_1,X_2],\ldots,[X_{l-1},X_l]$. They showed that for the positive solution $u(x,t)$ of (1.2) on $M\times[0,\infty)$, there exist constants C',C'',C''' and $\frac{1}{2}<\lambda<\frac{2}{3}$, such that for any $\delta>1$, $f(x,t)=\ln u\,(x,t)$ satisfies the following gradient estimate:

$$\sum_i|X_if|^2-\delta f_t+\sum_\alpha(1+|Y_\alpha f|^2)^\lambda\leq\frac{C'}{t}+C''\;+C'''t^{\frac{\lambda}{\lambda-1}} \tag{1.3}$$

with $\{Y_\alpha\}=\{[X_i,X_j]\}$.

We first compare Cao-Yau's notations with ours. Let J be a CR structure compatible with the contact bundle $\xi=\ker\theta$ and $\mathbf{T}$ be the Reeb vector field of the contact form θ in a closed pseudohermitian 3-manifold (M,J,θ). The CR structure J decomposes $\mathbf{C}\otimes\xi$ into the direct sum of $T_{1,0}$ and $T_{0,1}$, which are eigenspaces of J with respect to i and $-i$, respectively. By choosing a frame $\{\mathbf{T},Z_1,Z_{\bar{1}}\}$ of $TM\otimes\mathbf{C}$ with respect to the Levi form and $\{X_1,\ X_2\}$ such that

$$J(Z_1)=iZ_1\ \text{ and } J(Z_{\bar{1}})=-iZ_{\bar{1}}$$

and

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

it follows from (2.3) and (2.4) that

$$[X_1,X_2]=-2\mathbf{T}\quad\text{and}\quad\Delta_b=\frac{1}{2}(X_1^2+X_2^2)=\frac{1}{2}L.$$

Let W be the Tanaka-Webster curvature and A_{11} be the pseudohermitian torsion of (M,J,θ) with

$$W(Z,Z)=Wx^1x^{\bar{1}}\quad\text{and}\quad Tor(Z,Z)=2Re\ (iA_{\bar{1}\bar{1}}x^{\bar{1}}x^{\bar{1}})$$

for all $Z=x^1Z_1\in T_{1,0}$ (refer to section 2 for details). We also denote $\varphi_0=\mathbf{T}\varphi$ for a smooth function φ.

By using the arguments of [**LY**] and the CR Bochner formula ([**Gr**]), we are able to derive the CR version of Li-Yau gradient estimate for the positive solution of the CR heat equation (1.1) in a closed pseudohermitian 3-manifold with nonnegative Tanaka-Webster curvature.

THEOREM 1.1. *Let* (M^3, J, θ) *be a closed pseudohermitian* 3-*manifold. Suppose that*

$$(2W + Tor)(Z,\ Z) \geq 0 \tag{1.4}$$

for all $Z \in T_{1,0}$. *If* $u(x,t)$ *is the positive solution of* (1.1) *on* $M \times [0,\ \infty)$ *with*

$$[\Delta_b,\ \mathbf{T}]\, u = 0, \tag{1.5}$$

then $f(x,t) = \ln u(x,t)$ *satisfies the following subgradient estimate:*

$$\left[|\nabla_b f|^2 - 4f_t + \frac{1}{3}t(f_0)^2 \right] \leq \frac{16}{t}.$$

REMARK 1.2. 1. (1.4) is the CR analogue of the Ricci curvature tensors assumption in a closed Riemannian manifold.

2. Our subgradient estimates are more delicate due to the fact that the sub-Laplacian Δ_b is only subelliptic. In fact, by comparing with the Riemannian case, we obtain an extra gradient estimate in the so-called missing direction $\mathbf{T}$.

3. We observe that the main difference between the usual Riemannian Laplacian and the sub-Laplacian is the Reeb vector field $\mathbf{T}$. Then condition (1.5) is very natural due to the subellipticity of the sub-Laplacian in the method of Li-Yau gradient estimate. Furthermore, it follows from Lemma 3.4 (see section 3) that

$$[\Delta_b,\ \mathbf{T}]\, u = 2\mathrm{Im}Qu.$$

Here Q is the purely holomorphic second-order operator ([**GL**]) defined by

$$Qu = 2i(A_{\overline{11}}u_1)_1.$$

4. We want to emphasize that condition (1.5) is equivalent to

$$\mathrm{Im}Qu = 0.$$

If $\left(M^3,\ J,\ \theta\right)$ is a closed pseudohermitian 3-manifold with vanishing torsion (*i.e.* $A_{11} = 0$), condition (1.5) holds. However, it is not true vice versa.

5. In [**CSW**], its authors observe that condition (1.5) is related to the existence of pseudo-Einstein contact forms in a closed pseudohermitian $(2n+1)$-manifold with $n \geq 2$.

Corollary 1.3. *Let $\left(M^3,\ J,\ \theta\right)$ be a closed pseudohermitian 3-manifold with nonnegative Tanaka-Webster curvature and vanishing torsion. If $u\left(x,t\right)$ is the positive solution of* (1.1) *on $M\times[0,\ \infty)$, then $f\left(x,t\right)=\ln u\left(x,t\right)$ satisfies the following subgradient estimate:*

$$\left[|\nabla_b f|^2-4f_t+\frac{1}{3}t(f_0)^2\right]\leq\frac{16}{t}. \tag{1.6}$$

Remark 1.4. 1. Our estimate (1.6) is sharp in view of the Cao-Yau gradient estimate (1.3) in a closed pseudohermitian 3-manifold with nonnegative Tanaka-Webster curvature and vanishing torsion. As in the proof of Theorem 1.1 (see section 4), the coefficient t in front of $(f_0)^2$ in (1.6) is crucial for our estimate, which is different from the result of Li-Yau gradient estimate ([**LY**]).

2. The method of gradient estimate turns out to be useful in estimating the first eigenvalue of the Laplacian as in [**Li**] and [**LY1**]. In our case, we are able to apply the method of CR gradient estimate to prove the CR Obata Theorem completely. We refer to [**CC1**] and [**CC2**] for partial results. The complete proof will appear elsewhere ([**CK1**]).

3. In [**CCW**], the first author and his coauthors show that the torsion soliton of (1.7) has the contact form with vanishing torsion.

We should point out that the CR analogue of the Ricci curvature tensor is the pseudohermitian torsion A_{11}, which is complex. The result of Theorem 1.1 is new and considered to be of fundamental importance in the study of torsion flow. More precisely, let $\theta(t)$ be a family of smooth contact forms and $J(t)$ be a family of CR structures on (M,J_0,θ_0) with $J(0)=J_0$ and $\theta(0)=\theta_0$. We define the following so-called torsion flow ([**CCW**])

$$\left\{\begin{array}{l}\frac{\partial}{\partial t}J(t)=-2JA_{J,\theta}(t),\\ \frac{\partial}{\partial t}\theta(t)=-2W(t)\theta(t),\end{array}\right. \tag{1.7}$$

on $M\times[0,T)$ with $J(t)=i\theta^1\otimes Z_1-i\theta^{\overline{1}}\otimes Z_{\overline{1}}$ and $A_{J,\theta}(t)=-iA_{11}\theta^1\otimes Z_{\overline{1}}+iA_{\overline{1}\overline{1}}\theta^{\overline{1}}\otimes Z_1$. Here $\left\{\theta,\theta^1,\theta^{\bar{1}}\right\}$ is the coframe dual to $\{T,Z_1,Z_{\bar{1}}\}$.

In particular, if (M,J_0,θ_0) is a closed pseudohermitian 3-manifold with vanishing torsion,

$$\left\{\begin{array}{l}\frac{\partial}{\partial t}\theta(t)=-2W(t)\theta(t),\\ \theta(0)=\theta_0,\end{array}\right. \tag{1.8}$$

is the CR Yamabe flow. By using the same method of gradient estimate, we are able to obtain the CR Li-Yau-Hamilton inequality for the flow (1.8) in a closed spherical CR 3-manifold with positive Tanaka-Webster curvature and vanishing torsion ([**CK2**]).

Furthermore, in view of Theorem 1.1, we still have the following general subgradient estimate when we replace the lowerbound of curvature condition (1.4) by a negative constant.

THEOREM 1.5. *Let (M^3, J, θ) be a closed pseudohermitian 3-manifold with*

$$(2W + Tor)(Z,\ Z) \geq -2k|Z|^2 \tag{1.9}$$

for all $Z \in T_{1,0}$, where k is a positive constant. If $u(x,t)$ is the positive solution of (1.1) on $M \times [0,\ \infty)$ with

$$[\Delta_b,\ \mathbf{T}]\,u = 0,$$

then $f(x,t) = \ln u(x,t)$ satisfies the following subgradient estimate:

$$|\nabla_b f|^2 - (4 + 2k) f_t \leq \frac{(4+2k)^2(k+1)}{t} + \frac{(4+2k)^2(k+1)}{(3+2k)}. \tag{1.10}$$

Secondly, by using the arguments of [**LY**] and another CR Bochner formula (3.3) which involves the third order CR pluriharmonic operator P and CR Paneitz operator P_0 (see definition 2.1), we are able to derive another CR version of Li-Yau gradient estimate for the positive solution $u(x,t)$ of (1.1) on $M \times [0,\infty)$. We define the Kohn Laplacian $\Box_b$ on functions by $\Box_b\varphi = (-\Delta_b + i\mathbf{T})\varphi$.

THEOREM 1.6. *Let (M, J, θ) be a closed pseudohermitian 3-manifold with*

$$(2W + Tor)(Z, Z) \geq 0,$$

for all $Z \in T_{1,0}$. Let $u(x,t)$ be the positive smooth solution of (1.1) on $M \times [0,\infty)$ with

$$[\Delta_b,\ \mathbf{T}]\,u = 0.$$

If

$$\Box_b\overline{\Box}_b u(x,0) = 0 \tag{1.11}$$

at $t = 0$, then for $f(x,t) = \ln u(x,t)$,

$$|\nabla_b f|^2 + 3f_t \leq \frac{9}{t}$$

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

Now if $(M^3,\ J,\ \theta)$ is a closed pseudohermitian 3-manifold with vanishing torsion, it follows from Lemma 3.4 that condition (1.5) holds. Also we observe that $P_0 = 2\Box_b\overline{\Box}_b$. Then condition (1.11) is equivalent to $P_0u(x,0) = 0$. Furthermore, from (i) in Remark 2.2, we have that

$$P_0 u = 0 \iff Pu = 0$$

in a closed pseudohermitian 3-manifold with vanishing torsion. All these with Theorem 1.6 imply

COROLLARY 1.7. *Let (M, J, θ) be a closed pseudohermitian 3-manifold with nonnegative Tanaka-Webster curvature and vanishing torsion. If $u(x,t)$ is the positive solution of (1.1) on $M \times [0,\infty)$ such that u is the CR-pluriharmonic function*

$$Pu = 0$$

at $t = 0$, *then* $f(x,t) = \ln u(x,t)$ *satisfies the estimate*

$$|\nabla_b f|^2 + 3f_t \leq \frac{9}{t} \tag{1.12}$$

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

By combining the results of Theorem 1.1 and Theorem 1.6, we get the following subgradient estimate of the logarithm of the positive solution to (1.1) in a closed pseudohermitian 3-manifold.

THEOREM 1.8. *Let* (M, J, θ) *be a closed pseudohermitian* 3*-manifold with*

$$(2W + Tor)(Z, Z) \geq 0,$$

for all $Z \in T_{1,0}$. *Let* $u(x,t)$ *be the positive smooth solution of* (1.1) *on* $M \times [0, \infty)$ *with*

$$[\Delta_b,\ \mathbf{T}]\, u = 0.$$

If

$$\Box_b \overline{\Box}_b u(x,0) = 0$$

at $t = 0$, *then there exists a constant* C_1 *such that* u *satisfies the subgradient estimate*

$$\frac{|\nabla_b u|^2}{u^2} \leq \frac{C_1}{t} \tag{1.13}$$

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

As a consequence of Theorem 1.6, we have

COROLLARY 1.9. *Let* (M, J, θ) *be a closed pseudohermitian* 3*-manifold with nonnegative Tanaka-Webster curvature and vanishing torsion. If* $u(x,t)$ *is the positive solution of* (1.1) *on* $M \times [0, \infty)$ *such that*

$$Pu = 0$$

at $t = 0$, *then there exists a constant* C_2 *such that* u *satisfies the subgradient estimate*

$$\frac{|\nabla_b u|^2}{u^2} \leq \frac{C_2}{t}$$

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

Finally, we have the Harnack inequality and upper bound estimate for the heat kernel of (1.1). By Chow connectivity theorem [**Cho**], there always exists a horizontal curve (see definition 2.3) joining p and q, so the distance is finite. Now integrating (1.6) over $(\gamma(t), t)$ of a horizontal path $\gamma : [t_1, t_2] \to M$ joining points x_1, x_2 in M, we obtain the following CR version of Li-Yau Harnack inequality.

THEOREM 1.10. *Let (M, J, θ) be a closed pseudohermitian 3-manifold with nonnegative Tanaka-Webster curvature and vanishing torsion. If $u(x,t)$ is the positive solution of (1.1) on $M \times [0,\infty)$, then for any x_1, x_2 in M and $0 < t_1 < t_2 < \infty$, we have the inequality*

$$\frac{u(x_2,t_2)}{u(x_1,t_1)} \geq \left(\frac{t_2}{t_1}\right)^{-4} \exp(-\frac{d_{cc}(x_1,x_2)^2}{(t_2-t_1)}).$$

Here d_{cc} is the Carnot-Carathéodory distance.

As a consequence of Theorem 1.10 and [**CY**], we have the following upper bound estimate for the heat kernel of (1.1).

THEOREM 1.11. *Let (M, J, θ) be a closed pseudohermitian 3-manifold with nonnegative Tanaka-Webster curvature and vanishing torsion and $H(x,y,t)$ be the heat kernel of (1.1) on $M \times [0,\infty)$. Then for some constant $\delta > 1$ and $0 < \epsilon < 1$, $H(x,y,t)$ satisfies the estimate*

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

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

Let $u(x,t)$ be the positive solution of (1.1) on $M \times [0,\infty)$, and $g(x,t)$ be the function that satisfies

$$u(x,t) = \frac{e^{-g(x,t)}}{(4\pi t)^{16\times a}}$$

with $\int_M u d\mu = 1$. Here $a > 0$, to be determined later.

We first define the so-called Nash-type entropy ([**Na**]) (also [**CW**])

$$N(u,t) = -\int_M (\ln u) u d\mu \tag{1.14}$$

and

$$\widetilde{N}(u,t) = N(u,t) - (16 \times a)(\ln 4\pi t + 1). \tag{1.15}$$

Next, following Perelman ([**Pe1**]) (also [**Ni**], [**Li**]), we define

$$\mathcal{W}(u,t) = \int_M [t|\nabla_b g|^2 + g - (16 \times 2a)] u d\mu = \frac{d}{dt}[t\widetilde{N}(u,t)] \tag{1.16}$$

and

$$\widetilde{\mathcal{W}}(u,t) = \mathcal{W}(u,t) + \frac{1}{2}t^2 \int_M g_0^2 u d\mu. \tag{1.17}$$

Then, by applying Corollary 1.3, we obtain the following entropy formulae for $\widetilde{N}(u,t)$ and $\widetilde{\mathcal{W}}(u,t)$.

THEOREM 1.12. *Let (M, J, θ) be a closed pseudohermitian 3-manifold with nonnegative Tanaka-Webster curvature and vanishing torsion. Let*

$u(x,t)$ be the positive solution of (1.1) *on* $M\times[0,\infty)$ *with* $\int_M ud\mu=1$. *Then*

$$\frac{d}{dt}\widetilde{N}(u,t)=\int_M(|\nabla_b g|^2+4g_t+\frac{16\times 3a}{t})ud\mu\leq 0$$

for all $t\in(0,\infty)$ *and* $a\geq 1$.

Theorem 1.13. *Let* (M,J,θ) *be a closed pseudohermitian* 3*-manifold with nonnegative Tanaka-Webster curvature and vanishing torsion. Let* $u(x,t)$ *be the positive solution of* (1.1) *on* $M\times[0,\infty)$ *with* $\int_M ud\mu=1$. *Then*

$$\frac{d}{dt}\widetilde{\mathcal{W}}\leq -4t\int_M u|g_{11}|^2d\mu-t\int_M u(\Delta_b g)^2d\mu-2t\int_M uW|\nabla_b g|^2d\mu\leq 0$$

for all $t\in(0,\infty)$ *and* $a\geq 6$.

Note that all arguments here work as well in a closed pseudohermitian $(2n+1)$-manifold. We will pursue this issue elsewhere. Also we refer to [**SC**] and [**JS**] for other related topics.

We briefly describe the methods used in our proofs. In section 3, we will recall two CR versions of Bochner formulae and derive some key lemmas. In section 4, we derive two versions of Li-Yau gradient estimates and Harnack inequality for the CR heat equation. In section 5, by using the subgradient estimate in the previous section, we derive entropy formulae for the CR heat equation (1.1).

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2. Preliminary

We introduce some basic materials in a pseudohermitian 3-manifold (see [**L1**], [**L2**] for more details). Let M be a closed 3-manifold with an oriented contact structure ξ. There always exists a global contact form θ with $\xi=\ker\theta$, obtained by patching together local ones with a partition of unity. The Reeb vector field of θ is the unique vector field $\mathbf{T}$ such that $\theta(\mathbf{T})=1$ and $\mathcal{L}_T\theta=0$ or $d\theta(\mathbf{T},\cdot)=0$. A CR structure compatible with ξ is a smooth endomorphism $J:\xi\to\xi$ such that $J^2=-Id$. A pseudohermitian structure compatible with ξ is a CR-structure J compatible with ξ together with a global contact form θ. The CR structure J can extend to $\mathbf{C}\otimes\xi$ and decomposes $\mathbf{C}\otimes\xi$ into the direct sum of $T_{1,0}$ and $T_{0,1}$, which are eigenspaces of J with respect to i and $-i$, respectively.

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

Let $\{\mathbf{T}, Z_1, Z_{\bar{1}}\}$ be a frame of $TM \otimes \mathbf{C}$, where Z_1 is any local frame of $T_{1,0}$, $Z_{\bar{1}} = \overline{Z_1} \in T_{0,1}$. Then $\left\{\theta, \theta^1, \theta^{\bar{1}}\right\}$, the coframe dual to $\{T, Z_1, Z_{\bar{1}}\}$, satisfies

$$d\theta = ih_{1\bar{1}}\theta^1 \wedge \theta^{\bar{1}}$$

for some positive function $h_{1\bar{1}}$. Actually we can always choose Z_1 such that $h_{1\bar{1}} = 1$; hence, throughout this paper, we assume $h_{1\bar{1}} = 1$.

The pseudohermitian connection of (J, θ) is the connection ∇ on $TM \otimes \mathbf{C}$ (and extended to tensors) given in terms of a local frame $Z_1 \in T_{1,0}$ by

$$\nabla Z_1 = \theta_1{}^1 \otimes Z_1, \quad \nabla Z_{\bar{1}} = \theta_{\bar{1}}{}^{\bar{1}} \otimes Z_{\bar{1}}, \quad \nabla \mathbf{T} = 0,$$

where $\theta_1{}^1$ is the 1-form uniquely determined by the following equations:

$$\begin{aligned} d\theta^1 &= \theta^1 \wedge \theta_1{}^1 + \theta \wedge \tau^1 \\ \tau^1 &\equiv 0 \mod \theta^{\bar{1}} \\ 0 &= \theta_1{}^1 + \theta_{\bar{1}}{}^{\bar{1}}, \end{aligned} \tag{2.1}$$

where τ^1 is the pseudohermitian torsion. Put $\tau^1 = A^1{}_{\bar{1}}\theta^{\bar{1}}$. The structure equation for the pseudohermitian connection is

$$d\theta_1{}^1 = W\theta^1 \wedge \theta^{\bar{1}} + 2i\mathrm{Im}(A^{\bar{1}}{}_{1,\bar{1}}\theta^1 \wedge \theta), \tag{2.2}$$

where W is the Tanaka-Webster curvature.

We will denote components of covariant derivatives with indices preceded by a comma; thus write $A^{\bar{1}}{}_{1,\bar{1}}\theta^1 \wedge \theta$. The indices $\{0, 1, \bar{1}\}$ indicate derivatives with respect to $\{T, Z_1, Z_{\bar{1}}\}$. For derivatives of a scalar function, we will often omit the comma; for instance, $\varphi_1 = Z_1\varphi$, $\varphi_{1\bar{1}} = Z_{\bar{1}}Z_1\varphi - \theta_1^1(Z_{\bar{1}})Z_1\varphi$, $\varphi_0 = \mathbf{T}\varphi$ for a (smooth) function.

For a real-valued function φ, the subgradient ∇_b is defined by $\nabla_b\varphi \in \xi$ and $\langle Z, \nabla_b\varphi\rangle = d\varphi(Z)$ for all vector fields Z tangent to the contact plane. Locally, $\nabla_b\varphi = \varphi_{\bar{1}}Z_1 + \varphi_1 Z_{\bar{1}}$.

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

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

and

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

The sub-Laplacian Δ_b defined as the trace of the subhessian

$$\Delta_b\varphi = Tr\left((\nabla^H)^2\varphi\right) = (\varphi_{1\bar{1}} + \varphi_{\bar{1}1}). \tag{2.3}$$

Finally, we also need the following commutation relations ([**L1**]):

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

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

In the end, we recall some definitions.

Definition 2.1. Let (M, J, θ) be a closed pseudohermitian 3-manifold. We define ([**L1**])

$$P\varphi = (\varphi_{\bar{1}}{}^{\bar{1}}{}_1 + iA_{11}\varphi^1)\theta^1 = P\varphi = (P_1\varphi)\theta^1,$$

which is an operator that characterizes CR-pluriharmonic functions. Here $P_1\varphi = \varphi_{\bar{1}}{}^{\bar{1}}{}_1 + iA_{11}\varphi^1$ and $\overline{P}\varphi = (\overline{P}_1)\theta^{\bar{1}}$, the conjugate of P. The CR Paneitz operator P_0 is defined by

$$P_0\varphi = 4\left(\delta_b(P\varphi) + \bar{\delta}_b(\overline{P}\varphi)\right), \tag{2.5}$$

where δ_b is the divergence operator that takes $(1,0)$-forms to functions by $\delta_b(\sigma_1\theta^1) = \sigma_{1,}{}^1$, and similarly, $\bar{\delta}_b(\sigma_{\bar{1}}\theta^{\bar{1}}) = \sigma_{\bar{1},}{}^{\bar{1}}$.

We observe that

$$\int_M \langle P\varphi + \overline{P}\varphi, d_b\varphi\rangle_{L^*_\theta}\, d\mu = -\frac{1}{4}\int_M P_0\varphi \cdot \varphi\, d\mu \tag{2.6}$$

with $d\mu = \theta \wedge d\theta$. One can check that P_0 is self-adjoint. That is, $\langle P_0\varphi, \psi\rangle = \langle \varphi, P_0\psi\rangle$ for all smooth functions φ and ψ. For the details about these operators, the reader can make reference to [**GL**], [**Hi**], [**L1**], [**GG**], and [**FH**].

Remark 2.2. ([**Hi**], [**GL**]) (i) Let (M, J, θ) be a closed pseudohermitian 3-manifold with vanishing torsion. Then a smooth real-valued function φ satisfies $P_0\varphi = 0$ on M if and only if $P_1\varphi = 0$ on M.

(ii) Let $P_1\varphi = 0$. If M is the boundary of a connected strictly pseudoconvex domain $\Omega \subset C^2$, then φ is the boundary value of a pluriharmonic function u in Ω. That is, $\partial\overline{\partial}u = 0$ in Ω. Moreover, if Ω is simply connected, there exists a holomorphic function w in Ω such that $\mathrm{Re}(w) = u$ and $u|_M = \varphi$.

Definition 2.3. Let (M, J, θ) be a closed pseudohermitian 3-manifold with $\xi = \ker\theta$. A piecewise smooth curve $\gamma : [0,1] \to M$ is said to be horizontal if $\gamma'(t) \in \xi$ whenever $\gamma'(t)$ exists. The length of γ is then defined by

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

The Carnot-Carathéodory distance d_{cc} between two points $p, q \in M$ is defined by

$$d_{cc}(p,q) = \inf \{ l(\gamma) | \ \gamma \in C_{p,q} \},$$

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

3. The CR Bochner Formulae

In this section, we will recall two CR versions of Bochner formulae and derive some key lemmas in a closed pseudohermitian 3-manifold (M, J, θ). We first recall the following CR version of Bochner formula in a complete pseudohermitian 3-manifold.

LEMMA 3.1. *([**Gr**]) Let (M, J, θ) be a complete pseudohermitian 3-manifold. For a smooth real-valued function φ on (M, J, θ),*

(3.1)

$$\begin{aligned} \Delta_b |\nabla_b \varphi|^2 &= 2\left|\left(\nabla^H\right)^2 \varphi\right|^2 + 2\langle \nabla_b \varphi, \ \nabla_b \Delta_b \varphi\rangle \\ &+ (4W + 2Tor)\left((\nabla_b \varphi)_C, \ (\nabla_b \varphi)_C\right) + 4\langle J\nabla_b \varphi, \ \nabla_b \varphi_0\rangle . \end{aligned}$$

Here $(\nabla_b \varphi)_C = \varphi_{\bar{1}} Z_1$ is the corresponding complex $(1, \ 0)$-vector of $\nabla_b \varphi$.

Note that ([**CC1**])

$$\langle J\nabla_b \varphi, \ \nabla_b \varphi_0\rangle = -i(\varphi_1 \varphi_{0\bar{1}} - \varphi_{\bar{1}} \varphi_{01})$$

and

(3.2)

$$< P\varphi + \overline{P}\varphi, d_b\varphi >_{L_\theta^*} = (\varphi_{\bar{1}11}\varphi_{\bar{1}} + iA_{11}\varphi_{\bar{1}}\varphi_{\bar{1}}) + (\varphi_{1\bar{1}\bar{1}}\varphi_1 - iA_{\bar{1}\bar{1}}\varphi_1\varphi_1).$$

Then

$$\begin{aligned} -i(\varphi_1\varphi_{\bar{1}0} - \varphi_{\bar{1}}\varphi_{10}) &= -2 < P\varphi + \overline{P}\varphi, d_b\varphi >_{L_\theta^*} \\ &\quad -2Tor((\nabla_b\varphi)_{\mathbf{C}}, (\nabla_b\varphi)_{\mathbf{C}}) \\ &\quad + < \nabla_b\varphi, \nabla_b\Delta_b\varphi >_{L_\theta} . \end{aligned}$$

These and (3.1) imply

LEMMA 3.2. *([**CC1**]) Let (M, J, θ) be a complete pseudohermitian 3-manifold. For a smooth real-valued function φ on (M, J, θ),*

$$\begin{aligned} \Delta_b|\nabla_b\varphi|^2 &= 2|(\nabla^H)^2\varphi|^2 + 6 < \nabla_b\varphi, \nabla_b\Delta_b\varphi > \\ &\quad +[4W - 6Tor]((\nabla_b\varphi)_{\mathbf{C}}, (\nabla_b\varphi)_{\mathbf{C}}) \\ &\quad -8 < P\varphi + \overline{P\varphi}, d_b\varphi > . \end{aligned} \tag{3.3}$$

Here $d_b\varphi = \varphi_1\theta^1 + \varphi_{\bar{1}}\theta^{\bar{1}}$.

Now by applying the commutation relations (2.4), one obtains

LEMMA 3.3. *Let (M, J, θ) be a complete pseudohermitian 3-manifold. For a smooth real-valued function φ and any $\nu > 0$, we have*

$$\begin{aligned} \Delta_b |\nabla_b \varphi|^2 &\geq 4|\varphi_{11}|^2 + (\Delta_b \varphi)^2 + \varphi_0^2 + 2\langle \nabla_b \varphi, \ \nabla_b \Delta_b \varphi\rangle \\ &+ \left(4W + 2Tor - \tfrac{4}{\nu}\right)\left((\nabla_b \varphi)_C, \ (\nabla_b \varphi)_C\right) - 2\nu |\nabla_b \varphi_0|^2 . \end{aligned}$$

Proof. Note that

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

and for all $\nu > 0$

$$4\left\langle J\nabla_b\varphi,\ \nabla_b\varphi_0\right\rangle \geq -4\left|\nabla_b\varphi\right|\left|\nabla_b\varphi_0\right| \geq -\frac{2}{\nu}\left|\nabla_b\varphi\right|^2 - 2\nu\left|\nabla_b\varphi_0\right|^2.$$

Lemma 3.3 follows from Lemma 3.1 easily. q.e.d.

LEMMA 3.4. *Let (M, J, θ) be a complete pseudohermitian 3-manifold. For a smooth real-valued function $\varphi(x)$ defined on M, then*

$$\Delta_b\varphi_0 = \left(\Delta_b\varphi\right)_0 + 2\left[\left(A_{11}\varphi_{\bar{1}}\right)_{\bar{1}} + \left(A_{\bar{1}\bar{1}}\varphi_1\right)_1\right].$$

That is,

$$2ImQ\varphi = \left[\Delta_b,\ \mathbf{T}\right]\varphi.$$

Proof. By direct computation and the commutation relation (2.4), we have

$$\begin{aligned}
\Delta_b\varphi_0 &= \varphi_{01\bar{1}} + \varphi_{0\bar{1}1} \\
&= \left(\varphi_{10} + A_{11}\varphi_{\bar{1}}\right)_{\bar{1}} + \left(\varphi_{\bar{1}0} + A_{\bar{1}\bar{1}}\varphi_1\right)_1 \\
&= \varphi_{10\bar{1}} + \left(A_{11}\varphi_{\bar{1}}\right)_{\bar{1}} + \varphi_{\bar{1}01} + \left(A_{\bar{1}\bar{1}}\varphi_1\right)_1 \\
&= \varphi_{1\bar{1}0} + \varphi_{\bar{1}10} + 2\left[\left(A_{11}\varphi_{\bar{1}}\right)_{\bar{1}} + \left(A_{\bar{1}\bar{1}}\varphi_1\right)_1\right] \\
&= \left(\Delta_b\varphi\right)_0 + 2\left[\left(A_{11}\varphi_{\bar{1}}\right)_{\bar{1}} + \left(A_{\bar{1}\bar{1}}\varphi_1\right)_1\right].
\end{aligned}$$

This completes the proof. q.e.d.

Now we define

$$V : C^\infty(M) \to C^\infty(M)$$

by

$$V(\varphi) = \left(A_{11}\varphi_{\bar{1}}\right)_{\bar{1}} + \left(A_{\bar{1}\bar{1}}\varphi_1\right)_1 + A_{11}\varphi_{\bar{1}}\varphi_{\bar{1}} + A_{\bar{1}\bar{1}}\varphi_1\varphi_1.$$

LEMMA 3.5. *Let $\left(M^3,\ J,\ \theta\right)$ be a pseudohermitian 3-manifold. If $u(x,t)$ is the positive solution of (1.1) on $M \times [0,\infty)$, then $f(x,t) = \ln u(x,t)$ satisfies*

$$\Delta_b f_0 - f_{0t} = -2\left\langle \nabla_b f_0,\ \nabla_b f\right\rangle + 2V(f).$$

Proof. By Lemma 3.4, we have

$$\Delta_b f_0 = \left(\Delta_b f\right)_0 + 2\left[\left(f_1 A_{\bar{1}\bar{1}}\right)_1 + \left(f_{\bar{1}} A_{11}\right)_{\bar{1}}\right].$$

But

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

All these imply

$$\begin{aligned}
\Delta_b f_0 - f_{0t} &= \left(\Delta_b f\right)_0 - f_{t0} + 2\left[\left(A_{11}f_{\bar{1}}\right)_{\bar{1}} + \left(A_{\bar{1}\bar{1}}f_1\right)_1\right] \\
&= \left(\Delta_b f - f_t\right)_0 + 2\left[\left(A_{11}f_{\bar{1}}\right)_{\bar{1}} + \left(A_{\bar{1}\bar{1}}f_1\right)_1\right] \\
&= \left(-\left|\nabla_b f\right|^2\right)_0 + 2\left[\left(A_{11}f_{\bar{1}}\right)_{\bar{1}} + \left(A_{\bar{1}\bar{1}}f_1\right)_1\right] \\
&= -2\left\langle \nabla_b f_0,\ \nabla_b f\right\rangle + 2[\left(A_{11}f_{\bar{1}}\right)_{\bar{1}} + \left(A_{\bar{1}\bar{1}}f_1\right)_1 \\
&+ A_{11}f_{\bar{1}}f_{\bar{1}} + A_{\bar{1}\bar{1}}f_1f_1].
\end{aligned}$$

q.e.d.

LEMMA 3.6. *Let* $\left(M^3,\ J,\ \theta\right)$ *be a pseudohermitian* 3*-manifold. Suppose that*

$$[\Delta_b,\ \mathbf{T}]\, u = 0. \tag{3.4}$$

Then $f\,(x,t) = \ln u\,(x,t)$ *satisfies*

$$V\,(f) = 0.$$

Proof. It follows from Lemma 3.4 that

$$\begin{aligned} [\Delta_b,\ \mathbf{T}]\, u &= 2\mathrm{Im} Q u \\ &= 2\left[\left(A_{\bar{1}\bar{1}} u_1\right)_1 + \left(A_{11} u_{\bar{1}}\right)_{\bar{1}}\right]. \end{aligned} \tag{3.5}$$

Then

(3.6)

$$\begin{aligned} V\,(f) &= \left(f_1 A_{\bar{1}\bar{1}}\right)_1 + \left(f_{\bar{1}} A_{11}\right)_{\bar{1}} + A_{11} f_{\bar{1}} f_{\bar{1}} + A_{\bar{1}\bar{1}} f_1 f_1 \\ &= f_{11} A_{\bar{1}\bar{1}} + f_{\bar{1}\bar{1}} A_{11} + f_1 A_{\bar{1}\bar{1},1} + f_{\bar{1}} A_{11,\bar{1}} + A_{11} f_{\bar{1}} f_{\bar{1}} + A_{\bar{1}\bar{1}} f_1 f_1 \\ &= A_{\bar{1}\bar{1}} \left(\tfrac{u_{11}}{u} - \tfrac{u_1 u_1}{u^2}\right) + A_{11} \left(\tfrac{u_{\bar{1}\bar{1}}}{u} - \tfrac{u_{\bar{1}} u_{\bar{1}}}{u^2}\right) \\ &\quad + A_{\bar{1}\bar{1},1} \tfrac{u_1}{u} + A_{11,\bar{1}} \tfrac{u_{\bar{1}}}{u} + A_{\bar{1}\bar{1}} \tfrac{u_1 u_1}{u^2} + A_{11} \tfrac{u_{\bar{1}} u_{\bar{1}}}{u^2} \\ &= \tfrac{1}{u}\left[\left(A_{\bar{1}\bar{1}} u_1\right)_1 + \left(A_{11} u_{\bar{1}}\right)_{\bar{1}}\right] \\ &= \tfrac{1}{2u}\,[\Delta_b,\ \mathbf{T}]\, u \\ &= 0. \end{aligned}$$

This completes the proof. q.e.d.

4. Li-Yau Subgradient Estimate and CR Harnack Inequality

In this section, we derive CR versions of Li-Yau gradient estimates and classical Harnack inequality for the CR heat equation in a closed pseudohermitian 3-manifold.

Let u be the positive solution of (1.1) and denote

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

Then $f\,(x,t)$ satisfies the equation

$$\left(\Delta_b - \frac{\partial}{\partial t}\right) f\,(x,t) = -\left|\nabla_b f\,(x,t)\right|^2. \tag{4.1}$$

Now we define a real-valued function $F\,(x,t,\ a,\ c) : M \times [0,\ T] \times \mathbf{R}^* \times \mathbf{R}^+ \to \mathbf{R}$ by

$$F\,(x,t,\ a,\ c) = t\left(\left|\nabla_b f\right|^2(x) + a f_t + c t f_0^2\,(x)\right), \tag{4.2}$$

where $\mathbf{R}^*{=}\mathbf{R}\backslash\{0\}$ and $\mathbf{R}^+ = (0,\ \infty)$.

PROPOSITION 4.1. *Let* $\left(M^3,\ J,\ \theta\right)$ *be a pseudohermitian* 3*-manifold. Suppose that*

$$\left(2W + Tor\right)(Z,\ Z) \geq -2k\,|Z|^2 \tag{4.3}$$

for all $Z \in T_{1,0}$*, where* k *is a nonnegative constant. If* $u(x,t)$ *is the positive solution of* (1.1) *on* $M \times [0,\infty)$*, then*

(4.4)
$$\left(\Delta_b - \tfrac{\partial}{\partial t}\right) F \geq -\tfrac{1}{t}F - 2\langle \nabla_b f,\ \nabla_b F\rangle + t\Big[4|f_{11}|^2 + (\Delta_b f)^2 + (1-c) f_0^2 - \left(2k + \tfrac{2}{ct}\right)|\nabla_b f|^2 + 4ctf_0 V(f)\Big].$$

Proof. First we differentiate F with respect to the t-variable.

(4.5)
$$F_t = \tfrac{1}{t}F + t\left[2(1+a)\langle \nabla_b f,\ \nabla_b f_t\rangle + cf_0^2 + 2ctf_0 f_{0t} + a\Delta_b f_t\right].$$

By the assumption (4.3) and Lemma 3.3, one can compute

$$\begin{aligned}\Delta_b F &= t\left(\Delta_b |\nabla_b f|^2 + a\Delta_b f_t + ct\Delta_b f_0^2\right)\\ &\geq t\Big[4|f_{11}|^2 + (\Delta_b f)^2 + f_0^2 + 2\langle \nabla_b f,\ \nabla_b \Delta_b f\rangle - 2\left(k + \frac{1}{\nu}\right)|\nabla_b f|^2\\ &\quad -2\nu|\nabla_b f_0|^2 + a\Delta_b f_t + 2ctf_0\Delta_b f_0 + 2ct|\nabla_b f_0|^2\Big].\end{aligned}$$

Then, taking $\nu = ct$,

$$\Delta_b F \geq t\Big[4|f_{11}|^2 + (\Delta_b f)^2 + f_0^2 + 2\langle \nabla_b f,\ \nabla_b \Delta_b f\rangle - 2\left(k + \frac{1}{ct}\right)|\nabla_b f|^2 + a\Delta_b f_t + 2ctf_0\Delta_b f_0\Big]. \tag{4.6}$$

It follows from (4.5) and (4.6) that

$$\begin{aligned}\left(\Delta_b - \frac{\partial}{\partial t}\right) F \geq -\frac{1}{t}F + t[4|f_{11}|^2 + (\Delta_b f)^2\\ + \left(1 - c)f_0^2 - 2(k + \frac{1}{ct}\right)|\nabla_b f|^2\\ + 2\langle \nabla_b f,\ \nabla_b \Delta_b f\rangle + 2ctf_0(\Delta_b f_0 - f_{0t})\\ - 2(1+a)\langle \nabla_b f,\ \nabla_b f_t\rangle].\end{aligned} \tag{4.7}$$

By Lemma 3.5 and definition of F, we have

(4.8)
$$\begin{aligned}&2\langle \nabla_b f,\ \nabla_b \Delta_b f\rangle + 2ctf_0(\Delta_b f_0 - f_{0t}) - 2(1+a)\langle \nabla_b f,\ \nabla_b f_t\rangle\\ =\ &2\left\langle \nabla_b f,\ \nabla_b\left(f_t - |\nabla_b f|^2\right)\right\rangle - 2(1+a)\langle \nabla_b f,\ \nabla_b f_t\rangle\\ &+2ctf_0(-2\langle \nabla_b f_0,\ \nabla_b f\rangle + 2V(f))\\ =\ &-2a\langle \nabla_b f,\ \nabla_b f_t\rangle - 2\left\langle \nabla_b f,\ \nabla_b|\nabla_b f|^2\right\rangle\\ &-4ctf_0\langle \nabla_b f_0,\ \nabla_b f\rangle + 4ctf_0 V(f)\\ =\ &-2a\left\langle \nabla_b f,\ \nabla_b\left(\tfrac{1}{at}F - \tfrac{1}{a}|\nabla_b f|^2 - \tfrac{ct}{a}f_0^2\right)\right\rangle - 2\left\langle \nabla_b f,\ \nabla_b|\nabla_b f|^2\right\rangle\\ &-4ctf_0\langle \nabla_b f_0,\ \nabla_b f\rangle + 4ctf_0 V(f)\\ =\ &-\tfrac{2}{t}\langle \nabla_b f,\ \nabla_b F\rangle + 4ctf_0 V(f).\end{aligned}$$

Substitute (4.8) into (4.7):

$$\begin{aligned}\left(\Delta_b - \tfrac{\partial}{\partial t}\right) F \quad \geq \quad & -\tfrac{1}{t}F - 2\left\langle \nabla_b f,\ \nabla_b F\right\rangle + t\Big[4\left|f_{11}\right|^2 + \left(\Delta_b f\right)^2 \\ & + (1-c)\, f_0^2 - 2\left(k + \tfrac{1}{ct}\right)\left|\nabla_b f\right|^2 + 4ctf_0 V(f)\Big].\end{aligned}$$

This completes the proof. q.e.d.

Proposition 4.2. *Let* $\left(M^3,\ J,\ \theta\right)$ *be a pseudohermitian* 3*-manifold. Suppose that*

$$(2W + Tor)(Z,\ Z) \geq -2k\,|Z|^2$$

for all $Z \in T_{1,0}$*, where* k *is a nonnegative constant. If* $u(x,t)$ *is the positive solution of* (1.1) *on* $M \times [0,\infty)$*, then*

$$\begin{aligned}\left(\Delta_b - \frac{\partial}{\partial t}\right) F \geq\ & \frac{1}{a^2 t}F^2 - \frac{1}{t}F - 2\left\langle \nabla_b f,\ \nabla_b F\right\rangle + t\Big[4\left|f_{11}\right|^2 \\ & + \left(1 - c - \frac{2c}{a^2}F\right) f_0^2 \\ & + \left(-\frac{2(a+1)}{a^2 t}F - 2k - \frac{2}{ct}\right)\left|\nabla_b f\right|^2 + 4ctf_0 V(f)\Big].\end{aligned} \tag{4.9}$$

Proof. By definition of F and (4.1),

$$\begin{aligned}\Delta_b f &= f_t - \left|\nabla_b f\right|^2 \\ &= \frac{1}{at}F - \frac{a+1}{a}\left|\nabla_b f\right|^2 - \frac{ct}{a}f_0^2.\end{aligned}$$

Then

$$\begin{aligned}\left(\Delta_b f\right)^2 &= \left(\frac{1}{at}F - \frac{a+1}{a}\left|\nabla_b f\right|^2 - \frac{ct}{a}f_0^2\right)^2 \\ &= \frac{1}{a^2t^2}F^2 + \left(\frac{a+1}{a}\left|\nabla_b f\right|^2 + \frac{ct}{a}f_0^2\right)^2 \\ &\quad - \frac{2(a+1)}{a^2 t}F\left|\nabla_b f\right|^2 - \frac{2c}{a^2}F f_0^2 \\ &\geq \frac{1}{a^2t^2}F^2 - \frac{2(a+1)}{a^2 t}F\left|\nabla_b f\right|^2 - \frac{2c}{a^2}F f_0^2.\end{aligned}$$

It follows from (4.4) that

$$\begin{aligned}\left(\Delta_b - \frac{\partial}{\partial t}\right) F \geq\ & \frac{1}{a^2 t}F^2 - \frac{1}{t}F - 2\left\langle \nabla_b f,\ \nabla_b F\right\rangle \\ & + t\Big[4\left|f_{11}\right|^2 + \left(1 - c - \frac{2c}{a^2}F\right) f_0^2 \\ & + \left(-\frac{2(a+1)}{a^2 t}F - 2k - \frac{2}{ct}\right)\left|\nabla_b f\right|^2 + 4ctf_0 V(f)\Big].\end{aligned}$$

This completes the proof. q.e.d.

Proposition 4.3. *Let $\left(M^3,\ J,\ \theta\right)$ be a pseudohermitian 3-manifold. Suppose that*

$$(2W+Tor)(Z,\ Z)\geq -2k\,|Z|^2$$

for all $Z\in T_{1,0}$, where k is a nonnegative constant. Let $a,\ c,\ T<\infty$ be fixed. For each $t\in[0,T]$, let $(p(t),s(t))\in M\times[0,t]$ be the maximal point of F on $M\times[0,t]$. Then at $(p(t),s(t))$, we have

$$\begin{array}{lcl} 0 & \geq & \frac{1}{a^2t}F\left(F-a^2\right)+t\left[4\left|f_{11}\right|^2+\left(1-c-\frac{2c}{a^2}F\right)f_0^2\right.\\ & & \left.+\left(-\frac{2(a+1)}{a^2t}F-2k-\frac{2}{ct}\right)\left|\nabla_bf\right|^2+4ctf_0V(f)\right]. \end{array}\tag{4.10}$$

Proof. Since $F(p(t),s(t),\ a,\ c)=\max\limits_{(x,\mu)\in M\times[0,\ t]}F(x,\mu,\ a,\ c)$, the point $(p(t),s(t))$ is a critical point of $F(x,s(t),\ a,\ c)$. Then

$$\nabla_bF(p(t),s(t),\ a,\ c)=0.$$

On the other hand, since $(p(t),s(t))$ is a maximal point, we can apply the maximum principle at $(p(t),s(t))$ on $M\times[0,t]$:

$$\Delta_bF(p(t),s(t),\ a,\ c)\leq 0\tag{4.11}$$

and

$$\frac{\partial}{\partial t}F(p(t),s(t),\ a,\ c)\geq 0.\tag{4.12}$$

Now it follows from (4.11), (4.12), and (4.9) that

$$\begin{array}{lcl} 0 & \geq & \frac{1}{a^2t}F\left(F-a^2\right)+t\left[4\left|f_{11}\right|^2+\left(1-c-\frac{2c}{a^2}F\right)f_0^2\right.\\ & & \left.+\left(-\frac{2(a+1)}{a^2t}F-2k-\frac{2}{ct}\right)\left|\nabla_bf\right|^2+4ctf_0V(f)\right]. \end{array}$$

q.e.d.

Now we are ready to prove our main theorems.

Proof of Theorem 1.1. Let $\left(M^3,\ J,\ \theta\right)$ be a closed pseudohermitian 3-manifold. Suppose that

$$(2W+Tor)(Z,\ Z)\geq 0$$

for all $Z\in T_{1,0}$, and

$$[\Delta_b,\ T]\,u=0.$$

Recall that

$$F(x,\ t,\ a,\ c)=t\left(\left|\nabla_bf\right|^2(x)+af_t+ctf_0^2(x)\right).$$

We claim that for each fixed $T<\infty$,

$$F(p(T),s(T),\ -4,\ c)<\tfrac{16}{3c},$$

where we choose $a=-4$ and $0<c<\frac{1}{3}$ (see Remark 4.4). Here $(P(T),s(T))\in M\times[0,T]$ is the maximal point of F on $M\times[0,T]$.

We prove by contradiction. Suppose not; that is,

$$F(p(T), s(T), \ -4, \ c) \geq \tfrac{16}{3c}.$$

Due to Proposition 4.3, $(p(t), s(t)) \in M \times [0, t]$ is the maximal point of F on $M \times [0, t]$ for each $t \in [0, T]$. Since $F(p(t), s(t))$ is continuous in the variable t when a, c are fixed and $F(p(0), s(0)) = 0$, by Intermediate-value theorem there exists a $t_0 \in (0, \ T]$ such that

$$F(p(t_0), s(t_0), \ -4, \ c) = \tfrac{16}{3c}. \tag{4.13}$$

By assumption (1.5) and Lemma 3.6, we have $V(f) = 0$. Now we substitute (4.13) into (4.10) at the point $(p(t_0), s(t_0))$. Hence

$$\left(-\frac{2(a+1)}{a^2 t_0} F(p(t_0), s(t_0), \ -4, \ c) - \frac{2}{ct_0}\right) = 0$$

and

$$\begin{array}{rcl} 0 & \geq & \frac{1}{16s(t_0)} \frac{16}{3c} \left(\frac{16}{3c} - 16\right) + \left(1 - c - \frac{2c}{16} \frac{16}{3c}\right) s(t_0) f_0^2 \\ & = & \frac{16}{s(t_0)} \frac{1}{3c} \left(\frac{1}{3c} - 1\right) + \left(\frac{1}{3} - c\right) s(t_0) f_0^2. \end{array} \tag{4.14}$$

Since $0 < c < \frac{1}{3}$, (4.14) leads to a contradiction.

Hence

$$F(P(T), s(T), \ -4, \ c) < \tfrac{16}{3c}.$$

This implies that

$$\max_{(x, \ t) \in M \times [0, \ T]} t \left[|\nabla_b f|^2 (x) - 4 f_t + ct f_0^2 (x) \right] \ < \ \tfrac{16}{3c}.$$

When we fix on the set $\{T\} \times M$, we have

$$T \left[|\nabla_b f|^2 (x) - 4 f_t + cT f_0^2 (x) \right] \ < \ \tfrac{16}{3c}.$$

Since T is arbitrary, we obtain

$$\frac{|\nabla_b u|^2}{u^2} - 4\frac{u_t}{u} + ct\frac{u_0^2}{u^2} < \frac{16}{3ct}.$$

Finally, let $c \to \frac{1}{3}$; then we are done. This completes the proof. q.e.d.

Remark 4.4. In the previous proof, in fact we have

$$F \leq a^2$$

for all t with $a \leq -4$.

Proof of Theorem 1.5. Let $\left(M^3, \ J, \ \theta\right)$ be a closed pseudohermitian 3-manifold with

$$(2W + Tor)(Z, \ Z) \geq -2k |Z|^2$$

for all $Z \in T_{1,0}$, where k is a positive constant and

$$[\Delta_b, \ \mathbf{T}] u = 0.$$

Recall that

$$F(x, \ t, \ a, \ c) = t\left(|\nabla_b f|^2 (x) + a f_t + ct f_0^2 (x)\right).$$

We separate the proof into two parts:

(i) Again we use the same method as in the proof of Theorem 1.1. We first claim that for each fixed $T > 3 + 2k$,

$$F\left(p(T), s(T),\ -4-2k,\ \tfrac{1}{T}\right) < \tfrac{(4+2k)^2(k+1)T}{3+2k},$$

where we choose $a = (-4-2k)$ and $c = \frac{1}{T}$ (here c depends on T).

We prove by contradiction. Suppose not; that is,

$$F\left(p(T), s(T),\ -4-2k,\ \tfrac{1}{T}\right) \geq \tfrac{(4+2k)^2(k+1)T}{3+2k}.$$

Since $F(p(t), s(t))$ is continuous in the variable t when a, c are fixed and $F(p(0), s(0)) = 0$, by Intermediate-value theorem there exists a $t_0 \in (0,\ T]$ such that

$$F\left(p(t_0), s(t_0),\ -4-2k,\ \tfrac{1}{T}\right) = \tfrac{(4+2k)^2(k+1)T}{3+2k}. \tag{4.15}$$

By assumption (1.5) and Lemma 3.6, we have $V(f) = 0$. Now substitute (4.15) into (4.10) at the point $(p(t_0), s(t_0))$. Hence

$$\begin{aligned} 0 \ \geq\ & \tfrac{1}{(4+2k)^2 s(t_0)} \tfrac{(4+2k)^2(k+1)T}{3+2k}\left[\tfrac{(4+2k)^2(k+1)T}{3+2k} - (4+2k)^2\right] \\ & + \left(1 - \tfrac{1}{T} - \tfrac{2}{(4+2k)^2 T}\tfrac{(4+2k)^2(k+1)T}{3+2k}\right) s(t_0) f_0^2 \\ & + \left(\tfrac{2(3+2k)}{(4+2k)^2 s(t_0)}\tfrac{(4+2k)^2(k+1)T}{3+2k} - 2k - \tfrac{2T}{s(t_0)}\right) s(t_0) |\nabla_b f|^2 . \end{aligned}$$

Then

$$0 \ \geq\ \tfrac{(k+1)(4+2k)^2 T}{(3+2k)s(t_0)}\left[\tfrac{(k+1)T}{3+2k} - 1\right] + \left(1 - \tfrac{1}{T} - \tfrac{2(k+1)}{3+2k}\right) s(t_0) f_0^2. \tag{4.16}$$

But for $T > 3 + 2k$, we have

$$\tfrac{(k+1)T}{3+2k} - 1 > 0 \tag{4.17}$$

and

$$1 - \tfrac{1}{T} - \tfrac{2(k+1)}{3+2k} \ =\ \tfrac{1}{3+2k} - \tfrac{1}{T} \ >\ 0. \tag{4.18}$$

This leads to a contradiction to (4.16).

Hence

$$F\left(p(T), s(T),\ -4-2k,\ \tfrac{1}{T}\right) < \tfrac{(4+2k)^2(k+1)T}{3+2k}.$$

This implies that

$$\max_{(x,t)\in M\times[0,\ T]} t\left[|\nabla_b f|^2(x) - (4+2k) f_t + \tfrac{t}{T} f_0^2(x)\right] \ <\ \tfrac{(4+2k)^2(k+1)T}{3+2k}.$$

When we fix on the set $\{T\} \times M$, we have

$$T\left[|\nabla_b f|^2(x) - (4+2k) f_t + f_0^2(x)\right] \ <\ \tfrac{(4+2k)^2(k+1)T}{3+2k}.$$

Hence for any $t > 3 + 2k$, we obtain

$$\frac{|\nabla_b u|^2}{u^2} - (4+2k)\frac{u_t}{u} < \frac{(4+2k)^2(k+1)}{3+2k}. \tag{4.19}$$

(ii) Secondly, we consider the case when

$$T \leq 3 + 2k.$$

We claim that

$$F\left(p(T), s\left(T\right), \ -4-2k, \ c\right) < \tfrac{(4+2k)^2(k+1)}{(3+2k)c},$$

where we also choose $a = -4-2k$ and $c < \frac{1}{3+2k}$ (here c does *not* depend on T).

We prove by contradiction. Suppose not; that is,

$$F\left(p(T), s\left(T\right), \ -4-2k, \ c\right) \geq \tfrac{(4+2k)^2(k+1)}{(3+2k)c}.$$

Since $F\left(p(t), s\left(t\right)\right)$ is continuous in the variable t when a, c are fixed and $F\left(p(0), s\left(0\right)\right) = 0$, by Intermediate-value theorem there exists a $t_0 \in (0, \ T]$ such that

$$F\left(p(t_0), s\left(t_0\right), \ -4-2k, \ c\right) = \tfrac{(4+2k)^2(k+1)}{(3+2k)c}. \tag{4.20}$$

By assumption (1.5) and Lemma 3.6, we have $V\left(f\right) = 0$. Now substitute (4.20) into (4.10) at the point $\left(p(t_0), s\left(t_0\right)\right)$. Hence

$$\begin{aligned} 0 \ \geq \ & \tfrac{1}{(4+2k)^2 s(t_0)} \tfrac{(4+2k)^2(k+1)}{(3+2k)c}\left[\tfrac{(4+2k)^2(k+1)}{(3+2k)c} - (4+2k)^2\right] \\ & + \left(1 - c - \tfrac{2(k+1)}{(3+2k)}\right) s\left(t_0\right) f_0^2 \\ & + \left(\tfrac{2(3+2k)}{(4+2k)^2 s(t_0)} \tfrac{(4+2k)^2(k+1)}{(3+2k)c} - 2k - \tfrac{2}{cs(t_0)}\right) s\left(t_0\right) \left|\nabla_b f\right|^2. \end{aligned}$$

Then

$$0 \ \geq \ \tfrac{(k+1)(4+2k)^2}{(3+2k)s(t_0)c}\left[\tfrac{(k+1)}{(3+2k)c} - 1\right] + \left(\tfrac{1}{(3+2k)} - c\right) s\left(t_0\right) f_0^2. \tag{4.21}$$

But for $c < \frac{1}{3+2k}$, we have

$$\tfrac{1}{(3+2k)} - c > 0$$

and

$$\frac{(k+1)}{(3+2k)c} - 1 > k > 0.$$

This leads a contradiction to (4.21).

Hence

$$F\left(p(T), s\left(T\right), \ -4-2k, c\right) < \tfrac{(4+2k)^2(k+1)}{(3+2k)c}$$

for $c < \frac{1}{3+2k}$ and $T \leq 3 + 2k$.

By the same argument as above, we have

$$\frac{\left|\nabla_b u\right|^2}{u^2} - (4+2k)\frac{u_t}{u} < \frac{(4+2k)^2(k+1)}{(3+2k)ct} \tag{4.22}$$

for $c < \frac{1}{3+2k}$ and $t \leq 3 + 2k$.

(iii) Combining (4.19) and (4.22), we obtain that for any fixed $c < \frac{1}{3+2k}$,

$$\frac{|\nabla_b u|^2}{u^2} - (4+2k)\,\frac{u_t}{u} < \frac{(4+2k)^2\,(k+1)}{(3+2k)\,ct} + \frac{(4+2k)^2\,(k+1)}{(3+2k)}$$

for all $t > 0$.

Finally, let $c \to \frac{1}{3+2k}$; we are done. This completes the proof. q.e.d.

Finally, we derive another CR version of parabolic Li-Yau gradient estimate for the positive solution of the CR heat equation. We refer to [**CTW**] also. We first need the following lemmas.

LEMMA 4.5. *Let (M, J, θ) be a closed pseudohermitian 3-manifold. If $u(x,t)$ is a solution of*

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

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

$$[\Delta_b,\ \mathbf{T}]\, u = 0$$

and

$$\Box_b \overline{\Box}_b u(x,0) = 0$$

at $t = 0$, then

$$\Box_b \overline{\Box}_b u(x,t) = 0 \text{ and } u_{\bar{1}11}(x,t) = 0$$

for all $t \in (0,\infty)$.

Proof. Note that if $[\Delta_b,\ \mathbf{T}]\, u = 0$,

$$\Box_b \overline{\Box}_b u = [(\Delta_b + i\mathbf{T})(\Delta_b - i\mathbf{T})]u = (\Delta_b)^2 u + T^2 u.$$

It follows from the assumption that $\Delta_b \Box_b \overline{\Box}_b u = \Box_b \overline{\Box}_b \Delta_b u$. Applying $\Box_b \overline{\Box}_b$ to the heat equation, we obtain

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

on $M \times [0,\infty)$ with $\Box_b \overline{\Box}_b u(x,0) = 0$. It follows from the maximum principle that $\Box_b \overline{\Box}_b u(x,t) = 0$. That is,

$$u_{\bar{1}11\bar{1}} + u_{1\bar{1}\bar{1}1} = 0.$$

Next, by commutation relations (2.4) and Lemma 3.4,

$$\begin{array}{rcl} u_{\bar{1}11\bar{1}} & = & u_{1\bar{1}\bar{1}1} - i[(A_{\bar{1}\bar{1}}u_1)_1 + (A_{11}u_{\bar{1}})_{\bar{1}}] \\ & = & u_{1\bar{1}\bar{1}1} - \frac{1}{2} i\,[\Delta_b,\ \mathbf{T}]\,u \\ & = & u_{1\bar{1}\bar{1}1}. \end{array}$$

Hence

$$u_{1\bar{1}\bar{1}1} = 0.$$

It follows that

$$|u_{\bar{1}11}|^2 = u_{\bar{1}11} u_{1\bar{1}\bar{1}} = (u_{\bar{1}1} u_{1\bar{1}\bar{1}})_1 - u_{\bar{1}1} u_{1\bar{1}\bar{1}1} = (u_{\bar{1}1} u_{1\bar{1}\bar{1}})_1.$$

Integrate both sides and by divergence theorem ([**GL**, p713]), we get

$$u_{\bar{1}11} = 0.$$

q.e.d.

Lemma 4.6. *([**CTW**]) Let (M, J, θ) be a closed pseudohermitian 3-manifold. Let $f = \ln u$, for $u > 0$. Then*

$$4\left\langle Pf + \bar{P}f, d_b f\right\rangle_{L_\theta^*} = 4\frac{\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*}}{u^2} - 2 < \nabla_b f, \nabla_b |\nabla_b f|^2 > -2\frac{\Delta_b u}{u}|\nabla_b f|^2. \tag{4.23}$$

Proof. It follows from the straightforward computation. q.e.d.

Proof of Theorem 1.6. Denote that

$$G = t\left(|\nabla_b f|^2 + 3f_t\right). \tag{4.24}$$

First differentiating (4.24) w.r.t. the t-variable, we have

$$\begin{aligned} G_t &= \frac{1}{t}G + t\left(|\nabla_b f|^2 + 3f_t\right)_t \\ &= \frac{1}{t}G + t\left(4|\nabla_b f|^2 + 3\Delta_b f\right)_t \\ &= \frac{1}{t}G + t\left[8\langle\nabla_b f, \nabla_b f_t\rangle + 3\Delta_b f_t\right]. \end{aligned} \tag{4.25}$$

By using the CR version of Bochner formula (3.3) and Lemma 4.6, one obtains

$$\begin{aligned} \Delta_b G &= t\left(\Delta_b |\nabla_b f|^2 + 3\Delta_b f_t\right) \\ &= t[2|(\nabla^H)^2 f|^2 + 6\langle\nabla_b f, \nabla_b \Delta_b f\rangle \\ &\quad +2(2W - 3Tor)((\nabla_b f)_{\mathbf{C}}, (\nabla_b f)_{\mathbf{C}}) \\ &\quad -8\langle Pf + \overline{P}f, d_b f\rangle_{L_\theta^*} + 3\Delta_b f_t] \\ &\geq t[4|f_{11}|^2 + (\Delta_b f)^2 + 6\langle\nabla_b f, \nabla_b \Delta_b f\rangle \\ &\quad + 2(2W - 3Tor)((\nabla_b f)_{\mathbf{C}}, (\nabla_b f)_{\mathbf{C}}) \\ &\quad -8\langle Pf + \bar{P}f, d_b f\rangle_{L_\theta^*} + 3\Delta_b f_t] \\ &= t[4|f_{11}|^2 + (\Delta_b f)^2 + 6\langle\nabla_b f, \nabla_b \Delta_b f\rangle \\ &\quad + 2(2W - 3Tor)((\nabla_b f)_{\mathbf{C}}, (\nabla_b f)_{\mathbf{C}}) \\ &\quad -8u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*} + 4f_t|\nabla_b f|^2 \\ &\quad +4\left\langle\nabla_b f, \nabla_b|\nabla_b f|^2\right\rangle + 3\Delta_b f_t]. \end{aligned} \tag{4.26}$$

Here we have used the inequalities

$$\left|(\nabla^H)^2 f\right|^2 = 2\left|f_{11}\right|^2 + \frac{1}{2}(\Delta_b f)^2 + \frac{1}{2}f_0^2 \geq 2\left|f_{11}\right|^2 + \frac{1}{2}(\Delta_b f)^2,$$

and

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

Applying the formula

$$\Delta_b f = f_t - |\nabla_b f|^2 = \frac{1}{3t}G - \frac{4}{3}\left|\nabla_b f\right|^2 \tag{4.27}$$

and combining (4.25), (4.26), we conclude

$$\begin{aligned}\left(\Delta_b - \frac{\partial}{\partial t}\right)G \geq & -\frac{1}{t}G + t[4\left|f_{11}\right|^2 + (\Delta_b f)^2 + 6\left\langle \nabla_b f, \nabla_b \Delta_b f\right\rangle \\ & + 4\left\langle \nabla_b f, \nabla_b |\nabla_b f|^2\right\rangle - 8\langle \nabla_b f, \nabla_b f_t\rangle \\ & + 2(2W - 3Tor)((\nabla_b f)_{\mathbf{C}}, (\nabla_b f)_{\mathbf{C}}) \\ & + 4f_t|\nabla_b f|^2 - 8u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*}] \\ = & -\frac{1}{t}G + t[-\frac{2}{3t}\langle \nabla_b f, \nabla_b G\rangle - \frac{4}{3}\left\langle \nabla_b f, \nabla_b |\nabla_b f|^2\right\rangle \\ & + 4\left|f_{11}\right|^2 + (\Delta_b f)^2 \\ & + 4f_t|\nabla_b f|^2 + 2(2W - 3Tor)((\nabla_b f)_{\mathbf{C}}, (\nabla_b f)_{\mathbf{C}}) \\ & - 8u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*}].\end{aligned}$$

Now it is easy to see that

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

Thus

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

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

$$\begin{aligned}(4.28)\qquad \left(\Delta_b - \frac{\partial}{\partial t}\right) G \geq & -\frac{1}{t}G - \frac{2}{3}\langle \nabla_b f, \nabla_b G\rangle + t[(\Delta_b f)^2 \\ & + \frac{8}{3}\Delta_b f|\nabla_b f|^2 + \frac{32}{9}|\nabla_b f|^4 \\ & + 2(2W - 3Tor)((\nabla_b f)_{\mathbf{C}}, (\nabla_b f)_{\mathbf{C}}) \\ & - 8u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*}] \\ \geq & -\frac{2}{3}\langle \nabla_b f, \nabla_b G\rangle + \frac{1}{9t}G(G-9) \\ & + t[2(2W - 3Tor)((\nabla_b f)_{\mathbf{C}}, (\nabla_b f)_{\mathbf{C}}) \\ & - 8u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*}].\end{aligned}$$

Now from (3.2), we have

$$\begin{aligned}u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*} &= u^{-2}[(u_{\bar{1}11}u_{\bar{1}} + u_{1\bar{1}\bar{1}}u_1) + (iA_{11}u_{\bar{1}}u_{\bar{1}} - iA_{\bar{1}\bar{1}}u_1u_1)] \\ &= u^{-2}(u_{\bar{1}11}u_{\bar{1}} + u_{1\bar{1}\bar{1}}u_1) + (iA_{11}f_{\bar{1}}f_{\bar{1}} - iA_{\bar{1}\bar{1}}f_1f_1).\end{aligned}$$

Hence, from Lemma 4.5,

(4.29)

$$\begin{aligned}2(2W - 3Tor)&((\nabla_b f)_{\mathbf{C}}, (\nabla_b f)_{\mathbf{C}}) - 8u^{-2}\left\langle Pu + \bar{P}u, d_b u\right\rangle_{L_\theta^*} \\ &= 2(2W + Tor)((\nabla_b f)_{\mathbf{C}}, (\nabla_b f)_{\mathbf{C}}) - 8u^{-2}(u_{\bar{1}11}u_{\bar{1}} + u_{1\bar{1}\bar{1}}u_1) \\ &= 2(2W + Tor)((\nabla_b f)_{\mathbf{C}}, (\nabla_b f)_{\mathbf{C}}) \\ &\geq 0.\end{aligned}$$

It follows from (4.28), (4.29) that

$$(4.30)\qquad \left(\Delta_b - \frac{\partial}{\partial t}\right) G \geq -\frac{2}{3}\langle \nabla_b f, \nabla_b G\rangle + \frac{1}{9t}G(G-9).$$

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

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

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

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

and

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

Combining with (4.30), this implies

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

which is a contradiction. Hence $G \leq 9$ and Theorem 1.6 follows. q.e.d.

Proof of Theorem 1.10. Let γ be a horizontal curve with $\gamma(t_1) = x_1$ and $\gamma(t_2) = x_2$. We define $\eta : [t_1, t_2] \to M \times [t_1, t_2]$ by

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

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

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

Applying Theorem 1.1 to f_t, this yields

$$\begin{aligned} f(x_2, t_2) - f(x_1, t_1) &\geq \int_{t_1}^{t_2} \left\{ \frac{1}{4} |\nabla_b f|^2 - \frac{4}{t} + \langle \dot{\gamma}, \nabla_b f \rangle \right\} dt \\ &\geq -\int_{t_1}^{t_2} |\dot{\gamma}|^2 \, dt - 4 \ln(\frac{t_2}{t_1}). \end{aligned}$$

Now we choose

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

Then the inequality in Theorem 1.10 follows by taking exponentials of the above inequality.

q.e.d.

5. Perelman-Type Entropy Formulae

In this section, we prove the monotonicity formulae for $\widetilde{N}(u, t)$ and $\widetilde{\mathcal{W}}(u, t)$ under the CR heat equation (1.1):

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

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

Proof of Theorem 1.12. Let g be the function which satisfies

$$u(x, t) = \frac{e^{-g(x,t)}}{(4\pi t)^{16 \times a}}$$

with $\int_M u d\mu = 1$. Here $a > 0$, to be determined. Denote $f = \ln u$. Then

$$f = -g - (16 \times a) \ln(4\pi t).$$

Since

$$|\nabla_b f|^2 = |\nabla_b g|^2 \quad \text{and} \quad f_t = -g_t - \frac{16 \times a}{t}$$

and from Corollary 1.3,

$$|\nabla_b f|^2 - 4 f_t - \frac{16}{t} < 0.$$

It follows that

$$|\nabla_b g|^2 + 4g_t + \frac{16 \times (4a-1)}{t} < 0. \tag{5.1}$$

Hence

$$\begin{aligned}
\frac{d}{dt}N(u,t) &= -\frac{d}{dt}\int_M u \ln u d\mu = -\int_M u_t \ln u d\mu - \int_M u \frac{u_t}{u} d\mu \\
&= -\int_M \ln u \Delta_b u d\mu = -\int_M u \Delta_b \ln u d\mu \\
&= -\int_M (\Delta_b u - \frac{|\nabla_b u|^2}{u}) d\mu = \int_M (\frac{|\nabla_b u|^2}{u}) d\mu \\
&= \int_M u |\nabla_b g|^2 d\mu
\end{aligned}$$

and

$$\begin{aligned}
\frac{d}{dt}\widetilde{N}(u,t) &= \frac{d}{dt}N(u,t) - \frac{16 \times a}{t} \\
&= \int_M |\nabla_b g|^2 u d\mu - \frac{16 \times a}{t}.
\end{aligned}$$

But

$$\begin{aligned}
\int_M g_t u d\mu &= -\int_M f_t u d\mu - \frac{16 \times a}{t}\int_M u d\mu \\
&= -\int_M u_t d\mu - \frac{16 \times a}{t} \\
&= -\frac{16 \times a}{t}.
\end{aligned}$$

Thus

$$\frac{d}{dt}\widetilde{N}(u,t) = \int_M (|\nabla_b g|^2 + 4g_t + \frac{16 \times 3a}{t}) u d\mu.$$

Now if we choose

$$0 < 3a \leq 4a - 1,$$

that is,

$$a \geq 1,$$

it follows from (5.1) that

$$\frac{d}{dt}\widetilde{N}(u,t) < 0.$$

q.e.d.

Proof of Theorem 1.13. Compute

$$\begin{aligned}
\mathcal{W} &= \int_M [t|\nabla_b g|^2 - \ln u - (16\times a)\ln(4\pi t) - (16\times 2a)] u d\mu \\
&= \int_M (t|\nabla_b g|^2 - (16\times a)) u d\mu \\
&- [\int_M u\ln u d\mu + \int_M (16\times a)(\ln(4\pi t)+1) u d\mu] \\
&= t[\int_M (|\nabla_b g|^2 - \frac{16\times a}{t}) u d\mu] \\
&- [\int_M u\ln u d\mu + \int_M (16\times a)(\ln(4\pi t)+1) u d\mu] \\
&= t\frac{d}{dt}\widetilde{N}(u,t) + \widetilde{N}(u,t) \\
&= \frac{d}{dt}(t\widetilde{N}(u,t)).
\end{aligned} \tag{5.2}$$

Hence

$$\frac{d}{dt}\mathcal{W} = 2\frac{d}{dt}\widetilde{N}(u,t) + t\frac{d^2}{dt^2}\widetilde{N}(u,t).$$

It follows that

(5.3)

$$\begin{aligned}
\frac{d^2}{dt^2}\widetilde{N}(u,t) &= \frac{d}{dt}[-\int_M u\Delta_b \ln u d\mu - \frac{16\times a}{t}] \\
&= -\int_M u_t \Delta_b \ln u d\mu - \int_M u\frac{\partial}{\partial t}(\Delta_b \ln u) d\mu + \frac{16\times a}{t^2} \\
&= -\int_M \Delta_b u \Delta_b \ln u d\mu - \int_M u\frac{\partial}{\partial t}(\Delta_b \ln u) d\mu + \frac{16\times a}{t^2}.
\end{aligned}$$

Note that

$$\begin{aligned}
(\frac{\partial}{\partial t} - \Delta_b)(\Delta_b \ln u) &= \Delta_b(\frac{\partial}{\partial t} - \Delta_b)\ln u \\
&= \Delta_b[\frac{u_t}{u} - (\frac{\Delta_b u}{u} - \frac{|\nabla_b u|^2}{u^2})] \\
&= \Delta_b(|\nabla_b \ln u|^2).
\end{aligned}$$

Again, from the CR Bochner formula, we have

$$\begin{aligned}
\Delta_b(|\nabla_b \ln u|^2) &\geq 2|(\nabla^H)^2 \ln u|^2 + 2\langle \nabla_b \ln u,\ \nabla_b \Delta_b \ln u\rangle \\
&+ 2(W - \frac{1}{\nu})|\nabla_b \ln u|^2 - 2\nu|\nabla_b(\ln u)_0|^2
\end{aligned}$$

for all $\nu > 0$, where W is the Tanaka-Webster curvature. It follows from (5.3) that

$$\begin{aligned}\frac{d^2}{dt^2}\widetilde{N}(u,t) &= -\int_M \Delta_b u \Delta_b \ln u d\mu - \int_M u\frac{\partial}{\partial t}(\Delta_b \ln u)d\mu + \frac{16\times a}{t^2}\\ &= -\int_M \Delta_b u \Delta_b \ln u d\mu + \frac{16\times a}{t^2}\\ &\quad -\int_M u(\frac{\partial}{\partial t} - \Delta_b)\Delta_b \ln u d\mu - \int_M u\Delta_b(\Delta_b \ln u)d\mu\\ &\le -\int_M \Delta_b u(\Delta_b \ln u)d\mu + \frac{16\times a}{t^2} - 2\int_M u|(\nabla^H)^2 \ln u|^2 d\mu\\ &\quad - 2\int_M u\left\langle \nabla_b \ln u,\ \nabla_b\Delta_b \ln u\right\rangle d\mu\\ &\quad - 2\int_M u(W - \frac{1}{\nu})|\nabla_b \ln u|^2 d\mu\\ &\quad\ + 2\int_M \nu|\nabla_b(\ln u)_0|^2 u d\mu - \int_M u\Delta_b(\Delta_b \ln u)d\mu.\end{aligned}$$

Thus

$$\begin{aligned}\frac{d}{dt}\mathcal{W} &= t\frac{d^2}{dt^2}\widetilde{N}(u,t) + 2\frac{d}{dt}\widetilde{N}(u,t)\\ &\le -t\int_M \Delta_b u(\Delta_b \ln u)d\mu + \frac{16\times a}{t} - 2t\int_M u|(\nabla^H)^2 \ln u|^2 d\mu\\ &\quad - 2t\int_M u < \nabla_b \ln u, \nabla_b\Delta_b \ln u > d\mu\\ &\quad - 2t\int_M u(W - \frac{1}{\nu})|\nabla_b \ln u|^2 d\mu\\ &\quad + 2t\nu\int_M |\nabla_b(\ln u)_0|^2 u d\mu - t\int_M u\Delta_b(\Delta_b \ln u)d\mu\\ &\quad + 2\int_M |\nabla_b g|^2 u d\mu - \frac{16\times 2a}{t}.\end{aligned}$$

But

$$\int_M \Delta_b u \Delta_b \ln u d\mu = -\int_M < \nabla_b u, \nabla_b\Delta_b \ln u > d\mu$$

and

$$\int_M u\left\langle \nabla_b \ln u,\ \nabla_b\Delta_b \ln u\right\rangle d\mu = \int_M \left\langle \nabla_b u,\ \nabla_b\Delta_b \ln u\right\rangle d\mu.$$

This implies

$$\begin{aligned}-t\int_M \Delta_b u(\Delta_b \ln u)d\mu - 2t\int_M u\left\langle \nabla_b \ln u,\ \nabla_b\Delta_b \ln u\right\rangle d\mu - t\\ \int_M u\Delta_b(\Delta_b \ln u)d\mu = 0.\end{aligned}$$

Therefore

$$\begin{aligned}\frac{d}{dt}\mathcal{W} \leq & -2t\int_M u|(\nabla^H)^2\ln u|^2 d\mu - \frac{16\times a}{t} \\ & -2t\int_M u(W-\frac{1}{\nu})|\nabla_b \ln u|^2 d\mu + 2t\nu\int_M |\nabla_b(\ln u)_0|^2 u d\mu \\ & +2\int_M |\nabla_b g|^2 u d\mu.\end{aligned} \tag{5.4}$$

Now for some $\alpha > 0$, to be determined later such that $\frac{d}{dt}\widetilde{\mathcal{W}_\alpha} \leq 0$, we consider

$$\widetilde{\mathcal{W}_\alpha} = \int_M (t|\nabla_b g|^2 + g - (16\times 2a) + \alpha t^2 g_0^2)\frac{e^{-g(x,t)}}{(4\pi t)^{16\times a}}d\mu.$$

Thus

$$\begin{aligned}\frac{d}{dt}\widetilde{\mathcal{W}_\alpha} \leq & -2t\int_M u|(\nabla^H)^2\ln u|^2 d\mu + 2t\nu\int_M |\nabla_b(\ln u)_0|^2 u d\mu \\ & -2t\int_M u(W-\frac{1}{\nu})|\nabla_b\ln u|^2 d\mu + 2\int_M |\nabla_b g|^2 u d\mu \\ & +2\alpha t\int_M u g_0^2 d\mu + 2\alpha t^2\int_M u g_0 g_{0t} d\mu \\ & +\alpha t^2\int_M g_0^2\Delta_b u d\mu - \frac{16\times a}{t}.\end{aligned}$$

Now since

$$|(\nabla^H)^2 g|^2 = 2|g_{11}|^2 + \frac{1}{2}(\Delta_b g)^2 + \frac{1}{2}g_0^2$$

and

$$\ln u = -g - (16\times a)\ln(4\pi t),$$

hence

$$\begin{aligned}\frac{d}{dt}\widetilde{\mathcal{W}_\alpha} \leq & -4t\int_M u|g_{11}|^2 d\mu - t\int_M u(\Delta_b g)^2 d\mu - t\int_M u g_0^2 d\mu \\ & +2t\nu\int_M |\nabla_b g_0|^2 u d\mu - 2t\int_M u(W-\frac{1}{\nu})|\nabla_b g|^2 d\mu \\ & +2\int_M |\nabla_b g|^2 u d\mu + 2\alpha t\int_M u g_0^2 d\mu \\ & +2\alpha t^2\int_M u g_0 g_{0t} d\mu + \alpha t^2\int_M g_0^2\Delta_b u d\mu \\ & -\frac{16\times a}{t}.\end{aligned}$$

Since $u(x,t) = \frac{e^{-g(x,t)}}{(4\pi t)^{16\times a}}$, we have

$$\Delta_b g = g_t + |\nabla_b g|^2 + \frac{16\times a}{t}$$

and due to $A_{11} = 0$,

$$\begin{aligned}(g_t + \Delta_b g)_0 &= (2\Delta_b g - |\nabla_b g|^2 - \tfrac{16\times a}{t})_0 \\ &= 2\Delta_b g_0 - 2 < \nabla_b g,\ \nabla_b g_0 > .\end{aligned}$$

Then

$$\begin{aligned}&2\alpha t^2 \int_M u g_0 g_{0t} d\mu + \alpha t^2 \int_M g_0^2 \Delta_b u d\mu \\ &= 2\alpha t^2 \int_M u g_0 g_{0t} d\mu + 2\alpha t^2 \int_M g_0 \Delta_b g_0 u d\mu + 2\alpha t^2 \int_M |\nabla_b g_0|^2 u d\mu \\ &= 2\alpha t^2 \int_M u g_0 (g_t + \Delta_b g)_0 d\mu + 2\alpha t^2 \int_M |\nabla_b g_0|^2 u d\mu \\ &= 4\alpha t^2 \int_M u g_0 \Delta_b g_0 d\mu - 4\alpha t^2 \int_M u g_0 \left\langle \nabla_b g,\ \nabla_b g_0 \right\rangle d\mu + 2\alpha t^2 \\ &\quad \int_M |\nabla_b g_0|^2 u d\mu \\ &= -4\alpha t^2 \int_M u_0 \Delta_b g_0 d\mu - 4\alpha t^2 \int_M u g_0 \left\langle \nabla_b g,\ \nabla_b g_0 \right\rangle d\mu + 2\alpha t^2 \\ &\quad \int_M |\nabla_b g_0|^2 u d\mu \\ &= 4\alpha t^2 \int_M \left\langle \nabla_b u_0,\ \nabla_b g_0 \right\rangle d\mu - 4\alpha t^2 \int_M u g_0 \left\langle \nabla_b g,\ \nabla_b g_0 \right\rangle d\mu + 2\alpha t^2 \\ &\quad \int_M |\nabla_b g_0|^2 u d\mu \\ &= -4\alpha t^2 \int_M u |\nabla_b g_0|^2 d\mu - 4\alpha t^2 \int_M g_0 \left\langle \nabla_b u,\ \nabla_b g_0 \right\rangle d\mu \\ &\quad - 4\alpha t^2 \int_M u g_0 < \nabla_b g,\ \nabla_b g_0 > d\mu + 2\alpha t^2 \int_M |\nabla_b g_0|^2 u d\mu \\ &= -4\alpha t^2 \int_M u |\nabla_b g_0|^2 d\mu + 4\alpha t^2 \int_M g_0 u < \nabla_b g,\ \nabla_b g_0 > d\mu \\ &\quad - 4\alpha t^2 \int_M u g_0 < \nabla_b g,\ \nabla_b g_0 > d\mu + 2\alpha t^2 \int_M u |\nabla_b g_0|^2 d\mu \\ &= -2\alpha t^2 \int_M u |\nabla_b g_0|^2 d\mu.\end{aligned}$$

Therefore

$$\begin{aligned}\frac{d}{dt}\widetilde{\mathcal{W}_\alpha} &\leq -4t \int_M u |g_{11}|^2 d\mu - t \int_M u (\Delta_b g)^2 d\mu + (2\alpha - 1) t \int_M u g_0^2 d\mu \\ &\quad + (2t\nu - 2\alpha t^2) \int_M u |\nabla_b g_0|^2 d\mu - 2t \int_M u W |\nabla_b g|^2 d\mu \\ &\quad + (2 + \frac{2t}{\nu}) \int_M u |\nabla_b g|^2 d\mu - \frac{16 \times a}{t}.\end{aligned}$$

Choose $\alpha = \frac{1}{2}$ and $\nu = \frac{1}{2}t$; then

$$\widetilde{\mathcal{W}} = \widetilde{\mathcal{W}_{\frac{1}{2}}}$$

and

(5.5)

$$\frac{d}{dt}\widetilde{\mathcal{W}} \leq -4t\int_M u|g_{11}|^2 d\mu - t\int_M u(\Delta_b g)^2 d\mu - 2t\int_M uW|\nabla_b g|^2 d\mu + 6\int_M u|\nabla_b g|^2 d\mu - \frac{16 \times a}{t}.$$

But from Corollary 1.3,

$$\begin{array}{rcl} \int_M u|\nabla_b g|^2 d\mu & = & \int_M u|\nabla_b f|^2 d\mu \\ & < & 4\int_M u\frac{u_t}{u} d\mu + \frac{16}{t}\int_M u d\mu \\ & = & \frac{16}{t}. \end{array}$$

Then

$$6\int_M u|\nabla_b g|^2 d\mu = \frac{16 \times 6}{t}.$$

Now if we choose

$$a \geq 6,$$

it follows from (5.5) that

$$\frac{d}{dt}\widetilde{\mathcal{W}} \leq -4t\int_M u|g_{11}|^2 d\mu - t\int_M u(\Delta_b g)^2 d\mu - 2t\int_M uW|\nabla_b g|^2 d\mu.$$

If

$$W \geq 0 \quad \text{with} \quad a \geq 6,$$

then

$$\frac{d}{dt}\widetilde{\mathcal{W}}(u,t) \leq 0.$$

q.e.d.

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