A positive mass theorem in three dimensional Cauchy-Riemann geometry

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ABSTRACT. We define an ADM-like mass, called p-mass, for an asymptotically flat pseudohermitian manifold. The p-mass for the blow-up of a compact pseudohermitian manifold (with no boundary) is identified with the first nontrivial coefficient in the expansion of the Green function for the CR Laplacian. We deduce an integral formula for the p-mass, and we reduce its positivity to a solution of Kohn's equation. We prove that the p-mass is non-negative for (blow-ups of) compact 3-manifolds of positive CR Yamabe invariant and with non-negative CR Paneitz operator. Under these assumptions, we also characterize the zero mass case as the standard three dimensional CR sphere. We then show the existence of (non-embeddable) CR 3-manifolds having nonpositive Paneitz operator or negative p-mass through a second variation formula. Finally, we apply our main result to find solutions of the CR Yamabe problem with minimal energy.

Key Words: CR geometry, positive mass theorem, CR Paneitz operator, Tanaka-Webster curvature, CR Yamabe problem

AMS subject classification: 32V20, 53C17, 35J75, 35J20, 32V30

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1 Introduction and statement of the results

Around 1960 the three physicists R.Arnowitt, S.Deser, and C.Misner developed the Hamiltonian formulation for Einstein's general theory of relativity in a series of papers, see e.g. [2], [3]. The total energy was called the *ADM-mass* later in the literature. The positive mass conjecture asserts the non-negativity of such a quantity assuming non-negativity of the local energy density, and classifies the situation for the zero mass case. The conjecture was proved by R.Schoen and S.T.Yau using minimal surface theory ([37], [38], [39], [40]) and by Witten using the Dirac equation for spinors ([42]; a rigorous proof is given in [34]) in late 70's and early 80's.

The positive mass theorem was then used by Schoen in [36] to prove the Yamabe conjecture (finding conformal metrics with constant scalar curvature) in the cases left open in 1976 by T.Aubin ([4]), namely in dimension 3, 4, 5 or when the metric is locally conformally flat. As shown in [41], to solve the problem (in the *positive case*, the most difficult one) it is sufficient to show that the Yamabe quotient of the manifold is smaller than the one of $\mathbb{S}^n$. This was done both in [4] and in [36] using suitable test functions. In particular Schoen's argument consists in gluing a *standard bubble* near any $p \in M$ to $\mathcal{G}_p$, the Green's function of the conformal Laplacian with pole at p. It turns out that the regular part of $\mathcal{G}_p$ coincides with the mass of $(M \setminus \{p\}, \mathcal{G}_p^{\frac{4}{n-2}} g)$, the *blow-up* of M at p. The positive mass theorem played a key role in other problems in conformal geometry, for example in the compactness of the Yamabe equation or the Yamabe flow, see [7], [8], [30].

Since there is a strong analogy between CR geometry and conformal geometry, one may wonder about what happens in CR geometry correspondingly. The goal of this paper is to introduce a notion of asymptotically flat pseudohermitian manifold, define a *pseudohermitian mass* and to prove its positivity under suitable conditions. We give then applications concerning existence of minimizers for the CR Yamabe quotient, which is useful to study the CR analogue of the Yamabe quotient.

We consider a compact three dimensional pseudohermitian manifold (M, J, θ) (with no boundary) of *positive CR Yamabe invariant*. This means that the first eigenvalue of the *CR invariant sublaplacian*

$$L_b := -4\Delta_b + R,$$

is strictly positive. Here Δ_b stands for the sublaplacian of M and R for the Tanaka-Webster curvature, see Subsection 1.1 for their definition. The CR invariant sublaplacian has the following covariance property under a conformal change of contact form

$$\hat{L}_b(\varphi) = u^{-\frac{Q+2}{Q-2}} L_b(u\varphi); \qquad \hat{\theta} = u^2\theta,$$

where $Q = 4$ is the *homogeneous dimension* of the manifold. The CR invariant sublaplacian rules the change of the Tanaka-Webster curvature under the above conformal deformation, through the following formula

$$-4\Delta_b u + Ru = \hat{R} u^{\frac{Q+2}{Q-2}},$$

where $\hat{R}$ is the Tanaka-Webster curvature corresponding to the pseudohermitian structure $(J, \hat{\theta})$. The positivity of the CR Yamabe invariant is equivalent to the condition

$$\text{(1)} \qquad \mathcal{Y}(J) := \inf_{\hat{\theta}} \frac{\int_M R_{J,\hat{\theta}} \hat{\theta} \wedge d\hat{\theta}}{\left(\int_M \hat{\theta} \wedge d\hat{\theta}\right)^{\frac{1}{2}}} > 0,$$

where $\hat{\theta}$ is any contact form which annihilates ξ (the contact bundle). Under the assumption $\mathcal{Y}(J) > 0$ we have that L_b is invertible so for any $p \in M$ there exists a Green's function G_p for which

$$(-4\Delta_b + R)\, G_p = 16\delta_p.$$

One can show that in CR normal coordinates (z, t) (see Subsection A.2) G_p admits the following expansion

$$G_p = \frac{1}{2\pi}\rho^{-2} + A + O(\rho),$$

where A is some real constant and where we have set $\rho^4(z,t) = |z|^4 + t^2$, $z \in \mathbb{C}, t \in \mathbb{R}$. Having in mind the Riemannian construction for the blow-up of a compact manifold, we consider in Subsection 2.1 the new pseudohermitian manifold with a blow-up of contact form

$$N = (M \setminus \{p\}, J, \theta = G_p^2 \hat{\theta}), \tag{2}$$

where $\hat{\theta}$ is the contact form described in Proposition A.5. With an *inversion of coordinates* (described in Subsection 2.2) we then obtain a pseudohermitian manifold which has asymptotically the geometry of the Heisenberg group. Starting from this model, in Subsection 2.3 we give a definition of asymptotically flat pseudohermitian manifold and we introduce its *pseudohermitian mass* (p-mass) by the formula

$$m(J,\theta) := i \oint_{\infty} \omega_1^1 \wedge \theta := \lim_{\Lambda \to +\infty} i \oint_{S_\Lambda} \omega_1^1 \wedge \theta,$$

where we have set $S_\Lambda = \{\rho = \Lambda\}$, $\rho^4 = |z|^4 + t^2$, and where ω_1^1 stands for the connection form of the structure, see Subsection 1.1. The above quantity is indeed a natural candidate, since it satisfies a property analogous to the Einstein-Hilbert action (see (45) and Remark 2.4), and moreover it coincides with the zero-th order term in the expansion of the Green's function for L_b, see Lemma 2.5.

In our main theorem we give some general conditions which ensure the non-negativity of the p-mass for blow-ups of compact manifolds, characterizing also the zero case as (CR equivalent to) the standard CR sphere.

Theorem 1.1 *Let M be a smooth, strictly pseudoconvex three dimensional compact CR manifold. Suppose $\mathcal{Y}(J) > 0$, and that the CR Paneitz operator is non-negative. Let $p \in M$ and let θ be a blow-up of contact form as in* (2). *Then*

(a) $m(J,\theta) \geq 0$*;*

(b) *if $m(J,\theta) = 0$, M is CR equivalent (or, together with $\hat{\theta}$, isomorphic as pseudohermitian manifold) to S^3, endowed with its standard CR structure (and its standard contact form).*

In Subsection 2.3 we prove an integral formula for the p-mass, in the spirit of [42]. To state this formula we need to introduce another conformally covariant operator, the CR Paneitz operator

$$P\varphi := 4({\varphi_{\bar{1}}}^{\bar{1}}{}_1 + iA_{11}\varphi^1)^1$$

(where we are following the notation of Subsection 1.1). The operator P is a real self-adjoint operator ([24], [25]) and satisfies the covariance property ([25])

$$P_{(J,\hat{\theta})} = u^{-4} P_{(J,\theta)}; \qquad \hat{\theta} = u^2\theta. \tag{3}$$

In Proposition 2.6 we prove then the following integral formula, which holds for an asymptotically flat pseudohermitian manifold N

$$\frac{2}{3} m(J,\theta) = -\int_N |\Box_b \beta|^2 \theta \wedge d\theta + 2\int_N |\beta_{,\bar{1}\bar{1}}|^2 \theta \wedge d\theta + 2\int_N R|\beta_{,\bar{1}}|^2 \theta \wedge d\theta + \frac{1}{2}\int_N \overline{\beta} P\beta\, \theta \wedge d\theta. \tag{4}$$

Here $\beta : N \to \mathbb{C}$ is a function satisfying

$$\beta = \overline{z} + \beta_{-1} + O(\rho^{-2+\varepsilon}) \quad \text{near } \rho = \infty; \qquad \Box_b \beta = O(\rho^{-4}) \quad \text{near } \rho = \infty,$$

with $\Box_b \beta = -2\beta_{,\bar{1}1}$ and with β_{-1} a suitable function with homogeneity -1 in ρ, satisfying condition (35) below, which comes from a Taylor expansion of the $\Box_b$ operator at infinity. To explain the link between the spinor method in [42] and the $\Box_b$ operator, we refer the reader to the end of Section 2.

We prove Theorem 1.1 in Section 3. The assumptions we give here are CR invariant, and are needed to ensure the positivity of the right-hand side in (4). By the result in [12], the conditions on $\mathcal{Y}(J)$ and

P imply the embeddability of M: we use this property to find a solution of $\Box_b \beta = 0$ with the above asymptotics (and hence to make the first term in the right-hand side of (4) vanish): we first find an approximate solution through the expansion of $\Box_b \bar{z}$ at infinity, and then through the analysis of the Szegö projection of this quantity, see Subsection 3.2. To obtain the full solvability of $\Box_b \beta = 0$ we then employ a mapping theorem in weighted spaces from [26]. The positivity of the CR Paneitz operator is used instead to control the last term in the right-hand side of (4), showing that it is the sum of a non-negative term and a (negative) multiple of $m(J, \theta)$ which can be reabsorbed into the left-hand side, see Subsection 3.5. More comments on the relation between the embeddability and the non-negativity of P for manifolds of positive CR Yamabe invariant are given in Remark 1.4. As a matter of fact, non-negativity of the CR Paneitz operator is preserved under embedded analytic deformations.

Corollary 1.1 *Let M be a smooth, strictly pseudoconvex three dimensional compact CR manifold. Suppose M is an embedded, small enough, analytic deformation of the standard CR three sphere. Let $p \in M$ and let θ be a blow-up of contact form as in* (2)*. Then the same conclusions of Theorem 1.1 hold.*

In Section 4 we construct some examples of structures using the deformation formulas in Subsection A.1. First, using second variation formulas, in Subsection 4.1 we consider perturbations of the spherical structure for which P fails to be non-negative, see Proposition 4.1 (and also [12]). Then, in Subsection 4.2 we derive the first and second variations of the mass near the standard sphere. We also construct examples of manifolds with positive CR Yamabe invariant and negative mass (when the blow-up is done at suitable points), see Proposition 4.4. This is in striking contrast with the Riemannian case, where all perturbations of the sphere give rise to blown-up manifolds with positive mass (except for metrics conformally equivalent to the spherical one). We also describe an example of CR structure on $S^2 \times S^1$ with non-negative Paneitz operator and non-vanishing torsion, obtained as quotient of $\mathbb{H}^1 \setminus \{0\}$. This example is geometrically interesting. It is one of a few models for the class of S^1-invariant compact spherical CR 3-manifolds and plays an essential role in the classification problem.

Our next main goal is to apply Theorem 1.1 to the study of the CR Yamabe problem, namely finding conformal changes of contact form in order to obtain constant Tanaka-Webster curvature. As for the classical Yamabe problem, the cases $\mathcal{Y}(J) \leq 0$ are more directly treatable (see [20]), while the case $\mathcal{Y}(J) > 0$ is the most difficult one. Calling $\mathcal{Y}_0$ the quotient for the standard CR three sphere, by a result in [27] one always has

$$\mathcal{Y}(J) \leq \mathcal{Y}_0, \tag{5}$$

and if strict inequality holds, then the problem is solvable. The strict inequality is needed to ensure compactness of the minimizing sequences in (1). This condition was verified in [29] for $n \geq 2$ and non-spherical structures, in the spirit of [4] through some expansions involving the local geometry.

The positivity of the mass is instead a more global property, and it enters when G_p has the following expansion near p :

$$G_p = c_n \rho^{-2n} + A + O(\rho), \tag{6}$$

where ρ is the Heisenberg distance in CR normal coordinates. It turns out that the term A is a multiple of the mass defined for the blow-up M. We observe that (6) holds for $n = 1$ (dimension 3 case) and for N being spherical of all dimensions.

For such manifolds of $n \geq 2$ (some extra technical condition in dimension 5, $n = 2$) with positive CR Yamabe invariant, one can prove a positive mass theorem for A (and hence find solutions of the CR Yamabe problem with minimal energy) through another approach ([17]).

Our next result gives the strict Webster-Sobolev inequality (5) in the three dimensional case (the only one left), if M is not CR equivalent to the standard CR three-sphere, under the same assumptions as in the previous theorem.

Theorem 1.2 *Let M be a smooth, strictly pseudoconvex three dimensional compact CR manifold. Suppose $\mathcal{Y}(J) > 0$, and that the CR Paneitz operator is non-negative. Then either M is the standard CR three-sphere or if M is not CR equivalent to the standard CR three-sphere one has $\mathcal{Y}(J) < \mathcal{Y}_0$. In both cases, the CR Yamabe quotient admits a smooth minimizer.*

The CR Yamabe problem for the case of three-dimensional CR manifolds and for spherical CR manifolds was solved in [22] and [23] respectively (we also refer to [20] and [17]). While the proof in these papers relies on topological arguments and may not provide energy extremals, in the spirit of [5], our argument is based on direct minimization and gives an extra variational characterization on the solutions (see more comments in Remark 5.4). To prove strict inequality we follow Schoen's argument in [36], finding test functions which resemble a CR bubble at a small scale, and the Green's function G_p at a larger one. The construction is performed in Section 5. More in general, the analysis of the Yamabe problem in the CR case has been so far less precise than the Riemannian case: for example a basic difficulty is the lack of a moving plane method, which is useful in general to derive a priori estimates and to classify entire solutions.

In the Appendix we collect some useful tools: first the variations of some geometric quantities under a deformation of the CR structure, and then the CR normal coordinates introduced in [29]. The latter are needed here to derive asymptotic estimates on the Green's function near its singularity and on the geometric quantities on asymptotically flat manifolds.

1.1 Notation and preliminaries

We collect here some useful material: throughout this paper, we will mostly use notations taken from [31]. Consider a three dimensional CR manifold endowed with a contact structure ξ and a CR structure $J : \xi \to \xi$ such that $J^2 = -1$. We assume that there exists a global choice of contact form θ which annihilates ξ and for which $\theta \wedge d\theta$ is always nonzero. We define the *Reeb vector field* as the unique vector field T for which

$$\theta(T) \equiv 1; \qquad T \lrcorner\, d\theta = 0.$$

Given J as above, we have a local choice of a vector field Z_1 such that

$$JZ_1 = iZ_1; \qquad JZ_{\overline{1}} = -iZ_{\overline{1}} \qquad \text{where} \quad Z_{\overline{1}} = \overline{(Z_1)}. \tag{7}$$

We also define $(\theta, \theta^1, \theta^{\overline{1}})$ as the dual triple to $(T, Z_1, Z_{\overline{1}})$, so that

$$d\theta = ih_{1\overline{1}}\theta^1 \wedge \theta^{\overline{1}} \qquad \text{for some } h_{1\overline{1}} > 0 \quad (\text{possibly replacing } \theta \text{ by } -\theta).$$

In the following we will always assume that $h_{1\overline{1}} \equiv 1$.

The connection 1-form ω_1^1 and the torsion are uniquely determined by the equations

$$\begin{cases} d\theta^1 = \theta^1 \wedge \omega_1^1 + A^1_{\overline{1}}\theta \wedge \theta^{\overline{1}}; \\ \omega_1^1 + \omega_{\overline{1}}^{\overline{1}} = 0. \end{cases}$$

The *Tanaka-Webster curvature* is then defined by the formula

$$d\omega_1^1 = R\theta^1 \wedge \theta^{\overline{1}} \ (\text{mod } \theta).$$

In the (3-dimensional) Heisenberg group $\mathbb{H}^1$ standard choices for the dual forms are

$$\begin{cases} \overset{\circ}{\theta} = dt + izd\overline{z} - i\overline{z}dz; \\ \overset{\circ}{\theta}{}^1 = \sqrt{2}dz; \\ \overset{\circ}{\theta}{}^{\overline{1}} = \sqrt{2}d\overline{z}, \end{cases}$$

while for the vector fields we can take

$$
\begin{cases} \overset{\circ}{T} = \frac{\partial}{\partial t}; \\ \overset{\circ}{Z}_1 = \frac{1}{\sqrt{2}} \left(\frac{\partial}{\partial z} + i\bar{z} \frac{\partial}{\partial t} \right); \\ \overset{\circ}{Z}_{\bar{1}} = \frac{1}{\sqrt{2}} \left(\frac{\partial}{\partial \bar{z}} - iz \frac{\partial}{\partial t} \right). \end{cases} \tag{8}
$$

The standard contact structure ξ_0 on $\mathbb{H}^1$ is spanned by real and imaginary parts of $\overset{\circ}{Z}_1$ at each point. We define the standard CR structure $J_0 : \xi_0 \to \xi_0$ by $J_0 \overset{\circ}{Z}_1 = i \overset{\circ}{Z}_1$ on the complexification of ξ_0. $(\mathbb{H}^1, J_0, \overset{\circ}{\theta})$ is a pseudohermitian 3-manifold with $\omega_1^1 = A_{\bar{1}}^1 = R = 0$.

We recall the rules for the covariant differentiation with respect to ω_1^1. For a complex function f we set

$$
f_1 = f_{,1} \equiv Z_1 f; \qquad f_{,1\bar{1}} = Z_{\bar{1}} Z_1 f - \omega_1^1 (Z_{\bar{1}}) Z_1 f; \qquad f_{,0} = Tf, \ldots.
$$

We have the operators

$$
\Delta_b f = f_{,1}{}^1 + f_{,\bar{1}}{}^{\bar{1}} = f_{,1\bar{1}} + f_{,\bar{1}1}; \qquad \Box_b f = -\Delta_b f + iTf,
$$

where we have used $h^{1\bar{1}} = h_{1\bar{1}} = 1$ to raise or lower the indices. We also recall the commutation relations

$$
\begin{cases} c_{,1\bar{1}} - c_{,\bar{1}1} = ic_{,0} + kcR; \\ c_{,01} - c_{,10} = c_{,\bar{1}} A_{11} - kcA_{11,\bar{1}}; \\ c_{,0\bar{1}} - c_{,\bar{1}0} = c_{,1} A_{\bar{1}\bar{1}} + kcA_{\bar{1}\bar{1},1}, \end{cases} \tag{9}
$$

(see Lemma 2.3 in [32]; here we are considering the $n = 1$ case) where c is a tensor with 1 or $\bar{1}$ as subindices, k is the number of 1-subindices of c minus the number of $\bar{1}$-subindices of c and where, we recall, we are assuming that $h_{1\bar{1}} = 1$ (so $A_{\bar{1}\bar{1}} = A_{\bar{1}}^1$ and A_{11} is the complex conjugate of $A_{\bar{1}\bar{1}}$).

The CR Paneitz operator P is defined by

$$
P\varphi := 4(\varphi_{\bar{1}}{}^{\bar{1}}{}_1 + iA_{11}\varphi^1)^1. \tag{10}
$$

Let $\tilde{P}_3\varphi := \varphi_{\bar{1}}{}^{\bar{1}}{}_1 + iA_{11}\varphi^1$. The CR pluriharmonic functions are characterized by $\tilde{P}_3\varphi = 0$ ([32]) while P is identified with the compatibility operator for solving a certain degenerate Laplace equation (see [24]). The operator P is also a CR analogue of the Paneitz operator in conformal geometry (see [25] for the relation to a CR analogue of the Q-curvature and the log-term coefficient in the Szegö kernel expansion). On a compact pseudohermitian 3-dimensional manifold (M, J, θ), we call P *non-negative* if

$$
\int_M \varphi P \varphi \theta \wedge d\theta \geq 0 \tag{11}
$$

for all real (C^∞) smooth functions φ. When we want to emphasize the dependence of θ, we write P_θ instead of P. P is pseudohermitian covariant in the sense that

$$
P_{\hat{\theta}}\varphi = e^{4f} P_\theta \varphi \tag{12}
$$

for the contact form change $\theta = e^{2f}\hat{\theta}$ ([25]). The CR Paneitz operator enters in the assumptions of the following embeddability theorem.

Theorem 1.3 *([12]) Let M be a compact three-dimensional CR manifold. If P is non-negative and $R > 0$, then every eigenvalue $\lambda \neq 0$ of $\Box_b$ is greater or equal to $\min_M R$. In particular the range of $\Box_b$ is closed. If P is non-negative and $\mathcal{Y}(J) > 0$, then M can be embedded into $\mathbb{C}^N$, for some integer N.*

Remark 1.4 *For a large class of pseudohermitian structures close to the spherical one (see Theorem 1.9 in [12]) the non-negativity of P implies the embeddability of the structure. A partial converse is shown in [13], where non-negativity of the CR Paneitz operator and the condition $ker\tilde{P}_3 = ker P$ is shown to be preserved under embedded analytic deformations. The non-negativity of P is also used in [14] to obtain some hessian bounds on complex functions in terms of integral bounds on the sublaplacian.*

Examples with P non-negative include torsion-free (compact pseudohermitian) 3-manifolds (see Theorem 5.3 in [10]) and non torsion-free 3-manifolds like $S^2 \times S^1$, see Subsection 4.3.

In the systems of coordinates we will use below (both near zero or near infinity), we will set

$$\rho^4 = |z|^4 + t^2. \tag{13}$$

In the Heisenberg group $\mathbb{H}^1$ the function ρ has homogeneity 1 with respect to the natural dilation $(z,t) \mapsto (\lambda z, \lambda^2 t)$, $\lambda > 0$.

For a compact CR manifold M and for $q > 1$ we define the Folland-Stein space $\mathfrak{S}^{1,q}$ to be the completion of the (complex-valued) C^∞ functions on M with respect to the norm

$$\left(\int_M (u_{,1}\overline{u}_{,\overline{1}} + u_{,\overline{1}}\overline{u}_{,1})^{\frac{q}{2}} \theta \wedge d\theta \right)^{\frac{1}{q}} + \left(\int_M |u|^q \theta \wedge d\theta \right)^{\frac{1}{q}}.$$

We define the spaces $\mathfrak{S}^{k,q}$ ($k \in \mathbb{N}$) in a similar way, taking all possible combinations of 1 and $\overline{1}$ derivatives up to order k.

For $k \in \mathbb{Z}$ we denote by $\tilde{O}(\rho^k)$ a function $f(z, \overline{z}, t)$ for which $|f| \leq C\rho^k$ for some $C > 0$; we use instead the symbol $\tilde{O}'^k)$ for a function $f(z, \overline{z}, t)$ such that

$$|f| \leq C\rho^k, \qquad |\partial_z f| \leq C\rho^{k-1} |\partial_z \rho|, \qquad |\partial_{\overline{z}} f| \leq C\rho^{k-1} |\partial_{\overline{z}} \rho|, \qquad |\partial_t f| \leq C\rho^{k-2} |\partial_t \rho|.$$

One can define similarly the symbols $\tilde{O}''^k)$, $\tilde{O}'''^k)$, etc. We will use the symbol $O(\rho^k)$ for a function which is of the form $\tilde{O}^{(j)}(\rho^k)$ for every integer j, or for j large enough for our purposes.

Large positive constants are always denoted by C, and the value of C is allowed to vary from formula to formula and also within the same line. When we want to stress the dependence of the constants on some parameter (or parameters), we add subscripts to C, as C_δ, etc.. Also constants with this kind of subscripts are allowed to vary.

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2 Asymptotically flat pseudohermitian manifolds and definition of the p-mass

One of our main goals is to study compact manifolds with positive CR Yamabe invariant. For these, the CR invariant sublaplacian is positive definite, and therefore by classical arguments it admits a Green's function. By Proposition 5.2 (we refer to Subsection 5.1 for details), the Green's function G_p with pole at $p \in M$, namely the solution of

$$-4\Delta_b G_p + RG_p = 16\delta_p,$$

in CR normal coordinates (z,t)centered at p(see Subsection A.2) has the form

$$G_p = \frac{1}{2\pi\rho^2} + w,$$

where $w$is a function of class $C^{1,\alpha}$for any $\alpha \in (0,1)$and where, following our notation, $\rho^4 = |z|^4 + t^2$.

In fact, a more refined regularity property on w can be proved, see Appendix A of [26]: this fact will be needed to apply the main theorem there.

2.1 Blow-up through the Green's function

Let (M, J)be a CR three-manifold, and let $p \in M$. By Proposition A.5 (which relies on results by D.Jerison and J.Lee from [29]), we can find a contact form $\hat{\theta}$ near p and local coordinates (z, t) such that

$$\begin{cases} \hat{\theta} = \left(1 + O(\rho^4)\right) \overset{\circ}{\theta} + O(\rho^5) dz + O(\rho^5) d\overline{z}; \\ \hat{\theta}^1 = \sqrt{2} \left(1 + O(\rho^4)\right) dz + O(\rho^4) d\overline{z} + O(\rho^3) \overset{\circ}{\theta}, \end{cases}$$

where we recall

$$\overset{\circ}{\theta} = dt + iz d\overline{z} - i\overline{z} dz.$$

If $\hat{\theta}$is as above and if $\mathcal{Y}(J) > 0$we consider the following pseudohermitian manifold

$$\left(M \setminus \{p\}, J, \theta \equiv G_p^2 \hat{\theta}\right), \tag{14}$$

where we made a conformal change as in Subsection A.1.1, taking $f = \log G_p$. Then by (136) we also have

$$\theta^1 = G_p \left(\hat{\theta}^1 + 2i \left(\log G_p\right)_{,\overline{1}} \hat{\theta}\right). \tag{15}$$

By the expression of G_p (see Proposition 5.2), setting $A = w(0)$ we have that

$$G_p = \frac{1}{2\pi\rho^2} + A + O(\rho) \qquad \text{near } p. \tag{16}$$

Hence, from Proposition A.5 we have that

$$\begin{aligned} \theta &= G_p^2 \hat{\theta} = \left(\frac{1}{2\pi}\rho^{-2} + A + O(\rho)\right)^2 \left[\left(1 + O(\rho^4)\right) \overset{\circ}{\theta} + O(\rho^5) dz + O(\rho^5) d\overline{z}\right] \\ &= \left(\frac{1}{(2\pi)^2}\rho^{-4} + 2\frac{1}{2\pi} A\rho^{-2} + O(\rho^{-1})\right) \left[\left(1 + O(\rho^4)\right) \overset{\circ}{\theta} + O(\rho^5) dz + O(\rho^5) d\overline{z}\right] \\ &= \left(\frac{1}{(2\pi)^2}\rho^{-4} + 2\frac{1}{2\pi} A\rho^{-2} + O(\rho^{-1})\right) \overset{\circ}{\theta} + O(\rho) dz + O(\rho) d\overline{z}. \end{aligned} \tag{17}$$

Recall also the second equation in (15), which we rewrite as

$$\theta^1 = G_p \left[\hat{\theta}^1 + 2i \frac{(G_p)_{,\overline{1}}}{G_p} \hat{\theta}\right] = G_p \hat{\theta}^1 + 2i (G_p)_{,\overline{1}} \hat{\theta}.$$

Using the fact that

$$(\rho^{-2})_{,\overline{1}} = \frac{1}{\sqrt{2}} \frac{izv}{\rho^6} + O(\rho),$$

where $v = t + i|z|^2$, we get

$$(G_p)_{,\overline{1}} = \frac{1}{2\pi} \frac{1}{\sqrt{2}} \frac{izv}{\rho^6} + O(1), \tag{18}$$

from which we deduce

$$\begin{aligned} \theta^1 &= G_p \hat{\theta}^1 + 2i (G_p)_{,\overline{1}} \hat{\theta} \\ &= \left(\frac{1}{2\pi}\rho^{-2} + A + O(\rho)\right) \left(\sqrt{2} \left(1 + O(\rho^4)\right) dz + O(\rho^4) d\overline{z} + O(\rho^3) \overset{\circ}{\theta}\right) \\ &+ 2i \left(\frac{1}{2\pi} \frac{1}{\sqrt{2}} \frac{izv}{\rho^6} + O(1)\right) \left(\left(1 + O(\rho^4)\right) \overset{\circ}{\theta} + O(\rho^5) dz + O(\rho^5) d\overline{z}\right) \\ &= \left(\frac{1}{2\pi}\rho^{-2} + A + O(\rho)\right) \sqrt{2} dz + O(\rho^2) d\overline{z} + \left(-\frac{1}{\pi} \frac{1}{\sqrt{2}} \frac{zv}{\rho^6} + O(\rho)\right) \overset{\circ}{\theta}. \end{aligned} \tag{19}$$

Using (138), the new connection form becomes

$$\omega_1^1 = \hat{\omega}_1^1 + 3\left(\log G_p\right)_{,1}\hat{\theta}^1 - 3\left(\log G_p\right)_{,\bar{1}}\hat{\theta}^{\bar{1}} + i\left(\Delta_b\left(\log G_p\right) + 8\left(\log G_p\right)_{,1}\left(\log G_p\right)_{,\bar{1}}\right)\hat{\theta}. \tag{20}$$

From (18) we find

$$\begin{aligned}\left(\log G_p\right)_{,\bar{1}} &= \frac{(G_p)_{,\bar{1}}}{G_p} = \frac{\frac{1}{2\pi}\frac{1}{\sqrt{2}}\frac{izv}{\rho^6} + O(1)}{\frac{1}{2\pi}\rho^{-2} + A + O(\rho)} = \frac{\frac{1}{\sqrt{2}}\frac{izv}{\rho^4} + O(\rho^2)}{1 + 2\pi A\rho^2 + O(\rho^3)}\\ &= \frac{1}{\sqrt{2}}\frac{izv}{\rho^4} + O(\rho^2),\end{aligned}$$

which implies

$$\begin{aligned}&3\left(\log G_p\right)_{,1}\hat{\theta}^1 - 3\left(\log G_p\right)_{,\bar{1}}\hat{\theta}^{\bar{1}}\\ =\ &\left(-\frac{3i\overline{zv}}{\sqrt{2}\rho^4} + 3\sqrt{2}\pi A\frac{i\overline{zv}}{\rho^2} + O(\rho^2)\right)\left(\sqrt{2}dz + O(\rho^4)dz + O(\rho^4)d\bar{z} + O(\rho^3)\mathring{\theta}\right)\\ +\ &\left(-\frac{3izv}{\sqrt{2}\rho^4} + 3\sqrt{2}\pi A\frac{izv}{\rho^2} + O(\rho^2)\right)\left(\sqrt{2}d\bar{z} + O(\rho^4)dz + O(\rho^4)d\bar{z} + O(\rho^3)\mathring{\theta}\right).\end{aligned} \tag{21}$$

On the other hand, we also have that

$$\begin{aligned}\Delta_b\left(\log G_p\right) + 8\left(\log G_p\right)_{,1}\left(\log G_p\right)_{,\bar{1}} &= \left(\frac{(G_p)_{,1}}{G_p}\right)_{,\bar{1}} + \left(\frac{(G_p)_{,1}}{G_p}\right)_{,\bar{1}}\left(\frac{(G_p)_{,\bar{1}}}{G_p}\right)_{,1} + 8\frac{(G_p)_{,1}}{G_p}\frac{(G_p)_{,\bar{1}}}{G_p}\\ &= \frac{\Delta_b G_p}{G_p} + 6\frac{(G_p)_{,\bar{1}}(G_p)_{,1}}{G_p^2}.\end{aligned}$$

Letting $\mathring{\Delta}_b$ denote the standard sublaplacian in the Heisenberg group, from the choice of CR normal coordinates we find

$$\begin{aligned}\Delta_b &= \mathring{\Delta}_b + O(\rho^4)\mathring{Z}_1\mathring{Z}_1 + O(\rho^4)\mathring{Z}_1\mathring{Z}_{\bar{1}} + O(\rho^4)\mathring{Z}_{\bar{1}}\mathring{Z}_1 + O(\rho^4)\mathring{Z}_{\bar{1}}\mathring{Z}_{\bar{1}} + O(\rho^5)\mathring{Z}_1\partial_t + O(\rho^5)\mathring{Z}_{\bar{1}}\partial_t\\ &+ O(\rho^5)\partial_t\mathring{Z}_1 + O(\rho^5)\partial_t\mathring{Z}_{\bar{1}} + O(\rho^3)\mathring{Z}_1 + O(\rho^3)\mathring{Z}_{\bar{1}} + O(\rho^4)\partial_t.\end{aligned}$$

Using this expansion and the fact that $\mathring{\Delta}_b\rho^{-2} = 0$ in $\mathbb{H}^1$ we obtain

$$\frac{\Delta_b G_p}{G_p} = \frac{\Delta_b\left(\frac{1}{2\pi\rho^2} + A + O(\rho)\right)}{\frac{1}{2\pi\rho^2} + A + O(\rho)} = O(\rho) \qquad (\rho \text{ small}),$$

and

$$\begin{aligned}6\frac{(G_p)_{,\bar{1}}(G_p)_{,1}}{G_p^2} &= 6\frac{\left(\frac{1}{2\pi}\frac{1}{\sqrt{2}} - \frac{i\overline{zv}}{\rho^6} + O(1)\right)\left(\frac{1}{2\pi}\frac{1}{\sqrt{2}} + \frac{izv}{\rho^6} + O(1)\right)}{\left(\frac{1}{2\pi\rho^2} + A + O(\rho)\right)^2}\\ &= 6\frac{\left(\frac{1}{\sqrt{2}}\left(-\frac{i\overline{zv}}{\rho^4} + O(\rho^2)\right)\right)\left(\frac{izv}{\rho^4} + O(\rho^2)\right)}{\left(1 + 2\pi A\rho^2 + O(\rho^3)\right)^2} = 3\frac{|z|^2}{\rho^4} - 3\frac{|z|^2}{\rho^4}4\pi A\rho^2 + O(\rho).\end{aligned}$$

Therefore we get

$$\Delta_b\left(\log G_p\right) + 8\left(\log G_p\right)_{,1}\left(\log G_p\right)_{,\bar{1}} = 3\frac{|z|^2}{\rho^4} - 12\frac{|z|^2}{\rho^2}\pi A + O(\rho). \tag{22}$$

From (21) and (22), taking Proposition A.5 into account then one finds

$$
\begin{aligned}
\omega_1^1 &= -3i\frac{\overline{zv}}{\rho^4}dz - 3i\frac{zv}{\rho^4}d\overline{z} + 3i\frac{|z|^2}{\rho^4}\overset{\circ}{\theta} \\
&+ \left(3\sqrt{2}\pi Ai\frac{\overline{zv}}{\rho^2} + O(\rho^2)\right)\sqrt{2}dz + \left(3\sqrt{2}\pi Ai\frac{zv}{\rho^2} + O(\rho^2)\right)\sqrt{2}d\overline{z} \\
&+ \left(-12\pi Ai\frac{|z|^2}{\rho^2} + O(\rho)\right)\overset{\circ}{\theta}.
\end{aligned} \tag{23}
$$

2.2 CR inversion

Next we want to express θ and θ^1 in *inverted CR normal coordinates* (z_*, t_*). If (z,t) are CR normal coordinates in a neighborhood $\mathcal{U}$ of p, we define the inverted CR normal coordinates as

$$
z_* = \frac{z}{v}; \qquad t_* = -\frac{t}{|v|^2}; \qquad \text{on } \mathcal{U}\setminus\{p\}, \tag{24}
$$

where, as before, $v = t + i|z|^2$.

We have that

$$
v = t + i|z|^2 = -t_*|v|^2 + i|z_*v|^2 = |v|^2(-t_* + i|z_*|^2) = |v|^2(-\overline{v}_*),
$$

with $v_* = t_* + i|z_*|^2$. The following two identities hold

$$
1 = -\overline{v}\overline{v}_* \qquad \text{or} \qquad 1 = -vv_*,
$$

which imply

$$
z = -\frac{z_*}{v_*}; \qquad t = -\frac{t_*}{|v_*|^2}.
$$

We can write that

$$
dz = \frac{\partial z}{\partial z_*}dz_* + \frac{\partial z}{\partial \overline{z}_*}d\overline{z}_* + \frac{\partial z}{\partial t_*}dt_*; \qquad dt = \frac{\partial t}{\partial z_*}dz_* + \frac{\partial t}{\partial \overline{z}_*}d\overline{z}_* + \frac{\partial t}{\partial t_*}dt_*,
$$

so using elementary computations one finds

$$
\frac{\partial z}{\partial z_*} = -\frac{t_*}{v_*^2}; \qquad \frac{\partial z}{\partial \overline{z}_*} = i\frac{z_*^2}{v_*^2}; \qquad \frac{\partial z}{\partial t_*} = \frac{z_*}{v_*^2};
$$

$$
\frac{\partial t}{\partial z_*} = 2\frac{t_*|z_*|^2 z_*^{\overline{1}}}{|v_*|^4}; \qquad \frac{\partial t}{\partial \overline{z}_*} = 2\frac{t_* z_*^1|z_*|^2}{|v_*|^4}; \qquad \frac{\partial t}{\partial t_*} = \frac{t_*^2 - |z_*|^4}{|v_*|^4}.
$$

These relations imply

$$
\overset{\circ}{\theta} = \frac{(\overset{\circ}{\theta})_*}{|v_*|^2} = \frac{(\overset{\circ}{\theta})_*}{(\rho_*)^4}; \qquad \rho = \frac{1}{\rho_*}, \quad (\rho_*)^4 = (t_*)^2 + |z_*|^4, \tag{25}
$$

where $(\overset{\circ}{\theta})_* = dt_* + iz_*d\overline{z}_* - i\overline{z}_*dz_*$, and also

$$
dz = \frac{-t_*dz_* + iz_*^2d\overline{z}_* + z_*dt_*}{v_*^2} = \frac{z_*(\overset{\circ}{\theta})_* - \overline{v}_*dz_*}{v_*^2}. \tag{26}
$$

Now from (17) we have that

$$\begin{aligned}\theta &= G_p^2\hat{\theta} = \left(\frac{1}{(2\pi)^2}\rho^{-4} + 2\frac{1}{2\pi}A\rho^{-2} + O(\rho^{-1})\right)\overset{\circ}{\theta} + O(\rho)dz + O(\rho)d\overline{z} \\ &= \left(\frac{1}{(2\pi)^2}\rho_*^4 + 2\frac{1}{2\pi}A\rho_*^2 + O(\rho_*)\right)\frac{(\overset{\circ}{\theta})_*}{(\rho_*)^4} + O(\rho_*^{-1})\frac{z_*(\overset{\circ}{\theta})_* - \overline{v}_*dz_*}{(v_*)^2} + O(\rho_*^{-1})\frac{\overline{z}_*(\overset{\circ}{\theta})_* - v_*d\overline{z}_*}{(\overline{v}_*)^2} \\ &= \left(\frac{1}{(2\pi)^2} + \frac{1}{\pi}A\rho_*^{-2} + O(\rho_*^{-3})\right)(\overset{\circ}{\theta})_* + O(\rho_*^{-3})dz_* + O(\rho_*^{-3})d\overline{z}_*\end{aligned}$$

as $\rho \to 0$ and $\rho_* \to \infty$. Similarly from (19) we deduce

$$\begin{aligned}\theta^1 &= \left(\frac{1}{2\pi}\rho^{-2} + A + O(\rho)\right)\sqrt{2}dz + O(\rho^2)d\overline{z} + \left(-\frac{1}{\pi}\frac{1}{\sqrt{2}}\frac{zv}{\rho^6} + O(\rho)\right)\overset{\circ}{\theta} \\ &= \left(\frac{1}{2\pi}\rho_*^2 + A + O(\rho_*^{-1})\right)\sqrt{2}\left(\frac{z_*(\overset{\circ}{\theta})_* - \overline{v}_*dz_*}{(v_*)^2}\right) + O(\rho_*^{-2})\left(\frac{\overline{z}_*(\overset{\circ}{\theta})_* - v_*d\overline{z}_*}{(\overline{v}_*)^2}\right) \\ &+ \left(-\frac{1}{\pi}\frac{1}{\sqrt{2}}\frac{z_*(\rho_*)^6}{(v_*)^2} + O(\rho_*^{-1})\right)\frac{(\overset{\circ}{\theta})_*}{\rho_*^4} \\ &= \left(\sqrt{2}\frac{Az_*}{v_*^2} + O(\rho_*^{-5})\right)(\overset{\circ}{\theta})_* + O(\rho_*^{-4})d\overline{z}_* + \left(-\frac{1}{\sqrt{2}\pi}\rho_*^2\frac{\overline{v}_*}{(v_*)^2} - A\sqrt{2}\frac{\overline{v}_*}{v_*^2} + O(\rho_*^{-3})\right)dz_*.\end{aligned}$$

It is irrelevant to multiply the form θ^1 by a complex unitary factor, which we can choose to be $-\frac{v_*^3}{\rho_*^6} := e^{i\varphi}$. In this way the new θ^1, which we will denote as θ_n^1 is given by

$$\theta_n^1 = \left(-\sqrt{2}\frac{Az_*v_*}{\rho_*^6} + O(\rho_*^{-5})\right)(\overset{\circ}{\theta})_* + O(\rho_*^{-4})d\overline{z}_* + \left(\frac{1}{\sqrt{2}\pi} + A\sqrt{2}\rho_*^{-2} + O(\rho_*^{-3})\right)dz_*.$$

Under this complex rotation the connection form changes according to the law

$$\omega_1^1 \mapsto (\omega_1^1)_n = \omega_1^1 + id\varphi.$$

The function φ is defined by

$$i\varphi = \log\left(-\rho_*^2\frac{\overline{v}_*}{v_*^2}\right) = \log\left(\rho^{-2}v^2\overline{v}^{-1}\right) = 2\log v - 2\log\rho - \log\overline{v}.$$

By elementary computations one finds

$$\overset{\circ}{Z}_1\varphi = \frac{1}{\sqrt{2}}\frac{3\overline{zv}}{\rho^4}; \qquad \partial_t\varphi = -3\frac{|z|^2}{\rho^4}.$$

Hence, using Proposition A.5 one has

$$\begin{aligned}d\varphi &= \varphi_{,1}\hat{\theta}^1 + \varphi_{,\overline{1}}\hat{\theta}^{\overline{1}} + \varphi_{,0}\hat{\theta} \\ &= \frac{1}{\sqrt{2}}\frac{3\overline{zv}}{\rho^4}\sqrt{2}dz + \frac{1}{\sqrt{2}}\frac{3zv}{\rho^4}\sqrt{2}d\overline{z} - 3\frac{|z|^2}{\rho^4}\overset{\circ}{\theta} + O(\rho^3)dz + O(\rho^3)d\overline{z} + O(\rho^2)\overset{\circ}{\theta}.\end{aligned} \tag{27}$$

By (23) and (27) we then obtain

$$(\omega_1^1)_n = 6\pi Ai\frac{\overline{zv}}{\rho^2}dz + 6\pi Ai\frac{zv}{\rho^2}d\overline{z} - 12\pi Ai\frac{|z|^2}{\rho^2}\overset{\circ}{\theta} + O(\rho^2)dz + O(\rho^2)d\overline{z} + O(\rho)\overset{\circ}{\theta}. \tag{28}$$

From (24) and (26) one then gets

$$6\pi Ai\frac{\overline{zv}}{\rho^2}dz + 6\pi Ai\frac{zv}{\rho^2}d\overline{z} = -6\pi A\frac{\overline{z_*}(|z_*|^2 + it_*)}{\rho_*^6}dz_* - 6\pi A\frac{z_*(-|z_*|^2 + it_*)}{\rho_*^6}d\overline{z}_* + 12i\pi A\frac{|z_*|^2}{\rho_*^6}(\overset{\circ}{\theta})_*,$$

and the coefficient of $(\overset{\circ}{\theta})_*$ cancels with

$$-12\pi Ai\frac{|z|^2}{\rho^2}\overset{\circ}{\theta} = -12\pi Ai\frac{|z_*|^2}{\rho_*^2}(\overset{\circ}{\theta})_*.$$

In conclusion, using also (25), in inverted CR coordinates we obtain
(29)

$$(\omega_1^1)_n = \left[-6\pi A\frac{\overline{z_*}(|z_*|^2+it_*)}{\rho_*^6} + O(\rho_*^{-4})\right]dz_* + \left[-6\pi A\frac{z_*(-|z_*|^2+it_*)}{\rho_*^6} + O(\rho_*^{-4})\right]d\overline{z}_* + O(\rho_*^{-5})(\overset{\circ}{\theta})_*.$$

We can finally rescale by the constant factor $e^f = 2\pi$ to get the new forms (where we omit the normalization symbol)

$$\theta = \left(1+4\pi A\rho_*^{-2} + O(\rho_*^{-3})\right)(\overset{\circ}{\theta})_* + O(\rho_*^{-3})dz_* + O(\rho_*^{-3})d\overline{z}_*; \tag{30}$$

$$\theta^1 = \left(-2\sqrt{2}\pi A\frac{z_* v_*}{\rho_*^6} + O(\rho_*^{-5})\right)(\overset{\circ}{\theta})_* + O(\rho_*^{-4})d\overline{z}_* + \left(1+2\pi A\rho_*^{-2}+O(\rho_*^{-3})\right)\sqrt{2}dz_*. \tag{31}$$

Notice that by (138) the connection form will stay invariant.

Later on, in Subsection 3.1, we will also expand the adapted frame associated to this triple $(\theta,\theta^1,\theta^{\overline{1}})$.

2.3 Definition of p-mass and an integral formula

Having in mind the previous expansions, and in particular formulas (30), (31), we give the following definition of asymptotically flat manifold. Recall (see Subsection 1.1) that $\mathbb{H}^1$ denotes the (3-dimensional) Heisenberg group with standard pseudohermitian structure $(J_0,\overset{\circ}{\theta})$. Let B_{ρ_0} denote the Heisenberg ball of radius ρ_0.

Definition 2.1 *A three dimensional pseudohermitian manifold (N,J,θ) is said to be asymptotically flat pseudohermitian if $N = N_0 \cup N_\infty$, with N_0 compact and N_∞ diffeomorphic to $\mathbb{H}^1 \setminus B_{\rho_0}$ in which (J,θ) is close to $(J_0,\overset{\circ}{\theta})$ in the sense that*

$$\theta = \left(1+4\pi A\rho^{-2}+O(\rho^{-3})\right)\overset{\circ}{\theta} + O(\rho^{-3})dz + O(\rho^{-3})d\overline{z};$$

$$\theta^1 = O(\rho^{-3})\overset{\circ}{\theta} + O(\rho^{-4})d\overline{z} + (1+2\pi A\rho^{-2}+O(\rho^{-3}))\sqrt{2}dz$$

for some unitary coframe θ^1 and some $A\in\mathbb{R}$ in some system of coordinates (called asymptotic coordinates). We also require that $R\in L^1(N)$.

Remark 2.2 *From Definition 2.1 and the structure equations in Subsection 1.1, we can then have*

$$\theta^1 = \left(-2\sqrt{2}\pi A\frac{zv}{\rho^6} + O(\rho^{-4})\right)\overset{\circ}{\theta} + O(\rho^{-4})d\overline{z} + \left(1+2\pi A\rho^{-2}+O(\rho^{-3})\right)\sqrt{2}dz,$$

and

$$\omega_1^1 = \left[-6\pi A\frac{i\overline{zv}}{\rho^6} + O(\rho^{-4})\right]dz + \left[-6\pi A\frac{izv}{\rho^6}+O(\rho^{-4})\right]d\overline{z} + O(\rho^{-5})\overset{\circ}{\theta}.$$

We look for an expansion of the vector field Z_1 of the type

$$Z_1 = (1+a)\overset{\circ}{Z_1} + b\overset{\circ}{Z_{\overline{1}}} + c\overset{\circ}{T}$$

(recall the notation in (8)). From the three relations

$$0 = \theta(Z_1) = (1+a)O(\rho^{-3}) + bO(\rho^{-3}) + c\left(1+4\pi A\rho^{-2}+O(\rho^{-3})\right);$$

$$1 = \theta^1(Z_1) = (1+a)\left(1 + 2\pi A\rho^{-2} + O(\rho^{-3})\right) + bO(\rho^{-4}) + c\left(-2\sqrt{2}\pi A\frac{zv}{\rho^6} + O(\rho^{-3})\right);$$

$$0 = \theta^{\bar 1}(Z_1) = (1+a)O(\rho^{-4}) + b\left(1 + 2\pi A\rho^{-2} + O(\rho^{-3})\right) + c\left(-2\sqrt{2}\pi A\frac{\overline{zv}}{\rho^6} + O(\rho^{-4})\right)$$

we deduce that

$$c = O(\rho^{-3}); \qquad a = -2\pi A\rho^{-2} + O(\rho^{-3}); \qquad b = O(\rho^{-4}).$$

Similarly we obtain

$$T = (1 - 4\pi A\rho^{-2} + O(\rho^{-3}))\overset{\circ}{T} + \left(2\sqrt{2}\pi A\frac{zv}{\rho^6} + O(\rho^{-4})\right)\overset{\circ}{Z}_1 + \left(2\sqrt{2}\pi A\frac{\bar z\bar v}{\rho^6} + O(\rho^{-4})\right)\overset{\circ}{Z}_{\bar 1}.$$

By our conventions about the quantities of the type $O(\rho^k)$, we also have that

$$A_{11} = O(\rho^{-4}); \qquad R = \underbrace{Z_1(\omega_1^1(Z_{\bar 1})) - Z_{\bar 1}(\omega_1^1(Z_1))}_{O(\rho^{-4})} + i\underbrace{\omega_1^1(T)}_{O(\rho^{-5})} + 2\underbrace{\omega_1^1(Z_1)\omega_1^1(Z_{\bar 1})}_{O(\rho^{-6})}.$$

Note that if we use $1 + O(\rho^{-2})$ as the $\sqrt{2}dz$-coefficient of θ^1 in Definition 2.1, then only the real part of $O(\rho^{-2})$ (namely, $2\pi A\rho^{-2}$) is determined. But then the $\overset{\circ}{\theta}$-coefficient of ω_1^1 is not $O(\rho^{-5})$ (only $O(\rho^{-4})$). On the other hand, we may relax the conditions in Definition 2.1 for other purposes in the future.

After this definition we are ready to introduce the notion of p-mass using a variational characterization, in the same spirit of (45). Considering a one-parameter family of CR structures $J(s)$ and using the notation of Subsection A.1.2, we have that

$$\dot J = 2E = 2E_{11}\theta^1 \otimes Z_{\bar 1} + 2E_{\bar 1\bar 1}\theta^{\bar 1} \otimes Z_1.$$

Denoting by $R(s)$ the corresponding Tanaka-Webster curvature and using (141)-(142) we then find

$$\begin{aligned}
&\frac{d}{ds}_{|s=0}\int_N R(s)\,\theta\wedge d\theta = \int_N \dot R\,\theta\wedge d\theta\\
=\ & \int_N \left[i\left(E_{11},_{\bar 1\bar 1} - E_{\bar 1\bar 1},_{11}\right) - (A_{11}E_{\bar 1\bar 1} + A_{\bar 1\bar 1}E_{11})\right]\theta\wedge d\theta\\
=\ & -\int_N d\left(E_{11,1}\,\theta\wedge\theta^1\right) + \text{conj.} - \int_N (A_{11}E_{\bar 1\bar 1} + \text{conj.})\,\theta\wedge d\theta\\
=\ & -\oint_\infty E_{11,\bar 1}\,\theta\wedge\theta^1 + \text{conj.} - \int_N (A_{11}E_{\bar 1\bar 1} + \text{conj.})\,\theta\wedge d\theta\\
=\ & \oint_\infty i\dot\omega_1^1\wedge\theta - \int_N (A_{11}E_{\bar 1\bar 1} + \text{conj.})\,\theta\wedge d\theta.
\end{aligned}$$

This formula leads us to the following definition.

Definition 2.3 *Let N be an asymptotically flat manifold. Then we define the p-mass of (N, J, θ) as*

$$m(J,\theta) := i\oint_\infty \omega_1^1\wedge\theta := \lim_{\Lambda\to+\infty} i\oint_{S_\Lambda}\omega_1^1\wedge\theta,$$

where we have set $S_\Lambda = \{\rho = \Lambda\}$.

Remark 2.4 *By the above computations one finds*

$$\frac{d}{ds}_{|s=0}\left(-\int_N R(s)\,\theta\wedge d\theta + m(J(s),\theta)\right) = \int_N (A_{11}E_{\bar 1\bar 1} + A_{\bar 1\bar 1}E_{11})\,\theta\wedge d\theta,$$

which is the counterpart of (45), as desired. Apparently the definition of the p-mass depends on a choice of asymptotic coordinates and a (co)frame θ^1. Whether the p-mass is independent of the choice of asymptotic coordinates or an admissible *(co)frame is an interesting problem. But we will not pursue it in this paper.*

First, we show that $m(J,\theta)$ can be expressed in terms of the constant A appearing in Definition 2.1.

Lemma 2.5 *If $m(J,\theta)$ is as in Definition 2.3 and if A is as in* (16)*, then*

$$m(J,\theta) = 48\pi^2 A.$$

Proof. By (29) and some elementary estimates one finds

$$\begin{aligned} m(J,\theta) &= \oint_\infty i\omega_1^1 \wedge \theta = -3i2\pi A \oint_\infty \rho^{-6}\left[(|z|^2\overline{z} + i\overline{z}t)dz - (|z|^2 z - izt)d\overline{z}\right] \wedge \overset{\circ}{\theta} \\ &= -6i\pi A \oint_S |z|^2(\overline{z}dz - zd\overline{z}) \wedge \overset{\circ}{\theta} - 6i\pi A \oint_S (i\overline{z}tdz + iztd\overline{z}) \wedge \overset{\circ}{\theta}, \end{aligned}$$

where we have set

$$S = \{\rho = 1\}.$$

Using the relations

$$z = re^{i\varphi}; \qquad dz = e^{i\varphi}(dr + ird\varphi); \qquad \overline{z}dz - zd\overline{z} = 2ir^2 d\varphi, \tag{32}$$

we get

$$\begin{aligned} m(J,\theta) &= -6i\pi A \oint_S \left[2ir^4 d\varphi + 2itrdr\right] \wedge \overset{\circ}{\theta} = 12\pi A \oint_S \left[r^4 d\varphi \wedge dt + tr(dr \wedge dt + 2r^2 dr \wedge d\varphi)\right] \\ &= 12\pi A \oint_S \left(r^4 d\varphi \wedge dt + trdr \wedge dt + 2tr^3 dr \wedge d\varphi\right). \end{aligned}$$

On S we have $4r^3dr + 2tdt = 0$, so the last formula becomes

$$m(J,\theta) = 12\pi A \oint_S \left(r^4 d\varphi \wedge dt - t^2 dt \wedge d\varphi\right) = 12\pi A \oint_S d\varphi \wedge dt = 48\pi^2 A.$$

Therefore we obtain the conclusion. ■

We derive next an integral formula for the p-mass.

Proposition 2.6 *Let (N,J,θ) be an asymptotically flat pseudohermitian 3-manifold. Let $\beta : N \to \mathbb{C}$ be a C^∞-smooth complex-valued function such that*

$$\beta = \overline{z} + \beta_{-1} + O(\rho^{-2+\varepsilon}) \qquad \textit{near } \infty, \tag{33}$$

and

$$\Box_b \beta = O(\rho^{-4}), \tag{34}$$

where β_{-1} is a term with the homogeneity of ρ^{-1} satisfying

$$(\beta_{-1})_{,\overline{1}} = -2\sqrt{2}\pi A \frac{1}{\rho^2} - \frac{\sqrt{2}A}{|z|^2 + it} \tag{35}$$

near infinity, where $\varepsilon \in (0,1)$. Then one has

$$\frac{2}{3} m(J,\theta) = -\int_N |\Box_b \beta|^2 \theta \wedge d\theta + 2\int_N |\beta_{,\overline{1}\overline{1}}|^2 \theta \wedge d\theta + 2\int_N R|\beta_{,\overline{1}}|^2 \theta \wedge d\theta + \frac{1}{2}\int_N \overline{\beta} P\beta\, \theta \wedge d\theta, \tag{36}$$

where

$$P\beta := \bar{\Box}_b \Box_b \beta + 4i(A_{11}\beta_{,\overline{1}})_{,\overline{1}}$$

is the CR Paneitz operator (equivalent to the definition given by (10)).

Remark 2.7 *We will show in Section 3 that it is indeed possible to find a solution of* (34) *satisfying* (33) *and condition* (35).

Proof. By the commutation rules (9) we have that

$$\beta_{,\bar{1}1\bar{1}} = \beta_{,\bar{1}\bar{1}1} + i\beta_{,\bar{1}0} - R\beta_{,\bar{1}}.$$

Multiply by $\overline{\beta}_{,1}$ to obtain

$$\begin{aligned} \beta_{,\bar{1}1\bar{1}}\overline{\beta}_{,1} + R\beta_{,\bar{1}}\overline{\beta}_{,1} &= \beta_{,\bar{1}\bar{1}1}\overline{\beta}_{,1} + i\beta_{,\bar{1}0}\overline{\beta}_{,1} \\ &= (\beta_{,\bar{1}\bar{1}}\overline{\beta}_{,1})_{,1} - \beta_{,\bar{1}\bar{1}}\overline{\beta}_{,11} + i(\beta_{,\bar{1}0}\overline{\beta})_{,1} - i\beta_{,\bar{1}01}\overline{\beta}. \end{aligned} \tag{37}$$

Integrating by parts we get

$$\int_N (\beta_{,\bar{1}\bar{1}}\overline{\beta}_{,1})_{,1}\theta\wedge d\theta + \text{conj.} = i\oint_\infty (Z_{\bar{1}}\beta_{,\bar{1}})\overline{\beta}_{,1}\theta^{\bar{1}}\wedge\theta + \text{conj.} + i\oint_\infty \omega_1^1(Z_{\bar{1}})|\beta_{,\bar{1}}|^2\theta^{\bar{1}}\wedge\theta + \text{conj.}.$$

Regarding the first integral on the right-hand side of the last formula we have that

$$i\oint_\infty (Z_{\bar{1}}\beta_{,\bar{1}})\overline{\beta}_{,1}\theta^{\bar{1}}\wedge\theta + \text{conj.} = i\oint_\infty Z_{\bar{1}}\beta_{,\bar{1}}d\bar{z}\wedge(dt - i\bar{z}dz) + \text{conj.},$$

while for the second using the definition of $m(J,\theta)$ we find

$$i\oint_\infty \omega_1^1(Z_{\bar{1}})|\beta_{,\bar{1}}|^2\theta^{\bar{1}}\wedge\theta + \text{conj.} = \frac{1}{2}m(J,\theta).$$

For the second divergence term in (37) and recalling the asymptotics of ω_1^1 in Remark 2.2 we get

$$\begin{aligned} \int_N i(\beta_{,\bar{1}0}\overline{\beta})_{,1}\theta\wedge d\theta + \text{conj.} &= -\oint_\infty \beta_{,\bar{1}0}\overline{\beta}\theta^{\bar{1}}\wedge\theta + \text{conj.} \\ &= -\oint_\infty (T\beta_{,\bar{1}})\overline{\beta}\theta^{\bar{1}}\wedge\theta + \text{conj.} + \oint_\infty \omega_1^1(T)(\overline{\beta}_{,1}\beta\theta^1\wedge\theta - \beta_{,\bar{1}}\overline{\beta}\theta^{\bar{1}}\wedge\theta) \\ &= -\oint_\infty (T\beta_{,\bar{1}})\overline{\beta}\theta^{\bar{1}}\wedge\theta + \text{conj.}. \end{aligned} \tag{38}$$

We have the Paneitz operator appearing if we use the formulas (the boundary terms vanish after integration by parts)

$$\begin{aligned} -\int_N \frac{1}{4}(P\beta)\overline{\beta}\theta\wedge d\theta + \text{conj.} &= -\int_N (\beta_{,\bar{1}11} + iA_{11}\beta_{,\bar{1}})_{,\bar{1}}\overline{\beta}\theta\wedge d\theta + \text{conj.} \\ &= -\int_N \beta_{,\bar{1}1}\overline{\beta}_{,\bar{1}1}\theta\wedge d\theta + \int_N \left(-i(A_{11}\beta_{,\bar{1}})_{,\bar{1}}\overline{\beta} + \text{conj.}\right)\theta\wedge d\theta, \end{aligned}$$

and (from (9) we have $i\overline{\beta}_{,0} = \overline{\beta}_{,1\bar{1}} - \overline{\beta}_{,\bar{1}1}$)

$$\begin{aligned} -i\int_N \beta_{,\bar{1}01}\overline{\beta}\theta\wedge d\theta + \text{conj.} &= -i\int_N \left(\beta_{,\bar{1}10}\overline{\beta} + (\beta_{,\bar{1}}A_{11})_{,\bar{1}}\overline{\beta}\right)\theta\wedge d\theta + \text{conj.} \\ &= \int_N \left(|\beta_{,\bar{1}1}|^2 - \frac{1}{4}(P\beta)\overline{\beta}\right)\theta\wedge d\theta + \text{conj.}. \end{aligned}$$

We will show next the following two identities

$$i\oint_\infty Z_{\bar{1}}\beta_{,\bar{1}}d\bar{z}\wedge(dt - i\bar{z}dz) + \text{conj.} = \frac{7}{12}m(J,\theta); \tag{39}$$

$$-\oint_{\infty}(T\beta_{,\bar 1})z\sqrt{2}d\bar z\wedge(dt-i\bar z dz)+\text{conj.}=-\frac{5}{12}m(J,\theta). \tag{40}$$

To prove (39) we notice that (modulo $O(\rho^{-3+\epsilon})$)

$$\begin{aligned}\beta_{,\bar 1} &= (1-2\pi A\rho^{-2})\overset{\circ}{Z}_{\bar 1}(\bar z)+(\beta_{-1})_{,\bar 1}=\frac{1}{\sqrt{2}}-\sqrt{2}\pi A\rho^{-2}-2\sqrt{2}\pi A\frac{1}{\rho^2}-\frac{\sqrt{2}A}{|z|^2+it}\\ &= \frac{1}{\sqrt{2}}-3\sqrt{2}\pi A\frac{1}{\rho^2}-\frac{\sqrt{2}A}{|z|^2+it}.\end{aligned}$$

By elementary computations one finds

$$Z_{\bar 1}\beta_{,\bar 1}=-3\pi Az\frac{(it-|z|^2)}{\rho^6}+\frac{2Az(|z|^2-it)^2}{\rho^8}=\pi Az\frac{3|z|^2-3it}{\rho^6}+\frac{2Az(|z|^2-it)^2}{\rho^8},$$

Then, by a scaling argument, we obtain

$$\begin{aligned}& i\oint_{\infty}Z_{\bar 1}\beta_{,\bar 1}d\bar z\wedge(dt-i\bar z dz)+\text{conj.}\\ =\;& i\pi A\oint_S\left[(3|z|^2-3it)zd\bar z\wedge(dt-i\bar z dz)-(3|z|^2+3it)\bar z dz\wedge(dt+izd\bar z)\right]\\ +\;& 2Ai\oint_S\left[(|z|^2-it)^2zd\bar z\wedge(dt-i\bar z dz)-(|z|^2+it)^2\bar z dz\wedge(dt+izd\bar z)\right]\end{aligned} \tag{41}$$

(recall that $S=\{\rho=1\}$). By straightforward computations, and in particular the fact (cf. (32)) that

$$zd\bar z+\bar z dz=2rdr; \qquad dz\wedge d\bar z=2ird\varphi\wedge dr \tag{42}$$

we find (using also that on S, $4r^3dr+2tdt=0$)

$$\begin{aligned} i\oint_{\infty}Z_{\bar 1}\beta_{,\bar 1}d\bar z\wedge(dt-i\bar z dz)+\text{conj.} &= 2\pi A\int_S 3|z|^4d\varphi\wedge dt-2\pi A\int_S(-3)t^2d\varphi\wedge dt\\ &+ 8\pi A\int_{-1}^{1}\sqrt{1-t^2}dt.\end{aligned} \tag{43}$$

We then get

$$i\oint_{\infty}Z_{\bar 1}\beta_{,\bar 1}d\bar z\wedge(dt-i\bar z dz)+\text{conj.}=24\pi^2A+8\pi A\int_{-1}^{1}\sqrt{1-t^2}dt=28\pi^2A=\frac{7}{12}m(J,\theta),$$

which is (39).

To prove (40) instead we use the following formula, which can be obtained from the expansion of T in Remark 2.2

$$\begin{aligned}T\beta_{,\bar 1} &= 3\sqrt{2}\pi A\frac{t}{\rho^6}+\frac{iA\sqrt{2}}{(|z|^2+it)^2}+O(\rho^{-5+\varepsilon})\\ &= -\sqrt{2}\pi Ai\frac{3it}{\rho^6}+\frac{iA\sqrt{2}(|z|^2-it)^2}{\rho^8}+O(\rho^{-5+\varepsilon}),\end{aligned}$$

Using again a scaling and elementary computations (some of which are similar to those for the proof of (39)) one gets

$$\begin{aligned}&-\oint_{\infty}(T\beta_{,\bar 1})z\sqrt{2}d\bar z\wedge(dt-i\bar z dz)+\text{conj.}\\ =\;& 2i\pi A\oint_S\left[3itzd\bar z\wedge(dt-i\bar z dz)+3it\bar z dz\wedge(dt+izd\bar z)\right]-\frac{1}{12}m(J,\theta).\end{aligned}$$

Exactly as for (41) and (43) we deduce

$$\begin{aligned}
& -\oint_\infty (T\beta_{,\bar 1}) z\sqrt{2} d\bar z \wedge (dt - i\bar z dz) + \text{conj.} \\
= \quad & -4\pi A \int_S 3t^2 d\varphi \wedge dt - \frac{1}{12} m(J,\theta) \\
= \quad & -16\pi^2 A - \frac{1}{12} m(J,\theta) = -\frac{1}{3} m(J,\theta) - \frac{1}{12} m(J,\theta),
\end{aligned}$$

which proves also (40).

Using all the above formulas and the fact that P is real we then obtain

$$\begin{aligned}
& -2\int |\beta_{,\bar 1 1}|^2 \theta \wedge d\theta + 2\int_N R|\beta_{,\bar 1}|^2 \theta \wedge d\theta \\
= \quad & \frac{2}{3} m(J,\theta) - 2\int_N |\beta_{,\bar 1 \bar 1}|^2 \theta \wedge d\theta + 2\int_N |\beta_{,\bar 1 1}|^2 \theta \wedge d\theta - \frac{1}{2}\int_N \overline{\beta}(P\beta)\,\theta \wedge d\theta.
\end{aligned}$$

Since $\Box_b \beta = -2\beta_{,\bar 1 1}$, we finally get the conclusion. ■

In Proposition 3.1, we prove the existence of β satisfying (33), (34) in Proposition 2.6. Moreover, in Subsection 3.4, we prove the existence of β such that $\Box_b \beta = 0$. Substituting this in (36) (plus an argument on the Paneitz term), we finally get the non-negativity of the p-mass.

We recall next some well known definitions and facts in General Relativity, referring to [33] for more details. A Riemannian manifold N (of dimension n) with a smooth metric g is called *asymptotically flat* of order $\tau > 0$ if N decomposes as $N = N_0 \cup N_\infty$, where N_0 is compact and N_∞ is diffeomorphic to $\mathbb{R}^n \setminus B_R(0)$ for some $R > 0$, and if g on N_∞ satisfies $g_{ij} = \delta_{ij} + O(|x|^{-\tau})$, $|\partial g_{ij}| = O(|x|^{-\tau-1})$, $|\partial^2 g_{ij}| = O(|x|^{-\tau-2})$ as $|x| \to +\infty$, in some system of coordinates. Such coordinates are called *asymptotic coordinates*. One then considers the Einstein-Hilbert action

$$\mathcal{A}(g) := -\int_N S_g dV_g,$$

where S_g is the scalar curvature of (N,g). Given a smooth variation g_s of the metric with $\frac{d}{ds}|_{s=0} g_s = v$, $v = (v_{ij})$, one has

$$\frac{d}{ds}|_{s=0}(S_{g_s} dV_{g_s}) = -\left(v^{ij} G_{ij} + \nabla^* \xi\right) dV_g,$$

where $G_{ij} = R_{ij} - \frac{1}{2} S_g g_{ij}$ is the Einstein tensor and where $\xi = (v_{jk,}{}^{k} - v^k_{k,j}) dx^j$. Then, if one defines the *mass* $m(g)$ to be

$$m(g) = \lim_{R\to+\infty} \omega_n^{-1} \oint_{\Sigma_R} \mu \lrcorner dV_g \qquad \mu = (\partial_i g_{ij} - \partial_j g_{ii})\partial_j, \quad \Sigma_R = \{|x| = R\}. \tag{44}$$

varying the metric it turns out that

$$\frac{d}{ds}(\mathcal{A}(g_s) + m(g_s)) = \int_N v^{ij} G_{ij} dV_g. \tag{45}$$

To explain the link between the spinor method in [42] and the $\Box_b$ operator, let us consider a general spin^c structure on a contact bundle ξ over an asymptotically flat pseudohermitian manifold M of dimension $2n+1$. Let W denote the spinor bundle with a spin^c connection ∇ compatible with the pseudohermitian connection $\nabla^{p.h.}$. Let e_1, ..., e_{2n} denote an orthonormal basis of ξ with respect to the Levi metric. Denote the contact Dirac operator D_ξ by

$$D_\xi \psi = \sum_{a=1}^{2n} \Gamma(e_a) \nabla_{e_a} \psi$$

for a section ψ of W, where Γ denotes the Clifford multiplication. Let T denote the Reeb vector field associated to the contact form θ. Let D_ξ^*, ∇^* denote the adjoint operator of D_ξ, ∇, resp.. We then have the following formula

$$
\begin{aligned}
D_\xi^* D_\xi \psi &= \sum_{a=1}^{2n} \nabla_{e_a}^* \nabla_{e_a} \psi - 2\sum_{\alpha=1}^{n} \Gamma(e_\alpha e_{n+\alpha}) \nabla_T \psi \\
&\quad + \sum_{a<b} \Gamma(e_a)\Gamma(e_b) R^\nabla(e_a, e_b)\psi
\end{aligned} \tag{46}
$$

where $1 \leq a, b \leq 2n$ and $R^\nabla(e_a, e_b)$, the curvature operator, is defined by

$$R^\nabla(e_a, e_b) := \nabla_{e_a}\nabla_{e_b} - \nabla_{e_b}\nabla_{e_a} - \nabla_{[e_a, e_b]}.$$

Decompose $R_{ab}^\nabla := R^\nabla(e_a, e_b)$ as a sum of the trace free part $\mathring{R}_{ab}^\nabla$ and the trace part $2^{-n} tr_W R_{ab}^\nabla$. A standard deduction shows that

$$\sum_{a<b} \Gamma(e_a)\Gamma(e_b)\mathring{R}_{ab}^\nabla \psi = \frac{1}{4} R\psi$$

where, again, R denotes the Tanaka-Webster scalar curvature. On the other hand, $2^{-n} tr_W R_{ab}^\nabla = F_A(e_a, e_b)$ in which the curvature 2-form $F_A := dA$ and $2A$ is the connection form of an associated line bundle L_Γ ($\det W = L_\Gamma^{\otimes 2^{n-1}}$). Therefore we can reduce (46) to

$$
\begin{aligned}
D_\xi^* D_\xi \psi &= \sum_{a=1}^{2n} \nabla_{e_a}^* \nabla_{e_a} \psi - 2\sum_{\alpha=1}^{n} \Gamma(e_\alpha e_{n+\alpha}) \nabla_T \psi \\
&\quad + \frac{1}{4} R\psi + \rho(F_A)\psi
\end{aligned} \tag{47}
$$

where $\rho(F_A) = \sum_{a<b} \Gamma(e_a)\Gamma(e_b) F_A(e_a, e_b)$.

To deal with the T-derivative term in (47), we consider the canonical spin^c structure with $W = \Lambda^{0,*}$, the bundle of all $(0, q)$-forms. In particular, we take $\psi = \bar{\partial}_b u = \sum_{\beta=1}^{n} u_{,\bar{\beta}} \theta^{\bar{\beta}}$, a $(0, 1)$-form with components being derivatives of a complex function u. Then we have

$$D_\xi \psi = (\bar{\partial}_b + \bar{\partial}_b^*)\bar{\partial}_b u = \bar{\partial}_b^* \bar{\partial}_b u = \frac{1}{2}\Box_b u$$

where $\Box_b := 2(\bar{\partial}_b \bar{\partial}_b^* + \bar{\partial}_b^* \bar{\partial}_b)$ is Kohn's Laplacian. Note that $\bar{\partial}_b^* u = 0$. To solve the contact Dirac equation $D_\xi \psi = 0$ for ψ with suitably asymptotic behaviour at the infinity is reduced to solving $\Box_b u = 0$ for u with corresponding behaviour at the infinity. Associated to the T-derivative term is a term involving so-called CR Paneitz operator P after integration. Observe that for $n \geq 2$ (i.e. in real dimension $2n + 1$ ≥ 5), P is non-negative (for closed M and open M with suitably decaying test functions) (see [11], [24]). In dimension 3, the embeddability of the underlying CR structure is necessary for its non-negativity, see Remark 1.4.

On the other hand, in dimension 3, the trace curvature term $\rho(F_A)\psi$ is absorbed in the scalar curvature term. So by further assuming $R \geq 0$, we can have the non-negativity of the p-mass (which we pick up from the boundary terms).

3 Proof of Theorem 1.1

We are now in position to prove our main theorem. For doing this, we need to introduce some notation and preliminary facts. For two functions $f_1, f_2 \in L^1(\mathbb{H}^1)$ we define the convolution operator

$$(f_1 * f_2)(Z) = \int_{\mathbb{H}^1} f_1(ZW^{-1}) f_2(W)dW = \int_{\mathbb{H}^1} f_1(W) f_2(W^{-1}Z)dW; \qquad Z = (z, t), \quad W = (w, s),$$

with

$$W^{-1}Z = (z-w, t-s-2\,\mathrm{Im}\,\overline{z}w)\,; \qquad dW = \left(\overset{\circ}{\theta} \wedge d\overset{\circ}{\theta}\right)(W),$$

see the notation in Subsection 1.1.

By the solvability theory of $\overset{\circ}{\Box}_b$ in $\mathbb{H}^1$ (see Chapter 10 in [15]) we have that

$$\overset{\circ}{\Box}_b \mathcal{K} = \mathcal{K}\overset{\circ}{\Box}_b = Id - \mathcal{S} \qquad \text{on } L^2(\mathbb{H}^1), \tag{48}$$

where $\mathcal{S}$ is the Szegö projection

$$\mathcal{S}h = \lim_{\varepsilon\to 0} \frac{1}{4\pi^2} h * \eta_\varepsilon^{-2}; \qquad \eta_\varepsilon = |z|^2 + \varepsilon^2 - it,$$

and where

$$\mathcal{K}\,h = h * \Phi; \qquad \Phi = \frac{1}{8\pi^2} \log\left(\frac{|z|^2 - it}{|z|^2 + it}\right)(|z|^2 - it)^{-1}.$$

Define now

$$\mathfrak{f} = 4\pi A \frac{\overline{z}(|z|^2 + it)}{\rho^6}, \tag{49}$$

and let $\chi : \mathbb{H}^1 \to \mathbb{R}$ be a cutoff function, weakly monotone in ρ, satisfying

$$\begin{cases} \chi(z,t) = 0 & \text{in a neighborhood of } (0,0); \\ \chi(z,t) = 1 & \text{near infinity.} \end{cases}$$

Our next goal is to find a function β_{-1} which has the homogeneity of ρ^{-1} near infinity and such that

$$\overset{\circ}{\Box}_b \beta_{-1} = -\chi\mathfrak{f} \qquad \text{near infinity.} \tag{50}$$

This function will be useful to solve (34) and to determine the asymptotics of a function β as in Proposition 2.6. We can exhibit indeed two functions $\hat{g}$ and $\tilde{g}$ which satisfy

$$\overset{\circ}{\Box}_b g = -4\pi A \frac{\overline{z}(|z|^2 + it)}{\rho^6} \qquad \text{in } \mathbb{H}^1 \tag{51}$$

pointwise almost everywhere, but which are not continuous. The two functions are

$$\hat{g}(z,t) = \begin{cases} -4i\pi A\left(\frac{\rho^2}{vz} - \frac{1}{z}\right) & \text{for } t > 0; \\ -4i\pi A\left(\frac{\rho^2}{vz} + \frac{1}{z}\right) & \text{for } t < 0, \end{cases} \tag{52}$$

and

$$\tilde{g}(z,t) = -4i\pi A \frac{\rho^2}{vz} \qquad \text{for } z \neq 0, \tag{53}$$

where we recall

$$v = v(z,t) = t + i|z|^2. \tag{54}$$

The function $\hat{g}$ is not continuous on the plane $\{t = 0\}$, while $\tilde{g}$ is not continuous on the axis $\{z = 0\}$. By this reason, $\hat{g}$ and $\tilde{g}$ should be considered spurious solutions of (51): however, it turns out that they are useful in some integral estimates, see in particular Subsections 3.2 and 3.3 below.

The proof of our main theorem relies on the next proposition, where a solution of $\Box_b\beta = 0$ with a precise asymptotic behavior is found.

Proposition 3.1 *If N is an asymptotically flat pseudohermitian manifold of dimension 3, there exists a C^∞-smooth solution β of*

$$\Box_b \beta = O(\rho^{-4}) \qquad \text{on } N$$

satisfying (33)*, that is,*

$$\beta = \overline{z} + \beta_{-1} + O(\rho^{-2+\varepsilon}) \qquad \text{near } \infty.$$

More precisely, if $\varepsilon \in (0,1)$ and if $\mathfrak{f}$ is as in (49)*, we can choose a C^∞-smooth β_{-1} so that*

$$\beta_{-1} = \mathcal{K}(-\chi \mathfrak{f}) + O(\rho^{-2+\varepsilon}) \qquad \text{for } \rho \text{ large,} \tag{55}$$

and

$$(\beta_{-1})_{,\overline{1}} = -2\sqrt{2}\pi A \frac{1}{\rho^2} - \frac{\sqrt{2}A}{|z|^2 + it} \tag{56}$$

near infinity. Moreover, if N is the blow-up of an embeddable compact three dimensional CR manifold with $\mathcal{Y}(J) > 0$, then there exists a C^∞-smooth solution β of $\Box_b \beta = 0$ satisfying (33).

The proof of Proposition 3.1 is given in the next four subsections.

3.1 Expansion of $\Box_b \overline{z}$ near infinity

To study equation (34), we begin finding a correction to $\overline{z}$ by evaluating first $\Box_b$ on $\overline{z}$. The following asymptotic expansion holds.

Lemma 3.2 *If N is an asymptotically flat pseudohermitian manifold of dimension 3, then*

$$\Box_b \overline{z} = 4\pi A \frac{\overline{z}}{\rho^6}(|z|^2 + it) + O(\rho^{-4}) \qquad \text{near infinity.}$$

Proof. We want to express Z_1 and ω_1^1 in asymptotic coordinates, recalling that

$$\mathring{Z}_1 = \frac{1}{\sqrt{2}} \left(\frac{\partial}{\partial z} + i\overline{z} \frac{\partial}{\partial t} \right); \qquad \mathring{\omega}_1^{\,1} = 0.$$

Recall also that, from the expansions in Section 2

$$\theta = \left(1 + 4\pi A \rho^{-2} + O(\rho^{-3})\right) \mathring{\theta} + O(\rho^{-3}) dz + O(\rho^{-3}) d\overline{z};$$

$$\theta^1 = \left(-2\sqrt{2}\pi A \frac{zv}{\rho^6} + O(\rho^{-5}) \right) \mathring{\theta} + O(\rho^{-4}) d\overline{z} + \left(1 + 2\pi A \rho^{-2} + O(\rho^{-3})\right) \sqrt{2} dz.$$

Recalling also the estimates on the functions a, b, c from Remark 2.2 we also have

$$\begin{aligned} Z_1 Z_{\overline{1}} + \omega_1^1(Z_1) Z_{\overline{1}} &= \left[(1+a)\mathring{Z}_1 + b\mathring{Z}_{\overline{1}} + c\mathring{T} \right] \left[(1+a)\mathring{Z}_{\overline{1}} + b\mathring{Z}_1 + c\mathring{T} \right] + \omega_1^1(Z_1) Z_{\overline{1}} \\ &= \mathring{Z}_1 \mathring{Z}_{\overline{1}} + (\mathring{Z}_1 a)\mathring{Z}_{\overline{1}} + 2a\mathring{Z}_1 \mathring{Z}_{\overline{1}} + \omega_1^1(Z_1) Z_{\overline{1}} + \mathcal{R}_{\Box_b}, \end{aligned}$$

where the remainder term $\mathcal{R}_{\Box_b}$ satisfies

$$\begin{aligned} \mathcal{R}_{\Box_b} &= O(\rho^{-4})\mathring{Z}_1 \mathring{Z}_{\overline{1}} + O(\rho^{-4})\mathring{Z}_{\overline{1}}^2 + O(\rho^{-4})\mathring{Z}_1^2 + O(\rho^{-8})\mathring{Z}_{\overline{1}}\mathring{Z}_1 + O(\rho^{-3})\mathring{Z}_1\mathring{T} + O(\rho^{-5})\mathring{Z}_{\overline{1}}\mathring{T} \\ &+ O(\rho^{-6})\mathring{T}^2 + O(\rho^{-7})\mathring{T}\mathring{Z}_1 + O(\rho^{-3})\mathring{T}\mathring{Z}_{\overline{1}} + O(\rho^{-5})\mathring{Z}_1 + O(\rho^{-5})\mathring{Z}_{\overline{1}} + O(\rho^{-4})\mathring{T}. \end{aligned}$$

Recall that, by Remark 2.2 one has

$$\omega_1^1 = \left[-\overline{g}_{-3}\sqrt{2} + O(\rho^{-4})\right] dz + \left[g_{-3}\sqrt{2} + O(\rho^{-4})\right] d\overline{z} + O(\rho^{-5})\theta_0,$$

where

$$g_{-3} = \frac{\pi A\sqrt{2}}{\rho^6} z(3|z|^2 - 3it).$$

Noticing that $a = -2\pi A\rho^{-2} + O(\rho^{-3})$ implies

$$\mathring{Z}_1 a + O(\rho^{-4}) = -2\pi A\mathring{Z}_1\rho^{-2} + O(\rho^{-4}) = 2\pi A\frac{1}{\sqrt{2}}\frac{i\overline{zv}}{\rho^6} + O(\rho^{-4}),$$

we obtain the expansion of $\mathcal{E} := \Box_b - \mathring{\Box}_b$

$$\begin{aligned}
\mathcal{E} &= -4a\mathring{Z}_1\mathring{Z}_{\overline{1}} - 2(\mathring{Z}_1 a)\mathring{Z}_{\overline{1}} + 2\overline{g}_{-3}\mathring{Z}_{\overline{1}} - 2\mathcal{R}_{\Box_b} \\
&= 8\pi A\rho^{-2}\mathring{Z}_1\mathring{Z}_{\overline{1}} - 4\pi A\frac{1}{\sqrt{2}}\frac{i\overline{zv}}{\rho^6}\mathring{Z}_{\overline{1}} + 2\overline{g}_{-3}\mathring{Z}_{\overline{1}} - 2\mathcal{R}_{\Box_b} \\
&= 8\pi A\rho^{-2}\mathring{Z}_1\mathring{Z}_{\overline{1}} + 2\sqrt{2}\pi A\frac{\overline{z}}{\rho^6}(3|z|^2 + 3it - i\overline{v})\mathring{Z}_{\overline{1}} - 2\mathcal{R}_{\Box_b} \\
&= 8\pi A\rho^{-2}\mathring{Z}_1\mathring{Z}_{\overline{1}} + 4\sqrt{2}\pi A\frac{\overline{z}}{\rho^6}(|z|^2 + it)\mathring{Z}_{\overline{1}} - 2\mathcal{R}_{\Box_b}.
\end{aligned}$$

Applying this operator to the function $\overline{z}$ we have that

$$\mathcal{E}\overline{z} = 8\pi A\rho^{-2}\mathring{Z}_1(1) + 4\pi A\frac{\overline{z}}{\rho^6}(|z|^2 + it) + O(\rho^{-4}) = 4\pi A\frac{\overline{z}}{\rho^6}(|z|^2 + it) + O(\rho^{-4}), \tag{57}$$

which gives the desired conclusion. ■

3.2 proof of (55)

We have the following result concerning approximate orthogonality of $\mathfrak{f}$ to the Szegö projection.

Lemma 3.3 *If $\mathfrak{f}$ is defined as in* (49) *then*

$$(\mathcal{S}(\chi\mathfrak{f}))(z,t) = O(\rho^{-4}) \qquad \text{as } \rho \to +\infty.$$

Proof. Let $\hat{g}(z,t)$ be as in (52). Then one has

$$\mathring{\Box}_b\hat{g} = -\mathfrak{f} \qquad \text{for } t \neq 0.$$

Since

$$\mathring{Z}_{\overline{1}}\left(\frac{1}{z}\right) = 0; \qquad \mathring{Z}_{\overline{1}}\left(i\frac{\rho^2}{vz}\right) = \rho^{-2}$$

we have that $\mathring{Z}_{\overline{1}}\hat{g}$ extends smoothly to $t = 0$ except for $\rho = 0$. We consider the function

$$\hat{\mathfrak{f}} = -\mathring{\Box}_b(\chi\hat{g}),$$

which coincides with $\mathfrak{f}$ outside a compact set containing the origin of $\mathbb{H}^1$.

We then compute

$$\begin{aligned}
-(\mathcal{S}\hat{\mathfrak{f}})(Z) &= -\frac{1}{4\pi^2}\lim_{\varepsilon\to 0}\int_{\mathbb{H}^1}\hat{\mathfrak{f}}(W)\eta_\varepsilon^{-2}(W^{-1}Z)dW = -\frac{1}{2\pi^2}\lim_{\varepsilon\to 0}\int_{\mathbb{H}^1}(\chi\hat{g})_{\overline{1}1}(W)\eta_\varepsilon^{-2}(W^{-1}Z)dW \\
&= -\frac{1}{2\pi^2}\lim_{\varepsilon\to 0}\int_{\mathbb{H}^1}\left((\chi\hat{g})_{\overline{1}}(W)\eta_\varepsilon^{-2}(W^{-1}Z)\right)_{,1}dW + \frac{1}{2\pi^2}\lim_{\varepsilon\to 0}\int_{\mathbb{H}^1}(\chi\hat{g})_{\overline{1}}(W)(\eta_\varepsilon^{-2}(W^{-1}Z))_{,1}dW \\
&= -\frac{1}{2\pi^2}\lim_{\varepsilon\to 0}\int_{\mathbb{H}^1}\left((\chi\hat{g})_{\overline{1}}(W)\eta_\varepsilon^{-2}(W^{-1}Z)\right)_{,1}dW.
\end{aligned}$$

In the above equalities we used the fact that η_ε^{-2} is a conjugate CR function in W. Integrating by parts we then get

$$\begin{aligned}
& \lim_{\varepsilon\to 0}\int_{\mathbb{H}^1} \overset{\circ}{\square}_b(\chi\hat{g})\eta_\varepsilon^{-2}(W^{-1}Z)dW \\
= \ & \frac{i}{2\pi^2}\lim_{\varepsilon\to 0}\left[\oint_{t=0^+}(\chi\hat{g})_{\overline{1}}(W)\eta_\varepsilon^{-2}(W^{-1}Z)(\theta\wedge\theta^{\overline{1}})(W) - \oint_{t=0^-}(\chi\hat{g})_{\overline{1}}(W)\eta_\varepsilon^{-2}(W^{-1}Z)(\theta\wedge\theta^{\overline{1}})(W)\right] \\
= \ & \frac{1}{2\pi^2}\lim_{\varepsilon\to 0}\left[\oint_{t=0^+}(\chi\hat{g})_{\overline{1}}(W)\eta_\varepsilon^{-2}(W^{-1}Z)\frac{\overline{z}}{\sqrt{2}}dw\wedge d\overline{w} - \oint_{t=0^-}(\chi\hat{g})_{\overline{1}}(W)\eta_\varepsilon^{-2}(W^{-1}Z)\frac{\overline{z}}{\sqrt{2}}dw\wedge d\overline{w}\right].
\end{aligned}$$

Since $(\chi\hat{g})_{\overline{1}}$ is smooth outside a compact set, we have vanishing of the difference of the boundary integrands outside a compact set. We also have that

$$\lim_{\varepsilon\to 0}\eta_\varepsilon^{-2}(W^{-1}Z) = O(\rho^{-4})(Z) \qquad \text{for } W \text{ in any given compact set of } \mathbb{H}^1.$$

The last two formulas then imply

$$(\mathcal{S}\hat{\mathfrak{f}})(Z) = O(\rho^{-4})(Z).$$

By the same reason, since $\chi\mathfrak{f}$ and $\hat{\mathfrak{f}}$ coincide outside a compact set we have that as well

$$\mathcal{S}(\chi\mathfrak{f})(Z) = O(\rho^{-4})(Z),$$

which is the desired conclusion. ■

Take $\beta = \chi\overline{z} - \mathcal{K}(\chi\mathfrak{f})$. From (48), (57), and Lemma 3.3, we compute, near infinity,

$$\begin{aligned}
\square_b\beta &= \square_b(\overline{z} - \mathcal{K}(\chi\mathfrak{f})) \\
&= \mathfrak{f} - \chi\mathfrak{f} + \mathcal{S}(\chi\mathfrak{f}) - \mathcal{E}(\mathcal{K}(\chi\mathfrak{f})) + O(\rho^{-4}) \\
&= 0 + O(\rho^{-4}).
\end{aligned}$$

By scaling arguments, one finds that $\mathcal{K}(\chi\mathfrak{f})$ is the sum of a function with the homogeneity of ρ^{-1} and a function of order $\rho^{-2+\varepsilon}$, concluding the proof of (55).

3.3 Proof of (56)

Since

$$(\tilde{g})_{\overline{1}} = -2\sqrt{2}\pi A\frac{1}{\rho^2} \qquad (z\neq 0)$$

extends continuously to $\mathbb{H}^1\setminus\{0\}$, to show (56) it is sufficient to prove that

$$(\mathcal{K}(-\chi\mathfrak{f}))_{\overline{1}} + \frac{\sqrt{2}A}{|z|^2+it} = (\tilde{g})_{\overline{1}} + O(\rho^{-3}) \qquad \text{for } z\neq 0 \text{ and } \rho \text{ large.} \tag{58}$$

To obtain this estimate we use a distributional argument. First of all, we remark that $\frac{1}{z}$ is well defined, as a distribution, by the formula

$$\langle\frac{1}{z},\varphi\rangle = -\int_{\mathbb{H}^1}\log|z|^2\frac{\partial\varphi}{\partial z}\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta},$$

for any test function $\varphi\in C_c^\infty(\mathbb{H}^1)$. We have now the following result.

Lemma 3.4 *If $\tilde{g}$ is defined as in* (53) *then one has*

$$\overset{\circ}{\square}_b\,\tilde{g} = -\mathfrak{f} - 4\sqrt{2}i\pi^2 A\frac{\rho^2}{v}\overset{\circ}{Z}_1\delta_{\{z=0\}} \qquad \textit{in the distributional sense of } \mathbb{H}^1\setminus\{0\}. \tag{59}$$

Proof. We have

$$\overset{\circ}{Z}_{\bar 1}\tilde g = -4i\pi A \overset{\circ}{Z}_{\bar 1}\left(\frac{\rho^2}{v}\right)\frac{1}{z} - 4i\pi A\frac{\rho^2}{v}\overset{\circ}{Z}_{\bar 1}\left(\frac{1}{z}\right). \tag{60}$$

We next notice that, for any function $\varphi \in C_c^\infty(^1)$

$$\begin{aligned}
\langle \overset{\circ}{Z}_{\bar 1}\frac{1}{z},\varphi\rangle &= \langle \frac{1}{z}, \overset{\circ}{Z}{}^*_{\bar 1}\varphi\rangle = \langle \frac{1}{z}, -\overset{\circ}{Z}_1\varphi\rangle = \frac{1}{\sqrt 2}\int_{^1}\log|z|^2\overline{[\partial_{\bar z}(\partial_z\varphi + i\bar z\partial_t\varphi)]}\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta}\\
&= \frac{1}{\sqrt 2}\int_{^1}\log|z|^2\overline{\frac{1}{4}\Delta_{\mathbb{R}^2}\varphi}\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta} = \frac{1}{4\sqrt 2}\langle \Delta_{\mathbb{R}^2}\log|z|^2,\varphi\rangle\\
&= \frac{1}{4\sqrt 2}\cdot 4\pi\langle_{\{z=0\}},\varphi\rangle = \frac{\pi}{\sqrt 2}\langle_{\{z=0\}},\varphi\rangle.
\end{aligned}$$

Therefore by (60) we have

$$\overset{\circ}{Z}_{\bar 1}\tilde g = -4i\pi A\overset{\circ}{Z}_{\bar 1}\left(\frac{\rho^2}{v}\right)\frac{1}{z} + 4\pi A i\pi\frac{1}{\sqrt 2}\frac{\rho^2}{v}{}_{\{z=0\}} \qquad ((z,t)\neq(0,0)).$$

Using the (distributional) formulas

$$\overset{\circ}{Z}_1\frac{1}{z} = -\frac{1}{\sqrt 2}\frac{1}{z^2}; \qquad \overset{\circ}{Z}_1\left(\frac{\rho^2}{v}\right) = -\frac{i}{\sqrt 2}\frac{z(t-i|z|^2)}{\rho^6}$$

and the fact that $\bar z_{\{z=0\}} = 0$ we find

$$\begin{aligned}
-2\overset{\circ}{Z}_1\overset{\circ}{Z}_{\bar 1}\tilde g &= -\mathfrak{f} - 4\sqrt 2\pi^2 iA\overset{\circ}{Z}_1\left(\frac{\rho^2}{v}\right)\delta_{\{z=0\}} - 4\sqrt 2\pi^2 iA\frac{\rho^2}{v}\overset{\circ}{Z}_1\delta_{\{z=0\}}\\
&= -\mathfrak{f} - 4\sqrt 2\pi^2 iA\frac{\rho^2}{v}\overset{\circ}{Z}_1\delta_{\{z=0\}} \qquad ((z,t)\neq(0,0)),
\end{aligned}$$

which is the desired conclusion. ■

The previous lemma implies clearly that

$$\Box_b(\chi\tilde g) = \chi\left(-\mathfrak{f} - 4\sqrt 2 i\pi^2 A\frac{\rho^2}{v}Z_1\delta_{\{z=0\}}\right) + \tau,$$

where τ is a distribution with compact support A_τ.

We next consider a sequence of smooth nonincreasing cutoff functions $\chi_j = \chi_j(\rho)$ such that

$$\chi_j(\rho) = 1 \quad \text{for } \rho \le j; \qquad \chi_j(\rho) = 0 \quad \text{for } \rho \ge j+1,$$

and another sequence of nondecreasing cutoff functions $\tilde\chi_j = \tilde\chi_j(|z|)$ satisfying

$$\tilde\chi_j(|z|) = 1 \quad \text{for } |z| \ge \frac{1}{j}; \qquad \tilde\chi_j(|z|) = 0 \quad \text{for } |z| \le \frac{1}{2j}.$$

We then define the sequence

$$\tilde g_j(z,t) = \tilde\chi_j(|z|)\chi_j(\rho)\chi(z,t)\tilde g(z,t).$$

Since the $\tilde g_j$'s converge to $\tilde g$ locally in L^1 we have that

$$\overset{\circ}{\Box}_b\tilde g_j = -\chi_j\chi\mathfrak{f} + \zeta_j + \xi_j, \tag{61}$$

where ζ_j is a sequence of functions supported in $\{1 \leq \rho \leq j+1\} \cap \{|z| \leq 1/j\}$ satisfying

$$\zeta_j \overset{\mathcal{D}'}{\to} -4\sqrt{2}i\pi^2 A \frac{\rho^2}{v} Z_1 \delta_{\{z=0\}}, \tag{62}$$

on every open bounded set of $\mathbb{H}^1$ which does not intersect $\{\rho \geq 2\}$, and where ξ_j is supported in $\{1 \leq \rho \leq 2\} \cup \{j \leq \rho \leq j+1\}$, with order $O(\rho^{-3})$. For $z \neq 0$ we now compute

$$\begin{aligned} Z_{\bar{1}}(\mathcal{K}(\mathring{\Box}_b \tilde{g}_j))(Z) &= \int_{\mathbb{H}^1} (\mathring{\Box}_b \tilde{g}_j)(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW = \int_{\mathbb{H}^1} (\chi_j \chi \mathfrak{f})(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW \\ &+ \int_{\mathbb{H}^1} \zeta_j(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW + \int_{\mathbb{H}^1} \xi_j(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW. \end{aligned} \tag{63}$$

Lemma 3.5 *The following three formulas hold*

$$\int_{\mathbb{H}^1} (\chi_j \chi \mathfrak{f})(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW = Z_{\bar{1}} \mathcal{K}(\chi \mathfrak{f})(Z) + o_j(1) O(\rho^{-3}); \tag{64}$$

$$\int_{\mathbb{H}^1} \zeta_j(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW = \frac{\sqrt{2}A}{|z|^2 + it} + O(\rho^{-3}) + o_j(1); \tag{65}$$

$$\int_{\mathbb{H}^1} \xi_j(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW = O(\rho^{-3}) + o_j(1). \tag{66}$$

Proof. To prove (64) we notice that clearly

$$\begin{aligned} \int_{\mathbb{H}^1} (\chi_j \chi \mathfrak{f})(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW &= \int_{\mathbb{H}^1} (\chi \mathfrak{f})(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW \\ &+ \int_{\mathbb{H}^1} ((1-\chi_j)\chi \mathfrak{f})(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW, \end{aligned}$$

so it is sufficient to show

$$\int_{\mathbb{H}^1} ((1-\chi_j)\chi \mathfrak{f})(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW = o_j(1) O(\rho^{-3}).$$

We first notice that

$$Z_{\bar{1}} \Phi(W^{-1}Z) = \frac{\sqrt{2}}{8\pi^2} \frac{w - z}{(\rho(W^{-1}Z))^4} = O(\rho^{-3}(W^{-1}Z)), \tag{67}$$

which implies

$$\left| \int_{\mathbb{H}^1} ((1-\chi_j)\chi \mathfrak{f})(W) Z_{\bar{1}} \Phi(W^{-1}Z) \right| \leq C \int_{\{\rho(W) \geq j\}} (\rho(W))^{-3} (\rho(W^{-1}Z))^{-3} dW.$$

By a scaling argument one shows that

$$\int_{\{\rho(W) \geq j\}} (\rho(W))^{-3} (\rho(W^{-1}Z))^{-3} dW \leq C(\rho(Z))^{-2} \int_{\left\{\rho(W) \geq \frac{j}{\rho(Z)}\right\}} (\rho(W))^{-6} dW \leq \frac{C}{j} (\rho(Z))^{-3},$$

giving (64). Recalling the properties of the support of ζ_j, we can write that

$$\begin{aligned} \int_{\mathbb{H}^1} \xi_j(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW &= \int_{\{1 \leq \rho(W) \leq 2\}} \xi_j(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW \\ &+ \int_{\{j \leq \rho(W) \leq j+1\}} \xi_j(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW. \end{aligned}$$

An argument similar to the one for (64) gives the same estimate for the second integral in the last formula. To control the first one we use (67) to find

$$\left| \int_{\{1 \le \rho(W) \le 2\}} \xi_j(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW \right| \le C \int_{\{1 \le \rho(W) \le 2\}} (\rho(W^{-1}Z))^{-3} dW = O((\rho(Z))^{-3}),$$

which gives (66).

It remains to show (65). In this case, we divide the integral into the three regions

$$\mathcal{A}_1 = \{1 \le \rho \le 4\}; \qquad \mathcal{A}_2 = \{4 \le \rho \le j\}; \qquad \mathcal{A}_3 = \{j \le \rho \le j+1\}.$$

Letting W_1 denote 1-differentiation in the w-variable, using scaling arguments similar to the previous ones, (62), and the fact that

$$W_1 Z_{\bar{1}} \Phi(W^{-1}Z) = -\frac{1}{8\pi^2} \frac{1}{(|z-w|^2 + i(t-s-2\mathrm{Im}(\bar{z}w)))^2},$$

we easily obtain

$$\left| \int_{\mathcal{A}_1} \zeta_j(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW \right| = O((\rho(Z))^{-3}); \qquad \left| \int_{\mathcal{A}_3} \zeta_j(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW \right| = o_j(1).$$

On the other hand, from (62) and some elementary estimates one finds

$$\int_{\mathcal{A}_2} \zeta_j(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW = -4\sqrt{2} i \pi^2 A \int_{\mathcal{A}_2} \frac{\rho^2}{v} W_1 \delta_{\{w=0\}} Z_{\bar{1}} \Phi(W^{-1}Z) dW + o_j(1).$$

Using the facts that

$$Z_1\left(\frac{\rho^2}{s+i|w|^2}\right) = -i\frac{1}{\sqrt{2}} \frac{\overline{w}(s-i|w|^2)}{\rho^6} = 0; \qquad \frac{\rho^2}{s+i|w|^2} = \begin{cases} 1, & \text{for } s>0; \\ -1, & \text{for } s<0, \end{cases} \qquad \text{if } w=0,$$

we deduce

$$\begin{aligned} \int_{\mathcal{A}_2} \zeta_j(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW &= -4\sqrt{2} i \pi^2 A \int_{\mathcal{A}_2} \frac{\rho^2(W)}{s+i|w|^2} \left(W_1 \delta_{\{w=0\}}\right) Z_{\bar{1}} \Phi(W^{-1}Z) dW + o_j(1) \\ &= 4\sqrt{2} i \pi^2 A \int_{\mathcal{A}_2} \delta_{\{w=0\}} \left\{ \frac{s}{|s|} W_1 Z_{\bar{1}}(\Phi(W^{-1}Z)) \right\} dW + o_j(1). \end{aligned}$$

Using also the identity

$$W_1 Z_{\bar{1}} \Phi(W^{-1}Z) = -\frac{1}{8\pi^2} \frac{1}{(|z|^2 + i(t-s))^2}, \qquad \text{for } w=0,$$

we then find

$$\begin{aligned} \int_{\mathcal{A}_2} \zeta_j(W) Z_{\bar{1}} \Phi(W^{-1}Z) dW &= -\frac{\sqrt{2}}{2} iA \int_4^j \frac{1}{(|z|^2 + i(t-s))^2} ds \\ &+ \frac{\sqrt{2}}{2} iA \int_{-j}^{-4} \frac{1}{(|z|^2 + i(t-s))^2} ds + o_j(1) \\ &= \frac{\sqrt{2}A}{|z|^2 + it} + O(\rho^{-4}) + o_j(1), \end{aligned}$$

which gives (65). ■

Summing up, by (63) and Lemma 3.5 we obtained that

$$Z_{\overline{1}}(\mathcal{K}(\mathring{\Box}_b\tilde{g}_j)) = Z_{\overline{1}}\mathcal{K}(-\chi\mathfrak{f}) + \frac{\sqrt{2}A}{|z|^2+it} + O(\rho^{-3}) + o_j(1).$$

Since $\mathcal{K}\mathring{\Box}_b = Id - \mathcal{S}$ on distributions with compact support and since the image of the Szegö projection consists of CR functions, by Lemma 3.3 we deduce that for $z \neq 0$

$$Z_{\overline{1}}\tilde{g}_j = Z_{\overline{1}}\tilde{g}_j - Z_{\overline{1}}(\mathcal{S}\tilde{g}_j) = Z_{\overline{1}}\mathcal{K}(-\chi\mathfrak{f}) + \frac{\sqrt{2}A}{|z|^2+it} + O(\rho^{-3}) + o_j(1).$$

Letting $j \to +\infty$, this means

$$Z_{\overline{1}}\tilde{g} = Z_{\overline{1}}\mathcal{K}(\chi\mathfrak{f}) + \frac{\sqrt{2}A}{|z|^2+it} + O(\rho^{-3}) \qquad \text{for } z \neq 0 \text{ and } \rho \text{ large.}$$

This is precisely (58), concluding the proof of (56).

3.4 Existence of a solution to $\Box_b\beta = 0$

Below, for $\mu \in \mathbb{R}$ we denote by $\mathcal{E}(\rho^\mu)$ the set of smooth functions u on an asymptotically flat pseudohermitian manifold N for which near infinity one has

$$|\mathcal{Z}^{(\alpha)}u| \leq C_{\alpha,u}\,\rho^{\mu-|\alpha|},$$

where α is a multi-index and $\mathcal{Z}^{(\alpha)}$ is a composition of Z_1 and $Z_{\overline{1}}$ derivatives of order $|\alpha|$, and where $C_{\alpha,u}$ is a positive constant depending on α and u. The main tool to prove the existence part in Proposition 3.1 is the next result (notice that in [26] a different convention for θ is used). Define

$$\Box_{b,1} := G_p^2\Box_b; \quad m_1 := G_p^{-2}\theta\wedge d\theta.$$

Denote the space of square integrable functions with respect to the volume form m_1 by $L^2(m_1)$.

Theorem 3.6 *(Theorem 1.3 and Theorem 1.4 in [26]) Suppose N is the blow-up of an embeddable compact three dimensional CR manifold with $\mathcal{Y}(J) > 0$. Then*

$$\Box_{b,1} : Dom(\Box_{b,1}) \subseteq L^2(m_1) \to L^2(m_1)$$

has closed range, and the following decomposition holds

$$\Box_{b,1}\mathcal{K}_N + \mathcal{S}_N = Id \qquad \text{on } L^2(m_1),$$

where $\mathcal{K}_N$ denotes a partial inverse of $\Box_{b,1}$ and $\mathcal{S}_N$ the Szegö projection onto the kernel of $\Box_{b,1}$. Moreover, for every $\varepsilon \in (0,2)$, $\mathcal{K}_N$ and $\mathcal{S}_N$ can be extended continuously as maps

$$\mathcal{K}_N : \mathcal{E}(\rho^{2-\varepsilon}) \to \mathcal{E}(\rho^{-\varepsilon}); \qquad \mathcal{S}_N : \mathcal{E}(\rho^{2-\varepsilon}) \to \mathcal{E}(\rho^{2-\varepsilon})$$

and hence there holds

$$\Box_{b,1}\mathcal{K}_N + \mathcal{S}_N = Id \qquad \text{on } \mathcal{E}(\rho^{2-\varepsilon}).$$

Remark 3.7 *Note that $\Box_b$ may not have L^2 closed range with respect to the volume form $\theta\wedge d\theta$. This causes difficulty to solve the $\Box_b$ equation directly. In [26] the authors introduce the above weighted Kohn Laplacian $\Box_{b,1}$ and show that $\Box_{b,1}$ has L^2 closed range with respect to the weighted volume form m_1.*

We observe that near infinity, $\Box_{b,1} - \mathring{\Box}_{b,1} = G_p^2(\Box_b - \mathring{\Box}_b) + (G_p^2 - (\mathring{G}_p)^2)\mathring{\Box}_b$ maps $\mathcal{E}(\rho^\mu)$ to itself. We apply Theorem 3.6 with

$$h = -\Box_{b,1}(\chi\overline{z} + \mathcal{K}(-\chi\mathfrak{f})).$$

By Lemmas 3.2 and 3.3 (in fact, $O(\rho^{-4})$ in these two lemmas can be replaced by $\mathcal{E}(\rho^{-4})$) we have that $h \in \mathcal{E}(\rho^\varepsilon)$ and hence we can find $u = \mathcal{K}_N h \in \mathcal{E}(\rho^{-2+\varepsilon})$ such that $\Box_{b,1} u = h$ (note that $\mathcal{S}_N h = 0$, see Theorem 1.5 in [26]). Therefore the function

$$\beta = \chi\overline{z} + \mathcal{K}(-\chi\mathfrak{f}) + u$$

is a solution of $\Box_{b,1}\beta = 0$, hence $\Box_b\beta = 0$ (see also the deduction in the introduction of [26]). By scaling arguments, one finds that $\mathcal{K}(\chi\mathfrak{f})$ is the sum of a function with the homogeneity of ρ^{-1} and a function of order $\rho^{-2+\varepsilon}$. We have proved the last statement of Proposition 3.1.

3.5 The role of positivity of the CR Paneitz operator

We prove here that the positivity of P on the compact manifold implies positivity of the last term in (36) as well, up to a multiple of $m(J,\theta)$ (which can be reabsorbed into the left-hand side). We have the following proposition, which also exploits some result from [26].

Proposition 3.8 *Let N be the blow-up of a three dimensional CR manifold with positive CR Yamabe invariant and non-negative CR Paneitz operator. Let β be as in Proposition 2.6: then one has*

$$\frac{1}{2}\int_N \overline{\beta} P\beta\theta\wedge d\theta = \frac{1}{2}\int_N (\overline{\beta}_{-1} + \overline{\beta}_{-2+\varepsilon} + u)P(\beta_{-1} + \beta_{-2+\varepsilon} + \overline{u})\,\theta\wedge d\theta - \frac{2}{3}m(J,\theta) \tag{68}$$

where $u = O(\rho^{-3})$ and

$$\frac{4}{3}m(J,\theta) \geq -\int_N |\Box_b\beta|^2\theta\wedge d\theta + 2\int_N |\beta_{,\overline{1}\overline{1}}|^2\theta\wedge d\theta + 2\int_N R|\beta_{,\overline{1}}|^2\theta\wedge d\theta. \tag{69}$$

Moreover, if θ is chosen as in (2) *and β is chosen so that* $\Box_b\beta = 0$ *(this can be achieved by Proposition 3.1), then $R = 0$ and the above inequality is reduced to*

$$\frac{4}{3}m(J,\theta) \geq 2\int_N |\beta_{,\overline{1}\overline{1}}|^2\theta\wedge d\theta \geq 0. \tag{70}$$

Proof. We set

$$f = \overline{\partial}_b z \in \mathcal{E}(\rho^{-4}).$$

By Theorem 4.5 in [26], we can find $u \in \mathcal{E}(\rho^{-3})$ so that $\overline{\partial}_b u = \overline{\partial}_b z$ (note that in [26], the coordinates that authors use can be changed to ours by a CR inversion). Let us write β as

$$\beta = \overline{z} + \beta_{-1} + \beta_{-2+\varepsilon} = (\overline{z} - \overline{u}) + \beta_{-1} + \beta_{-2+\varepsilon} + \overline{u},$$

so

$$\overline{\beta} = (z - u) + \overline{\beta}_{-1} + \overline{\beta}_{-2+\varepsilon} + u.$$

We write the CR Paneitz operator $P\psi = 4(\psi_{\overline{1}11} + iA_{11}\psi_{\overline{1}})_{\overline{1}}$ as

$$P = P_3 \circ \overline{\partial}_b \qquad \text{or} \qquad P = \partial_b^* \circ \tilde{P}_3.$$

where

$$P_3(a_{\overline{1}}\theta^{\overline{1}}) = 4(a_{\overline{1},11} + iA_{11}a_{\overline{1}})_{,\overline{1}},$$

and

$$\tilde{P}_3(\psi) = 4(\psi_{\overline{1}11} + iA_{11}\psi_{\overline{1}})\theta^1.$$

Since P is real we have that $\int_N \overline{\beta} P\beta\, \theta\wedge d\theta = \int_N \beta P\overline{\beta}\,\theta\wedge d\theta \in \mathbb{R}$, and hence

$$\begin{aligned}&\int_N \left[(\overline{z}-\overline{u})+\beta_{-1}+\beta_{-2+\varepsilon}+\overline{u}\right] P(\overline{\beta}_{-1}+\overline{\beta}_{-2+\varepsilon}+u)\,\theta\wedge d\theta \\ = &\int_N \left[(z-u)+\overline{\beta}_{-1}+\overline{\beta}_{-2+\varepsilon}+u\right] P(\beta_{-1}+\beta_{-2+\varepsilon}+\overline{u})\,\theta\wedge d\theta.\end{aligned}$$

Integrating by parts, we move a $\overline{1}$ derivative to the first term in the integrand of the right-hand side, which annihilates $z-u$. In this way we get

$$\begin{aligned}&\int_N \left[(\overline{z}-\overline{u})+\beta_{-1}+\beta_{-2+\varepsilon}+\overline{u}\right] P(\overline{\beta}_{-1}+\overline{\beta}_{-2+\varepsilon}+u)\,\theta\wedge d\theta \\ = &-\int_N (\overline{\beta}_{-1}+\overline{\beta}_{-2+\varepsilon}+u)_{\overline{1}}\tilde{P}_3(\beta_{-1}+\beta_{-2+\varepsilon}+\overline{u})\,\theta\wedge d\theta + \oint_\infty zi\tilde{P}_3\beta_{-1}\,\theta\wedge\theta^1.\end{aligned}$$

For the last term we used the decay at infinity of the lower order terms in β, giving

$$\oint_\infty i((z-u)+\overline{\beta}_{-1}+\overline{\beta}_{-2+\varepsilon}+u)\tilde{P}_3(\beta_{-1}+\beta_{-2+\varepsilon}+\overline{u})\,\theta\wedge\theta^1 = \oint_\infty zi\tilde{P}_3\beta_{-1}\,\theta\wedge\theta^1.$$

Using the Stokes theorem again, we find

$$\begin{aligned}\oint_\infty zi\tilde{P}_3\beta_{-1}\,\theta\wedge\theta^1 &= \int_N ((z-u)+\overline{\beta}_{-1}+\overline{\beta}_{-2+\varepsilon}+u)P(\beta_{-1}+\beta_{-2+\varepsilon}+\overline{u})\,\theta\wedge d\theta \\ &+ \int_N (\overline{\beta}_{-1}+\overline{\beta}_{-2+\varepsilon}+u)_{\overline{1}}\tilde{P}_3(\beta_{-1}+\beta_{-2+\varepsilon}+\overline{u})\,\theta\wedge d\theta.\end{aligned}$$

From the last formulas we deduce

$$\begin{aligned}\int_N \beta P\overline{\beta}\,\theta\wedge d\theta &= \int_N (\overline{\beta}_{-1}+\overline{\beta}_{-2+\varepsilon}+u)P(\beta_{-1}+\beta_{-2+\varepsilon}+\overline{u})\,\theta\wedge d\theta \\ &+ \oint_\infty zi\tilde{P}_3\beta_{-1}\,(dt - i\overline{z}dz + izd\overline{z})\wedge\sqrt{2}dz. \qquad (71)\end{aligned}$$

Using the decay of A_{11} at infinity we find

$$\oint_\infty \tilde{P}_3\beta_{-1}\cdot zi(dt-i\overline{z}dz+izd\overline{z})\wedge\sqrt{2}dz = \oint_\infty 4(\beta_{-1})_{\overline{1}11}(i\sqrt{2}zdt\wedge dz - \sqrt{2}z^2 d\overline{z}\wedge dz). \qquad (72)$$

By our choice of β_{-1} we have that

$$-2(\beta_{-1})_{\overline{1}1} = \mathring{\Box}_b\beta_{-1} = -4\pi A\frac{\overline{z}}{\rho^6}\left\{|z|^2+it\right\} + O(\rho^{-4}),$$

and moreover

$$(\partial_z + i\overline{z}\partial_t)\left[\frac{\overline{z}}{\rho^6}\left(|z|^2+it\right)\right] = -3\overline{z}^2(|z|^2+it)^2\rho^{-6},$$

so we find

$$4(\beta_{-1})_{\overline{1}11} = -12\sqrt{2}A\pi\overline{z}^2\frac{(|z|^2+it)^2}{\rho^{10}}.$$

Inserting this expression into the boundary formula we get

$$\begin{aligned}&4\oint_\infty (\beta_{-1})_{\overline{1}11}(i\sqrt{2}zdt\wedge dz - \sqrt{2}z^2d\overline{z}\wedge dz) \\ = &-12\sqrt{2}\oint_\infty \pi A\left[|z|^4 - t^2 + 2it|z|^2\right]\rho^{-10}\overline{z}^2(i\sqrt{2}zdt\wedge dz - \sqrt{2}z^2d\overline{z}\wedge dz) \\ = &-24\pi A\oint_S \left[|z|^4-t^2+2it|z|^2\right]\overline{z}^2(izdt\wedge dz - z^2d\overline{z}\wedge dz).\end{aligned}$$

Using the fact that $r^4 + t^2 = 1$ on S and the relations (cf. (32) and (42))

$$dz \wedge d\overline{z} = -2ir dr \wedge d\varphi; \qquad dt \wedge dz = ire^{i\varphi} dt \wedge d\varphi,$$

one finds

$$\begin{aligned} & 4 \oint_{\infty} (\beta_{-1})_{\overline{1}11} (i\sqrt{2} z dt \wedge dz - \sqrt{2} z^2 d\overline{z} \wedge dz) \\ = \ & -24\pi A \int_S \left[|z|^4 - t^2 + 2it|z|^2 \right] r^2 \left(-r^2 dt \wedge d\varphi - 2ir^3 dr \wedge d\varphi \right) \\ = \ & -24\pi A \int_S \left[|z|^4 - t^2 + 2it|z|^2 \right] \left(r^4 d\varphi \wedge dt + 2ir^5 d\varphi \wedge dr \right) \\ = \ & -24\pi A \int_S \left[|z|^4 - t^2 + 2it|z|^2 \right] \left(r^4 d\varphi \wedge dt - ir^2 t d\varphi \wedge dt \right). \end{aligned}$$

The terms which are odd in t vanish after integration, so the last expression becomes

$$-48\pi^2 A \int_{-1}^{1} (1 - t^2) dt = -64\pi^2 A = -\frac{4}{3} m(J, \theta).$$

In conclusion, from (36), (71), (72) and the last formula we find

$$\begin{aligned} \frac{2}{3} m(J, \theta) &= -\int_N |\Box_b \beta|^2 \theta \wedge d\theta + 2 \int_N |\beta_{,\overline{1}\overline{1}}|^2 \theta \wedge d\theta + \frac{1}{2} \int_N \overline{\beta} P \beta \theta \wedge d\theta \\ &= -\int_N |\Box_b \beta|^2 \theta \wedge d\theta + 2 \int_N |\beta_{,\overline{1}\overline{1}}|^2 \theta \wedge d\theta \\ &+ \frac{1}{2} \int_N (\overline{\beta}_{-1} + \overline{\beta}_{-2+\varepsilon} + u) P (\beta_{-1} + \beta_{-2+\varepsilon} + \overline{u}) \, \theta \wedge d\theta - \frac{2}{3} m(J, \theta). \end{aligned}$$

Viewed as a function on M, $\beta_{-1} + \beta_{-2+\varepsilon} + \overline{u}$, vanishes at p, is of class $\mathfrak{S}^{2,2}(M)$, and is smooth on $M \setminus \{p\}$. Therefore, by the conformal invariance of P and its non-negativity we have

$$\begin{aligned} & \int_N (\overline{\beta}_{-1} + \overline{\beta}_{-2+\varepsilon} + u) P_\theta (\beta_{-1} + \beta_{-2+\varepsilon} + \overline{u}) \, \theta \wedge d\theta \\ = \ & \int_{M \setminus \{p\}} (\overline{\beta}_{-1} + \overline{\beta}_{-2+\varepsilon} + u) P_{\hat{\theta}} (\beta_{-1} + \beta_{-2+\varepsilon} + \overline{u}) \, \hat{\theta} \wedge d\hat{\theta} \geq 0. \end{aligned}$$

Notice that the non-negativity of P is assumed on smooth functions, but by approximation and integration by parts one also gets a sign condition on the integral of $v P_{\hat{\theta}} \overline{v}$ for v of class $\mathfrak{S}^{2,2}(M)$.

Summing up we then obtain

$$\begin{aligned} \frac{4}{3} m(J, \theta) &= -\int_N |\Box_b \beta|^2 \theta \wedge d\theta + 2 \int_N |\beta_{,\overline{1}\overline{1}}|^2 \theta \wedge d\theta + 2 \int_N R |\beta_{,\overline{1}}|^2 \theta \wedge d\theta \\ &+ \frac{1}{2} \int_{M \setminus \{p\}} (\overline{\beta}_{-1} + \overline{\beta}_{-2+\varepsilon} + u) P_{\hat{\theta}} (\beta_{-1} + \beta_{-2+\varepsilon} + \overline{u}) \, \hat{\theta} \wedge d\hat{\theta}, \end{aligned}$$

which implies (69). Formula (70) then follows immediately. ■

3.6 Conclusion of the proof of Theorem 1.1

The first statement of the theorem follows immediately from Proposition 3.8.

Suppose now that $m(J, \theta) = 0$. Then, from (70), Proposition 3.1 and (68) we have the following identities

(73) $$\beta_{,\overline{1}\overline{1}} \equiv 0; \qquad \beta_{,\overline{1}1} \equiv 0; \qquad P\beta \equiv 0.$$

The first two relations imply that $|\beta_{,\bar{1}}|^2$ is constant: in particular, from the behavior of $\beta_{,\bar{1}}$ at infinity we deduce that $|\beta_{,\bar{1}}|^2 \equiv \frac{1}{2}$. We also have then

$$R \equiv 0.$$

From $P\beta = 0$ we also deduce that $A_{11,\bar{1}} \equiv 0$. Let us now show that the torsion vanishes identically: in order to do this, we follow the arguments of Section 3 in [37]. Since the ideas here require rather straightforward modifications, we will be rather sketchy in this part.

We consider the flow φ_s generated by the Reeb vector field T of N, and we let

$$J_{(s)} = \varphi_s^* J \qquad (\dot{J} = L_T J = 2A_{J,\theta}),$$

where $A_{J,\theta} = -iA_{11}\theta^1 \otimes Z_{\bar{1}}$+conj.. By the variation formulas (141), (142) we have that

$$\frac{d}{ds} R_{J_{(s)},\theta} = -2|A_{11}|^2 + i(A_{11,\overline{11}} - A_{\overline{11},11}); \qquad \frac{d}{ds}(A_{11})_{J_{(s)},\theta} = iA_{11,0}. \tag{74}$$

Since for an asymptotically flat manifold we have $A_{11} = O(\rho^{-4})$ at infinity (see Remark 2.2) and since $A_{11,\bar{1}} \equiv 0$ at $s = 0$, from the second equation in (74) we derive (from a Taylor expansion in s and taking space derivatives) that

$$A_{11,\overline{11}} = O(s\rho^{-8}) \quad \text{for } s \text{ small and } \rho \text{ large.}$$

Then the first equation in (74) implies that for s small

$$R_{J_{(s)},\theta} \geq \begin{cases} -Cs & \text{everywhere on } N; \\ -C\frac{s}{\rho^8} & \text{at infinity.} \end{cases} \tag{75}$$

In particular, it turns out that the negative part of $R_{J_{(s)},\theta}$ is arbitrarily small as $s \to 0$. Similarly to Lemma 3.1 in [37] one has the Sobolev type inequality

$$\left(\int_N u^4 \theta \wedge d\theta \right)^{\frac{1}{2}} \leq C \int_N |\nabla_b u|^2 \theta \wedge d\theta; \qquad C > 0, u \in C_c^\infty(N)$$

where $|\nabla_b u|^2 := 2u_{,1}u_{,\bar{1}}$. This implies that

$$\begin{aligned} \int_N \left(4|\nabla_b u|^2 + R_{J_{(s)},\theta} u^2\right) \theta \wedge d\theta &\geq 4\int_N |\nabla_b u|^2 \theta \wedge d\theta - \left(\int_N R^2_{J_{(s)},\theta} \theta \wedge d\theta \right)^{\frac{1}{2}} \left(\int_N u^4 \theta \wedge d\theta \right)^{\frac{1}{2}} \\ &\geq (4 + o_s(1)) \int_N |\nabla_b u|^2 \theta \wedge d\theta \qquad \text{as } s \to 0. \end{aligned}$$

Therefore, the operator $-4\Delta_b + R_{J_{(s)},\theta}$ is coercive for s small. Estimates similar to (75) imply that $|R_{J_{(s)},\theta}| \leq C\rho^{-8}$ at infinity, and hence we can find a solution v_s of

$$-4\Delta_b v_s + R_{J_{(s)},\theta} v_s = R_{J_{(s)},\theta} \qquad \text{on } N,$$

which decays to zero at infinity. More precisely, using estimates similar to those of Lemma 3.2 in [37], together with Lemma 5.1 one finds that

$$v_s = \frac{1}{32\pi\rho^2} \int_N (R_{J_{(s)},\theta} - R_{J_{(s)},\theta} v_s)\theta \wedge d\theta + O(\rho^{-3}) \qquad \text{at infinity.}$$

The function $u_s = 1 - v_s$ then satisfies

$$-4\Delta_b u_s + R_{J_{(s)},\theta} u_s = 0 \qquad \text{on } N, \tag{76}$$

which means that the manifold $(N, J_{(s)}, u_s^2\theta)$ has zero Tanaka-Webster curvature and is asymptotically flat. By the asymptotic formula for v_s we deduce immediately

$$u_s = 1 - \frac{1}{32\pi\rho^2} \int_N R_{J_{(s)},\theta} u_s \theta \wedge d\theta + O(\rho^{-3}) \qquad \text{at infinity,}$$

and hence by Lemma 2.5 (see also the coefficient of θ in Definition 2.1) we have that

$$m(J_{(s)}, u_s^2\theta) = -\frac{3}{4}\int_N R_{J(s),\theta} u_s \theta \wedge d\theta. \tag{77}$$

Differentiating the last formula in s and using the fact that $u_0 \equiv 1$, together with (74), we find

$$\frac{d}{ds}|_{s=0} m(J_{(s)}, u_s^2\theta) = \frac{3}{2}\int_N |A_{11}|^2 \theta \wedge d\theta > 0 \qquad \text{in case } A_{11} \not\equiv 0 \text{ at } s = 0.$$

This implies that for s negative we obtain a manifold which is asymptotically flat, with zero Tanaka-Webster curvature and with negative mass.

We show that this is a contradiction to the first part of the theorem. In fact, the flow $\varphi_{(s)}$ on the manifold N corresponds to the one parameter family of diffeomorphisms $\hat{\varphi}_{(s)}$ on $(M, \hat{J}, \hat{\theta})$ generated by the vector field $(G_p)^{-2}\left[\hat{T} + 2i(\log G_p)_{,1}\hat{Z}_{\bar{1}} - 2i(\log G_p)_{,\bar{1}} Z_1\right]$, where G_p is the Green's function of L_b on M for $s = 0$, and $\hat{T}$ the corresponding Reeb vector field. Letting $\hat{J}_{(s)}$ denote $(\hat{\varphi}_{(s)})^*\hat{J}$, then one has clearly that $(G_p)_{(s)} = u_s G_p$ (since $u_s G_p \hat{\theta}$ has zero Tanaka-Webster curvature, and the correct asymptotics near the singularity). Hence we obtain $(N, J_{(s)}, u_s^2\theta)$ as blow-up of the compact manifold $(M, \hat{J}_{(s)}, \hat{\theta})$, through the Green's function $(G_p)_{(s)}$.

The contradiction will follow if we show that $(M, \hat{J}_{(s)}, \hat{\theta})$ satisfies the same assumptions of Theorem 1.1. Notice that we are pulling back the structure via the contact diffeomorphisms $\hat{\varphi}_{(s)}$, so the positivity of $L_{b,\hat{J}_{(s)},\hat{\theta}}$ and of $P_{\hat{J}_{(s)},\hat{\theta}}$ both follow from a change of variable and its conformal invariance. Therefore, we proved that $m(J, \theta) = 0$ also implies $A_{11} \equiv 0$.

To show that N coincides with Heisenberg, first we define a map from a neighborhood of infinity $\mathcal{U}$ in N to a neighborhood of infinity $\mathcal{V}$ in $\mathbb{H}^1$. From (73) we find that

$$d(\beta_{,\bar{1}}\theta^{\bar{1}}) = \beta_{,\bar{1}1}\theta^1 \wedge \theta^{\bar{1}} + \beta_{,\bar{1}0}\theta \wedge \theta^{\bar{1}} = 0,$$

which implies that $\beta_{,1\bar{1}} = \beta_{,11\bar{1}} = 0$, $\beta_{,11} = 0$, $|\beta_{,1}|^2 = \mathit{constant} = 0$, and hence $d\beta = \beta_{,\bar{1}}\theta^{\bar{1}}$. Taking $z = \overline{\beta}$ we have

$$d(\theta - iz d\bar{z} + i\bar{z} dz) = i\theta^1 \wedge \theta^{\bar{1}} - 2i dz \wedge d\bar{z} = 0.$$

Note that $dz \wedge d\bar{z} = |\beta_{,\bar{1}}|^2\theta^1 \wedge \theta^{\bar{1}}$ and $|\beta_{,\bar{1}}|^2 = \frac{1}{2}$ hence, if we take $\mathcal{U}$ simply connected (for example, $\{\rho \geq R\}$, $R \gg 1$, in inverted CR coordinates), there exists a function $\tilde{t}$ such that

$$d\tilde{t} = \theta - iz d\bar{z} + i\bar{z} dz.$$

So we get a pseudohermitian isomorphism between $\mathcal{U}$ and its image in $\mathbb{H}^1$, $\mathcal{V}$, if we send $q \in N$ into

$$q \mapsto (z(q), t(q)) = \left(\overline{\beta}(q), \int_{q_0}^{q} d\tilde{t}\right),$$

where we are taking curves connecting q_0 to q inside $\mathcal{U}$.

We call $\Psi : \mathcal{V} \to \mathcal{U}$ (sets which we can assume to be connected by arcs) the inverse of this map. Extend Ψ to a covering map $\tilde{\Psi} : \mathbb{H}^1 \mapsto N$. Observe that $\mathcal{V}$ is contained in a fundamental domain. If $\tilde{\Psi}$ is not 1-1, then there are at least two fundamental domains. But one of them has infinity volume while any other one has finite volume. The contradiction shows $\tilde{\Psi}$ is 1-1 and a pseudohermitian isomorphism between $\mathbb{H}^1$ and N. This concludes the proof.

Remark 3.9 *If J is spherical we have a different proof of the vanishing of A_{11}. In fact, if $\mathfrak{Q}$ stands for the Cartan tensor (see Subsection A.2), for spherical structures one has*

$$0 = \mathfrak{Q}_{11} = \frac{1}{6}R_{,11} + \frac{i}{2}RA_{11} - A_{11,0} - \frac{2}{3}iA_{11,\bar{1}1}.$$

Then (see Section A), since $A_{11,\bar{1}} = 0$ and $R = 0$ we find that

$$0 = iA_{11,0} = A_{11,1\bar{1}} - A_{11,\bar{1}1} - 2A_{11}R,$$

which implies $A_{11,1\bar{1}} = 0$. By integration we obtain

$$0 = -\int_N A_{11,1\bar{1}} A_{\bar{1}\bar{1}} \theta \wedge d\theta = \int_N A_{11,1} A_{\bar{1}\bar{1},\bar{1}} \theta \wedge d\theta = \int_N |A_{11,1}|^2 \theta \wedge d\theta,$$

which implies $A_{11,1} = 0$. Differentiating we get $|A_{11}|^2 = const.$ and the constant is zero at infinity, which implies $A_{11} \equiv 0$.

4 Some examples

In this section we describe some examples: first we find a structure close to the spherical one with nonpositive Paneitz operator. Then, we derive an example of manifold with positive Tanaka-Webster class but with negative mass. We finally describe a CR structure on $S^2 \times S^1$ with non-negative Paneitz operator.

4.1 Three dimensional CR manifolds with nonpositive CR Paneitz operator

Recall that from the commutation rules (9) one has

$$\square_b u = -\Delta_b u + iTu = -(u_{,1\bar{1}} + u_{,\bar{1}1}) + iu_{,0} = -2u_{,\bar{1}1} = -2Z_1(Z_{\bar{1}}u) - 2\omega_{\bar{1}}^{\bar{1}}(Z_1)Z_{\bar{1}}u. \tag{78}$$

Recall also that, along a deformation $J_{(s)}$ of the CR structure the following relations hold (see Subsection A.1.2)

$$\dot{Z}_1 = -iE_{11}Z_{\bar{1}}; \qquad \dot{\theta}^1 = -iE_{\bar{1}\bar{1}}\theta^{\bar{1}}, \tag{79}$$

$$\dot{\omega}_1^1 = i\left(A_{11}E_{\bar{1}\bar{1}} + A_{\bar{1}\bar{1}}E_{11}\right)\theta - i(E_{11,\bar{1}}\theta^1 + E_{\bar{1}\bar{1},1}\theta^{\bar{1}}); \qquad \dot{A}_{11} = iE_{11,0}. \tag{80}$$

$$-\dot{\Delta}_b = 2i\left(E_{11}Z_{\bar{1}}Z_{\bar{1}} + E_{11,\bar{1}}Z_{\bar{1}}\right) + \text{ conj.}. \tag{81}$$

We derive next the first and second variations of the Paneitz operator near the standard three dimensional pseudohermitian sphere. We can express the Paneitz operator P as follows

$$P\psi := \bar{\square}_b \square_b \psi + 4i(A_{11}\psi_{,\bar{1}})_{,\bar{1}} \tag{82}$$

for a smooth real function ψ. By (78) the expression (82) is equivalent to

$$P\psi = 4(\psi_{,\bar{1}11} + iA_{11}\psi_{,\bar{1}})_{,\bar{1}} \qquad \text{or} \qquad P\psi = \Delta_b^2\psi + T^2\psi + 4\,\mathrm{Im}\,(A_{\bar{1}\bar{1}}\psi_{,1})_{,1}. \tag{83}$$

Along the above deformation $J_{(s)}$, let $P_{(s)}$ denote the Paneitz operator associated to $(J_{(s)}, \theta)$. Let $(\cdot,\cdot)$ denote the L^2 inner product with respect to the volume form $\theta \wedge d\theta$. We then find

$$\frac{d}{ds}(P_{(s)}\psi,\psi) = 2(\dot{\Delta}_b\psi, \Delta_b\psi) - 4\,\mathrm{Im}\int_M \dot{A}_{\bar{1}\bar{1}}(\psi_{,1})^2\theta \wedge d\theta - 8\,\mathrm{Im}\int_M A_{\bar{1}\bar{1}}(\psi_{,1})^{\cdot}\psi_{,1}\theta \wedge d\theta \tag{84}$$

by (83). From (79) we have

$$(\psi_{,1})^{\cdot} = -iE_{11}\psi_{,\bar{1}}. \tag{85}$$

Substituting (80), (81), and (85) into (84), we obtain

$$
\begin{aligned}
(86)\qquad \frac{d}{ds}(P_{(s)}\psi,\psi) &= 4\int_M E_{\bar{1}\bar{1}}\psi_{,1}\left(-i\psi_{,1\bar{1}1}-i\psi_{,\bar{1}11}-\psi_{,10}+A_{11}\psi_{,\bar{1}}\right)\theta\wedge d\theta+\text{ conj.}\\
&= -8i\int_M E_{\bar{1}\bar{1}}\psi_{,1}(\psi_{,\bar{1}11}+iA_{11}\psi_{,\bar{1}})\theta\wedge d\theta+\text{ conj.}
\end{aligned}
$$

using an integration by parts and the commutation relations (9). Take $\psi\in KerP_{(0)}$, i.e.

$$
(87)\qquad 4(\psi_{,\bar{1}11}+iA_{11}\psi_{,\bar{1}})_{,\bar{1}}=0.
$$

If $J_{(0)}$ has transverse symmetry, then we can find a contact form $\theta_{(0)}$ such that $A_{11}=0$ with respect to $(J_{(0)},\theta_{(0)})$ (see [32]). By the transformation law (3) we have that $KerP_{(0)}$ and $(P_{(s)}\psi,\psi)$ are independent of the choice of contact form. So we may just take $\theta_{(0)}$ as the contact form in (87) to get $\psi_{,\bar{1}11\bar{1}}=0$. Multiplying this by $\psi_{,1\bar{1}}$ and integrating, we get

$$
\begin{aligned}
0 &= \int_M \psi_{,\bar{1}11\bar{1}}\psi_{,1\bar{1}}\theta_{(0)}\wedge d\theta_{(0)} = -\int_M \psi_{,\bar{1}11}\psi_{,1\bar{1}\bar{1}}\theta_{(0)}\wedge d\theta_{(0)}\\
&= -\int_M |\psi_{,\bar{1}11}|^2\theta_{(0)}\wedge d\theta_{(0)}
\end{aligned}
$$

using an integration by parts and the fact that ψ is real. It follows that $\psi_{,\bar{1}11}=0$, so from (86) we have

$$
(88)\qquad \frac{d}{ds}|_{s=0}(P_{(s)}\psi,\psi)=0
$$

for $\psi\in KerP_{(0)}$ if $J_{(0)}$ has transverse symmetry. For example we can take $J_{(0)}=\hat{J}$, the standard pseudohermitian structure compatible with $\hat{\xi}$ on $M=S^3$, where $(S^3,\hat{\xi})$ is the standard contact 3-sphere. Note that from the above argument, $\psi\in KerP_{(0)}$ implies that ψ is CR-pluriharmonic if $J_{(0)}$ has transverse symmetry. So by Proposition 3.4 in [32], we have

$$
(89)\qquad \psi_{,\bar{1}11}+iA_{11}\psi_{,\bar{1}}=0
$$

with respect to $J_{(0)}$ coupled with any contact form. Starting with (86) we compute

$$
(90)\qquad \frac{d^2}{ds^2}(P_{(s)}\psi,\psi)|_{s=0}=-8i\int_{S^3}E_{\bar{1}\bar{1}}\psi_{,1}\frac{d}{ds}\left(\psi_{,\bar{1}11}+iA_{11}\psi_{,\bar{1}}\right)|_{s=0}\theta_{(0)}\wedge d\theta_{(0)}+\text{ conj.}
$$

by (89). From (79) and (80) we obtain

$$
(91)\qquad \frac{d}{ds}\psi_{,\bar{1}1}=i[(E_{\bar{1}\bar{1}}\psi_{,1})_{,1}-(E_{11}\psi_{,\bar{1}})_{,\bar{1}}].
$$

We then have

$$
(92)\qquad \frac{d}{ds}\psi_{,\bar{1}11}=\left(\frac{d}{ds}Z_1\right)(\psi_{,\bar{1}1})+Z_1\left(\frac{d}{ds}\psi_{,\bar{1}1}\right)=-iE_{11}\psi_{,\bar{1}1\bar{1}}+i(E_{\bar{1}\bar{1}}\psi_{,1})_{,11}-i(E_{11}\psi_{,\bar{1}})_{,\bar{1}1}
$$

by (79) and (91). Substituting (92), the conjugate of (85), and $\dot{A}_{11}=iE_{11,0}$ into (90) we get

$$
\begin{aligned}
(93)\qquad \frac{d^2}{ds^2}(P_{(s)}\psi,\psi)|_{s=0} &= 8\int_{S^3}E_{\bar{1}\bar{1}}\psi_{,1}\left[(E_{\bar{1}\bar{1}}\psi_{,1})_{,11}-(E_{11}\psi_{,\bar{1}})_{,\bar{1}1}\right.\\
&\left.-E_{11}\psi_{,\bar{1}1\bar{1}}+iE_{11,0}\psi_{,\bar{1}}+iA_{11}E_{\bar{1}\bar{1}}\psi_{,1}\right]\theta_{(0)}\wedge d\theta_{(0)}+\text{ conj..}
\end{aligned}
$$

In view of the conjugate of (89) and the commutation relations (9), we compute

$$
(94)\qquad \psi_{,\bar{1}1\bar{1}}=\psi_{,1\bar{1}\bar{1}}-i\psi_{,0\bar{1}}=iA_{\bar{1}\bar{1}}\psi_{,1}-i\psi_{,\bar{1}0}-i\psi_{,1}A_{\bar{1}\bar{1}}=-i\psi_{,\bar{1}0}.
$$

Substituting (94) into (93), integrating by parts, and making use of the first commutation relation in (9):

$$i(E_{\bar{1}\bar{1}}\psi_{,1})_{,0} = (E_{\bar{1}\bar{1}}\psi_{,1})_{,1\bar{1}} - (E_{\bar{1}\bar{1}}\psi_{,1})_{,\bar{1}1} + (E_{\bar{1}\bar{1}}\psi_{,1})R,$$

hence we obtain

$$\begin{aligned}\frac{d^2}{ds^2}(P_{(s)}\psi,\psi)|_{s=0} &= 8\int_{S^3}\big(-[(E_{\bar{1}\bar{1}}\psi_{,1})_{,1}]^2 + 2|(E_{\bar{1}\bar{1}}\psi_{,1})_{,1}|^2 - |(E_{\bar{1}\bar{1}}\psi_{,1})_{,\bar{1}}|^2 \\ &\quad -R|E_{\bar{1}\bar{1}}\psi_{,1}|^2 + iA_{11}(E_{\bar{1}\bar{1}}\psi_{,1})^2\big)\,\theta_{(0)}\wedge d\theta_{(0)} + \text{ conj.} \\ &= 8\int_{S^3}\big(4|(E_{\bar{1}\bar{1}}\psi_{,1})_{,1}|^2 - [(E_{\bar{1}\bar{1}}\psi_{,1})_{,1}]^2 - [(E_{11}\psi_{,\bar{1}})_{,\bar{1}}]^2 \\ &\quad -2|(E_{\bar{1}\bar{1}}\psi_{,1})_{,\bar{1}}|^2 - 2R|E_{\bar{1}\bar{1}}\psi_{,1}|^2\big)\,\theta_{(0)}\wedge d\theta_{(0)}.\end{aligned} \tag{95}$$

In the last equality of (95) we have used $A_{11} = 0$. We now choose $E_{11} \neq 0$ such that

$$E_{11,\bar{1}} = 0 \tag{96}$$

Assuming (96), we reduce (95) to

$$\begin{aligned}\frac{d^2}{ds^2}(P_{(s)}\psi,\psi)|_{s=0} &= 8\int_{S^3}\big(4|E_{\bar{1}\bar{1}}\psi_{,11}|^2 - [E_{\bar{1}\bar{1}}\psi_{,11}]^2 - [E_{11}\psi_{,\bar{1}\bar{1}}]^2 \\ &\quad -2|(E_{\bar{1}\bar{1}}\psi_{,1})_{,\bar{1}}|^2 - 2R|E_{\bar{1}\bar{1}}\psi_{,1}|^2\big)\,\theta_{(0)}\wedge d\theta_{(0)}.\end{aligned} \tag{97}$$

Now on $(S^3,\, J_{(0)} = \hat{J},\, \theta_{(0)} = \hat{\theta})$, where

$$\hat{\theta} = i(\overline{\partial} - \partial)(|z_1|^2 + |z_2|^2) \tag{98}$$

is the standard contact form on $(S^3,\, \hat{\xi})$, we have that R is a positive constant. Note also that $Z_1 = \frac{1}{\sqrt{2}}\left(\bar{z}_2\frac{\partial}{\partial z_1} - \bar{z}_1\frac{\partial}{\partial z_2}\right)$, $Z_{\bar{1}} = \frac{1}{\sqrt{2}}\left(z_2\frac{\partial}{\partial \bar{z}_1} - z_1\frac{\partial}{\partial \bar{z}_2}\right)$. To make (97) negative, we choose $\psi = z_1 + \bar{z}_1$ where $(z_1,\, z_2) \in S^3 \subseteq \mathbb{C}^2$. It follows that

$$\psi_{,1} = \frac{1}{\sqrt{2}}\bar{z}_2; \qquad \psi_{,11} = 0; \qquad \psi_{,1\bar{1}} = -\frac{1}{2}z_1; \qquad \psi_{,\bar{1}\bar{1}} = 0. \tag{99}$$

Observing that the first three terms of the integrand in (97) vanish due to the fact that $\psi_{,11} = 0$ by (99), we have

$$\frac{d^2}{ds^2}(P_{(s)}\psi,\psi)|_{s=0} = 8\int_{S^3}\left(-\left|E_{\bar{1}\bar{1},\bar{1}}\bar{z}_2 - E_{\bar{1}\bar{1}}\frac{1}{\sqrt{2}}z_1\right|^2 - R|E_{\bar{1}\bar{1}}\bar{z}_2|^2\right)\hat{\theta}\wedge d\hat{\theta} < 0. \tag{100}$$

For example, we can take E_{11} to be a nonzero constant in (100), which satisfies (96). In view of (100), (88), and $(P_{(0)}\psi,\psi) = 0$, we can find $\varepsilon > 0$ small so that

$$(P_{(s)}\psi,\psi) < 0$$

for $0 < s \leq \varepsilon$. In conclusion we obtain the following result.

Proposition 4.1 *There exist CR structures on S^3 arbitrarily close to the spherical one for which the CR Paneitz operator is not non-negative.*

Remark 4.2 *In [1] and [35] some examples of non-embeddable structures were given, where E_{11} was taken to be a nonzero constant (the associated deformed CR structures are indicated by their type $(0,1)$ vector fields $Z_{\bar{1}} + \frac{iE_{\bar{1}\bar{1}}s}{\sqrt{1+|E_{\bar{1}\bar{1}}s|^2}}Z_1$), satisfying in particular (96). Observe that the tangency condition for the embeddability reads*

$$E = B_J(f) := (f_{,11} + iA_{11}f)\theta^1 \otimes Z_{\bar{1}} + (\overline{f}_{,\overline{1}\overline{1}} - iA_{\overline{1}\overline{1}}\overline{f})\theta^{\overline{1}} \otimes Z_1,$$

for some complex-valued function f ([16]). Since on the sphere the torsion vanishes, the condition simplifies as

$$E = f_{,11}\theta^1 \otimes Z_{\bar{1}} + \overline{f}_{,\bar{1}\bar{1}}\theta^{\bar{1}} \otimes Z_1 \tag{101}$$

for some complex-valued function f. For other embeddability criteria using a Fourier representation (or a suitable normal form) or a spectrum of $\Box_b$, see [6] and [9].

We notice that an E satisfying (96) *cannot correspond to any nonzero f in* (101)*. In fact if this would be the case, we would have that $f_{,11\bar{1}} = 0$. Multiplying this equation by $\overline{f}_{,\bar{1}}$ and integrating by parts we would get $\int_M |f_{,11}|^2\theta \wedge d\theta = 0$, which would also imply $E_{11} = 0$. Therefore we expect our examples to be non-embeddable ones. The same comments apply to the construction in the next subsection.*

Remark 4.3 *The statement of Proposition 4.1 can also be deduced by applying the results in [6] and [12]. In fact, in [12], the authors prove that a smooth, strictly pseudoconvex compact CR 3-manifold is embeddable if the CR Paneitz operator is non-negative and the CR Yamabe invariant is positive.*

4.2 First and second variations of the mass near the standard sphere

In this subsection we perturb the pseudohermitian structure of the standard sphere in order to understand the variation of the mass. We begin with a deformation in $\mathbb{H}^1$, which we will eventually transfer to a compact setting.

We consider a deformation $J(s)$ of the standard pseudohermitian structure of $\mathbb{H}^1$, namely such that $J(0)$ is as in (7). Recall the variation formulas for Δ_b and R in Subsection A.1.2. Assuming the deformation of J decays sufficiently fast (so that, say, (75) holds for $N = \mathbb{H}^1$, $\theta = \mathring{\theta}$) near infinity, we can find a scalar flat conformal contact form $\theta_s = u_s^2\mathring{\theta}$, with u_s satisfying (76), as in Subsection 3.6. Then the mass $m(J_{(s)}, u_s^2\theta)$ will be still given by formula (77). Differentiating this formula twice in s, taking into account that $u \equiv 1$ and $R \equiv 0$ for $s = 0$ we obtain, at $s = 0$

$$\ddot{m}(J,\theta) = -\frac{3}{4}\int_{\mathbb{H}^1} \ddot{R}\mathring{\theta} \wedge d\mathring{\theta} - \frac{3}{2}\int_{\mathbb{H}^1} \dot{R}\dot{u}\mathring{\theta} \wedge d\mathring{\theta}. \tag{102}$$

We choose a deformation $J(s)$ so that E_{11} (see the notation in Subsection A.1.2) is a CR function, namely $E_{11,\bar{1}} = 0$. We can take for example

$$E_{11}(z,\overline{z},t) = \frac{1}{(t + i(|z|^2+1))^k},$$

with k integer and large (to have a fast decay). By (142) we have then $\dot{R} = 0$, which by (102) implies

$$\ddot{m}(J,\theta) = -\frac{3}{4}\int_{\mathbb{H}^1} \ddot{R}\mathring{\theta} \wedge d\mathring{\theta}. \tag{103}$$

Reasoning as for (143), one can check that on $\mathbb{H}^1$

$$\begin{aligned} \ddot{R} &= -6|E_{11,\bar{1}}|^2 - 2|E_{11,1}|^2 - 3E_{11,\bar{1}1}E_{\bar{1}\bar{1}} - 3E_{\bar{1}\bar{1},1\bar{1}}E_{11} - E_{11}E_{\bar{1}\bar{1},\bar{1}1} - E_{\bar{1}\bar{1}}E_{11,1\bar{1}} \\ &- iE_{11,0}E_{\bar{1}\bar{1}} + iE_{\bar{1}\bar{1},0}E_{11}. \end{aligned}$$

Therefore, by our choice of E_{11} one has

$$\ddot{R} = -2|E_{11,1}|^2 - E_{11}E_{\bar{1}\bar{1},\bar{1}1} - E_{\bar{1}\bar{1}}E_{11,1\bar{1}} - iE_{11,0}E_{\bar{1}\bar{1}} + iE_{\bar{1}\bar{1},0}E_{11}.$$

Using the commutation rules (9) and again the fact that E_{11} is a CR function we obtain

$$\ddot{R} = -2|E_{11,1}|^2 - 2E_{11}E_{\bar{1}\bar{1},\bar{1}1} - 2E_{\bar{1}\bar{1}}E_{11,1\bar{1}}.$$

Then the above formula (103) implies

$$\ddot{m}(J,\theta) = \frac{3}{2}\int_{\mathbb{H}^1}\left(|E_{11,1}|^2 + E_{11}E_{\overline{11},\overline{1}1} + E_{\overline{11}}E_{11,1\overline{1}}\right)\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta},$$

so integrating by parts we obtain

$$\ddot{m}(J,\theta) = -\frac{3}{2}\int_{\mathbb{H}^1}|E_{11,1}|^2\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta} < 0.$$

We can transport the latter example on S^3 using the Cayley transform $\varpi : S^3 \setminus p \to \mathbb{H}^1$, $p = (0,1) \in \mathbb{C}^2$, defined as

$$\varpi(z_1, z_2) = \left(\frac{z_1}{1+z_2}, \mathrm{Re}\,\left(i\frac{1-z_2}{1+z_2}\right)\right),$$

where (z_1, z_2) are standard coordinates in $\mathbb{C}^2$. It turns out that

$$G_p(z_1,z_2) = \frac{1}{\pi}\left(\frac{(1+z_2)(1+\overline{z}_2)}{|z_1|^4 - (z_2-\overline{z}_2)^2}\right)^{\frac{1}{2}}.$$

As in Subsection 3.6, we can obtain $(\mathbb{H}^1, J_{(s)}, u_s^2\theta)$ as blow up of the structure $(S^3, \hat{J}_{(s)}, \hat{\theta})$ at the point p through the Green's function $(G_p)_s = (u_s \circ \varpi)G_p$. In conclusion, we derived the following result.

Proposition 4.4 *There exist compact three dimensional pseudohermitian manifolds of positive Tanaka-Webster class such that, once the contact form is blown-up as in* (14) *at proper points, the resulting asymptotically flat pseudohermitian manifold has negative mass.*

Remark 4.5 *For an arbitrary variation E_{11} we have*

$$\dot{R} = i\left(E_{11,\overline{11}} - E_{\overline{11},11}\right),$$

and

$$\dot{m}(J,\theta) = -\frac{3}{4}\int_{\mathbb{H}^1}\dot{R}\,\overset{\circ}{\theta}\wedge d\,\overset{\circ}{\theta} = -\frac{3}{4}i\int_{\mathbb{H}^1}\left(E_{11,\overline{11}} - E_{\overline{11},11}\right)\overset{\circ}{\theta}\wedge d\,\overset{\circ}{\theta}.$$

Assuming sufficiently fast decay to zero of E_{11} and its derivatives, integrating by parts we obtain $\dot{m}(J,\theta) = 0$, namely vanishing of the first variation of the p-mass under arbitrary perturbations (with sufficient decay and regularity).

4.3 A CR structure on $S^2 \times S^1$ with non-negative Paneitz operator and non-vanishing torsion

Consider the Heisenberg group $\mathbb{H}^1$ with it origin removed: endowing it with the standard CR structure J_0 and with the contact form

$$\check{\theta} = \rho^{-2}\overset{\circ}{\theta},$$

the transformation $(z,t) \mapsto (2z, 4t)$ defines a pseudohermitian isomorphism. Introducing then the equivalence relation

$$(z_1,t_1) \sim (z_2,t_2) \qquad \text{if and only if} \qquad z_1 = 2^k z_2 \text{ and } t_1 = 2^{2k}t_2 \text{ for some } k \in \mathbb{Z},$$

we obtain a pseudohermitian structure on $S^2 \times S^1$. Using (139), one finds that

$$\check{A}_{11} = i|z|^2\left(|z|^2 + it\right)^2\rho^{-6},$$

so the torsion of $(S^2 \times S^1, J_0, \check{\theta})$ is non-zero. Given any smooth function φ we would like to prove the non-negativity of $\int_{S^2\times S^1}\varphi P_{(J_0,\check{\theta})}\varphi\,\check{\theta}\wedge d\check{\theta}$.

Using the conformal covariance of P, see (3), we obtain

$$\int_{S^2\times S^1} \varphi P_{(J_0,\check{\theta})}\varphi\, \check{\theta}\wedge d\check{\theta} = \int_{\{\rho\in[1,2]\}} \varphi P_{(J_0,\mathring{\theta})}\varphi\, \mathring{\theta}\wedge d\mathring{\theta}. \tag{104}$$

Extend next φ by periodicity in $\log\rho$ to a smooth function $\tilde{\varphi}$ on $\mathbb{H}^1\setminus\{0\}$: for any positive integer n we obtain that

$$\int_{\{\rho\in[1,2]\}} \varphi P_{(J_0,\mathring{\theta})}\varphi\, \mathring{\theta}\wedge d\mathring{\theta} = \frac{1}{n}\int_{\{\rho\in[1,2^n]\}} \tilde{\varphi} P_{(J_0,\mathring{\theta})}\tilde{\varphi}\, \mathring{\theta}\wedge d\mathring{\theta}. \tag{105}$$

We next consider a smooth cut-off function χ, depending only on ρ, such that

$$\begin{cases} \chi(\rho)=0 & \text{for } \rho\leq\frac{5}{8};\\ \chi(\rho)=1 & \text{for } \rho\geq\frac{7}{8}, \end{cases}$$

and define the function $\tilde{\varphi}_n:\mathbb{H}^1\to\mathbb{R}$ as

$$\tilde{\varphi}_n := \chi(\rho)\left[1-\chi\left(2^{-(n+1)}\rho\right)\right]\tilde{\varphi}.$$

By the non-negativity of $P_{(J_0,\mathring{\theta})}$ (notice that the torsion vanishes identically) then we clearly have

$$\begin{aligned} 0 \quad \leq \quad & \int_{\mathbb{H}^1} \tilde{\varphi}_n P_{(J_0,\mathring{\theta})}\tilde{\varphi}_n\, \mathring{\theta}\wedge d\mathring{\theta} = \int_{\{\rho\in[1,2^n]\}} \tilde{\varphi} P_{(J_0,\mathring{\theta})}\tilde{\varphi}\, \mathring{\theta}\wedge d\mathring{\theta} \\ + \quad & \int_{\{\rho\in[1/2,1]\}} \tilde{\varphi}_n P_{(J_0,\mathring{\theta})}\tilde{\varphi}_n\, \mathring{\theta}\wedge d\mathring{\theta} + \int_{\{\rho\in[2^n,2^{n+1}]\}} \tilde{\varphi}_n P_{(J_0,\mathring{\theta})}\tilde{\varphi}_n\, \mathring{\theta}\wedge d\mathring{\theta}. \end{aligned}$$

By dilation invariance the last two terms in the above formula are uniformly bounded: therefore by (104), (105) we obtain that

$$\int_{S^2\times S^1} \varphi P_{(J_0,\check{\theta})}\varphi\, \check{\theta}\wedge d\check{\theta} = \lim_{n\to+\infty}\frac{1}{n}\int_{\mathbb{H}^1} \tilde{\varphi}_n P_{(J_0,\mathring{\theta})}\tilde{\varphi}_n\, \mathring{\theta}\wedge d\mathring{\theta} \geq 0,$$

which is the desired conclusion.

5 Proof of Theorem 1.2

The main goal of this section is to prove the inequality $\mathcal{Y}(J)<\mathcal{Y}_0$ for a manifold M as in Theorem 1.2. We first discuss the existence of the Green's function and provide some estimates near the singularity. Then we define suitable test functions for which the Sobolev quotient is below the value of the standard pseudohermitian sphere.

5.1 Green's function of L_b and test functions for the CR Yamabe quotient

Given a compact CR manifold M of positive CR Yamabe invariant and a point $p\in M$, let us consider the equation

$$-4\Delta_b G_p + RG_p = 16_p, \tag{106}$$

where $_p$ is the Dirac delta at the point p. We will use the classical method of the parametrix to construct the Green's kernel. The following result is well known (see [21] for instance).

Lemma 5.1 *In the Heisenberg group $\mathbb{H}^1$ one has*

$$\mathring{\Delta}_b\,\frac{1}{\rho^2} = -8\pi\delta_0.$$

To find a solution of (106), using CR normal coordinates at p, we are going to consider a function G_p of the form

$$G_p = \frac{1}{2\pi}\rho^{-2} + w; \qquad \rho^4 = |z|^4 + t^2,$$

where w has to be suitably chosen. First of all, we evaluate Δ_b on ρ^{-2}. Using the fact that

$$|Z_1 \rho^i| \leq C_i \rho^{i-1}, \qquad |T\rho^i| \leq C_i \rho^{i-2}; \qquad i \in \mathbb{Z}, i < 0,$$

together with Proposition A.5 in the Appendix, we obtain

$$\Delta_b(\rho^{-2}) = -8\pi\delta_p + g; \qquad g = O(1).$$

Therefore, we are reduced to solving the following equation for w

$$-4\Delta_b w + Rw = g - \frac{1}{2\pi} R\rho^{-2}.$$

From the choice of CR normal coordinates (see Subsection A.2) it follows that $R = O(\rho^2)$, which implies that w satisfies

$$-4\Delta_b w + Rw = \tilde{g}; \qquad \tilde{g} = O(1).$$

The operator on the left-hand side is subelliptic, while the right-hand side is in $L^q(M)$ for any $q > 1$. The regularity theory in [21] then implies that $w \in \mathfrak{S}^{2,q}(M)$ for any $q > 1$. By the Folland-Stein embeddings this also implies that $w \in C^{1,\gamma}(M)$ for any $\gamma \in (0,1)$. In conclusion we obtain the following result.

Proposition 5.2 *Suppose M is of positive CR Yamabe invariant, and that $p \in M$. Then the CR invariant sublaplacian admits a Green's function G_p with pole at p, and in CR normal coordinates one has*

$$G_p = \frac{1}{2\pi\rho^2} + w,$$

where w is a function of class $C^{1,\gamma}$ for any $\gamma \in (0,1)$.

By Theorem 1.1 we also deduce the following result.

Proposition 5.3 *Let M, p and G_p be as in Proposition 5.2. Suppose the CR Paneitz operator is non-negative. Then the following expansion holds*

$$G_p = \frac{1}{2\pi\rho^2} + A + \hat{w},$$

where $A \geq 0$ and $\hat{w} \in C^{1,\gamma}$ for any $\gamma \in (0,1)$, and $\hat{w}(p) = 0$. If $A = 0$, then $(M, J, \hat{\theta})$ is pseudohermitian equivalent to the standard three dimensional pseudohermitian sphere.

To find suitable test functions we follow Schoen's idea, see [36], and glue the Green's function to a *standard bubble*, which for the Heisenberg group is given by

$$\omega_\lambda(z,t) = \lambda\left[\lambda^4 t^2 + (1 + \lambda^2|z|^2)^2\right]^{-\frac{1}{2}} = \frac{1}{\lambda}\left(t^2 + |z|^4 + \frac{2}{\lambda^2}|z|^2 + \frac{1}{\lambda^4}\right)^{-\frac{1}{2}}; \qquad \lambda > 0.$$

This function satisfies

$$-\overset{\circ}{\Delta}_b \omega_\lambda = \omega_\lambda^3 \tag{107}$$

and $\mathbb{H}^1$, endowed with the contact form $\omega_\lambda^2\overset{\circ}{\theta}$ has constant positive Tanaka-Webster curvature (equal to $\frac{1}{4}$). Moreover, ω_λ realizes the CR Yamabe quotient on $\mathbb{H}^1$ in the sense that

$$\frac{\int_{\mathbb{H}^1}|\nabla_b\omega_\lambda|^2\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta}}{\left(\int_{\mathbb{H}^1}|\omega_\lambda|^4\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta}\right)^{\frac{1}{2}}}=\inf_{v\in\, C_c^\infty(\mathbb{H}^1)}\frac{\int_{\mathbb{H}^1}|\nabla_b v|^2\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta}}{\left(\int_{\mathbb{H}^1}|v|^4\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta}\right)^{\frac{1}{2}}}=\mathcal{Y}_0. \tag{108}$$

We now choose $\rho_0\gg\frac{1}{\lambda}$, and define a cutoff function ψ which satisfies

$$\psi(z,t)=1\quad\text{in }\{\rho\le\rho_0\};\qquad\qquad \psi(z,t)=0\quad\text{in }\{\rho\ge 2\rho_0\}.$$

Next, consider the following test function

$$u(z,t)=\begin{cases}\omega_\lambda(z,t) & \text{in }\{\rho\le\rho_0\};\\ \varepsilon_0\left(\tilde{G}_p(z,t)-\psi\tilde{w}(z,t)\right)+\psi(z,t)\frac{1}{\lambda}\varphi(z,t) & \text{in }\{\rho\in(\rho_0,2\rho_0]\};\\ \varepsilon_0\tilde{G}_p(z,t) & \text{in }M\setminus\{\rho\le 2\rho_0\},\end{cases} \tag{109}$$

where we have set

$$\varphi(z,t)=\left(t^2+|z|^4+\frac{2}{\lambda^2}|z|^2+\frac{1}{\lambda^4}\right)^{-\frac{1}{2}}-\rho^{-2};\qquad \tilde{G}_p=2\pi G_p;\qquad \tilde{w}=2\pi\hat{w}.$$

The constant ε_0 has to be chosen so that the function u is continuous, namely so that

$$\varepsilon_0=\frac{1}{\lambda(1+\tilde{A}\rho_0^2)};\qquad \tilde{A}=2\pi A. \tag{110}$$

5.2 Estimates on the CR Yamabe quotient $\mathcal{Y}(J)$

We now evaluate the Sobolev-type quotient

$$\frac{\int_M\left(|\nabla_b u|^2+\frac{1}{4}Ru^2\right)\theta\wedge d\theta}{\left(\int_M|u|^4\theta\wedge d\theta\right)^{\frac{1}{2}}} \tag{111}$$

on the test function in (109). We divide the estimate into four parts.

Recall from Subsection 2.1 that for CR normal coordinates of order $N=4$ one has

$$\begin{cases}\theta=\left(1+O(\rho^4)\right)\overset{\circ}{\theta}+O(\rho^5)dz+O(\rho^5)d\overline{z};\\ \theta^1=\sqrt{2}\left(1+O(\rho^4)\right)dz+O(\rho^4)d\overline{z}+O(\rho^3)d\overset{\circ}{\theta},\end{cases} \tag{112}$$

which implies

$$\theta\wedge d\theta=(1+O(\rho^4))\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta}, \tag{113}$$

and

$$\begin{cases}Z_1=\left(1+O(\rho^4)\right)\overset{\circ}{Z}_1+O(\rho^4)\overset{\circ}{Z}_{\overline{1}}+O(\rho^5)\overset{\circ}{T};\\ T=\left(1+O(\rho^4)\right)\overset{\circ}{T}+O(\rho^3)\overset{\circ}{Z}_1+O(\rho^3)\overset{\circ}{Z}_{\overline{1}}.\end{cases} \tag{114}$$

Since u is real, its squared subgradient is given by

$$|\nabla_b u|^2=2(Z_1u)(Z_{\overline{1}}u).$$

5.2.1 Integral estimate of $|\nabla_b u|^2$

First of all, we estimate $\int_{\{\rho\le\rho_0\}} |\nabla_b u|^2\theta\wedge d\theta$ in terms of the flat subgradient. We can write

$$
\begin{aligned}
&\int_{\{\rho\le\rho_0\}} |\nabla_b u|^2\theta\wedge d\theta \\
= \;& 2\int_{\{\rho\le\rho_0\}} (\mathring{Z}_1 u)(\mathring{Z}_{\bar 1} u)\mathring{\theta}\wedge d\mathring{\theta} + 2\int_{\{\rho\le\rho_0\}} ((Z_1 u)(Z_{\bar 1} u) - (\mathring{Z}_1 u)(\mathring{Z}_{\bar 1} u))\theta\wedge d\theta \\
+ \;& 2\int_{\{\rho\le\rho_0\}} (\mathring{Z}_1 u)(\mathring{Z}_{\bar 1} u)(\theta\wedge d\theta - \mathring{\theta}\wedge d\mathring{\theta}).
\end{aligned}
\tag{115}
$$

To evaluate the last term in the above expression we use (113), and the fact that

$$
2(\mathring{Z}_1 u)(\mathring{Z}_{\bar 1} u) = \frac{|z|^2\lambda^6}{((1+\lambda^2|z|^2)^2+\lambda^4 t^2)^2},
\tag{116}
$$

to obtain ($\tilde\rho = \lambda\rho$)

$$
\left|\int_{\{\rho\le\rho_0\}} (\mathring{Z}_1 u)(\mathring{Z}_{\bar 1} u)(\theta\wedge d\theta - \mathring{\theta}\wedge d\mathring{\theta})\right| \le C\int_0^{\rho_0} \frac{\rho^2\lambda^6\rho^4}{(1+\lambda^4\rho^4)^2}\rho^3 d\rho \le \frac{C}{\lambda^2}\int_0^{\lambda\rho_0} \tilde\rho d\tilde\rho \le C\frac{\rho_0^2}{\lambda^2}.
\tag{117}
$$

To evaluate instead the second term in the right hand side of (115), we use (112) and (114) to find

$$
\begin{aligned}
\int_{\{\rho\le\rho_0\}} \left|(Z_1 u)(Z_{\bar 1} u) - (\mathring{Z}_1 u)(\mathring{Z}_{\bar 1} u)\right| \theta\wedge d\theta \;\le\;& C\int_{\{\rho\le\rho_0\}} |\mathring{\nabla}_b\omega_\lambda| \left(\rho^4|\mathring{\nabla}_b\omega_\lambda| + \rho^5|\mathring{T}\omega_\lambda|\right)\mathring{\theta}\wedge d\mathring{\theta} \\
+\;& C\int_{\{\rho\le\rho_0\}} \left(\rho^8|\mathring{\nabla}_b\omega_\lambda|^2 + \rho^{10}|\mathring{T}\omega_\lambda|^2\right)\mathring{\theta}\wedge d\mathring{\theta}.
\end{aligned}
\tag{118}
$$

The first terms in the right hand side of the first line in (118) and in the second line in (118) can be treated exactly as for (117). For the remaining ones, we use the explicit expression

$$
\mathring{T}\omega_\lambda = -\frac{t\lambda^5}{((1+\lambda^2|z|^2)^2+\lambda^4t^2)^{\frac{3}{2}}},
$$

to find

$$
\int_{\{\rho\le\rho_0\}} |\mathring{\nabla}_b\omega_\lambda|\,\rho^5\,|\mathring{T}\omega_\lambda|\,\mathring{\theta}\wedge d\mathring{\theta} \le C\int_0^{\rho_0} \frac{\rho^8\lambda^8}{(1+\lambda^4\rho^4)^{\frac{5}{2}}}\rho^3 d\rho \le \frac{C}{\lambda^4}\int_0^{\lambda\rho_0} \frac{\tilde\rho^{11}}{(1+\tilde\rho^4)^{\frac{5}{2}}} d\tilde\rho \le \frac{C}{\lambda^2}\rho_0^2;
$$

$$
\int_{\{\rho\le\rho_0\}} \rho^{10}|\mathring{T}\omega_\lambda|^2\mathring{\theta}\wedge d\mathring{\theta} \le C\int_0^{\rho_0} \frac{\rho^{14}\lambda^{10}}{(1+\lambda^4\rho^4)^3}\rho^3 d\rho \le \frac{C}{\lambda^8}\int_0^{\lambda\rho_0} \frac{\tilde\rho^{17}}{(1+\tilde\rho)^{12}} d\tilde\rho \le C\frac{\rho_0^6}{\lambda^2}.
$$

In conclusion, using (115), (117), (118) and the last two formulas we obtain that

$$
\left|\int_{\{\rho\le\rho_0\}} |\nabla_b u|^2\theta\wedge d\theta - \int_{\{\rho\le\rho_0\}} |\mathring{\nabla}_b u|^2\mathring{\theta}\wedge d\mathring{\theta}\right| \le C\frac{\rho_0^2}{\lambda^2}.
\tag{119}
$$

5.2.2 Integral estimate of Ru^2

We estimate next the term $\int_{\{\rho\le\rho_0\}} Ru^2\theta\wedge d\theta$. For doing this, we first expand in Taylor series the Tanaka-Webster curvature R, using real CR normal coordinates. From the relations (see Subsection A.2)

$$
R = 0; \qquad R_{,1} = 0; \qquad \Delta_b R = R_{,1\bar 1} + R_{,\bar 1 1} = 0; \qquad R_{,0} = 0
\tag{120}
$$

at p, and the fact that for a smooth function f one has

$$\overset{\circ}{\Delta}_b f = f_{xx} + f_{yy} + 2y f_{xt} - 2x f_{yt} + 4|z|^2 f_{tt} \qquad \text{at } p,$$

we can write

$$R(z,t) = \frac{1}{2}\left(R_{xx}x^2 + R_{yy}y^2 + 2R_{xy}xy\right) + O(\rho^3), \qquad \text{with} \quad R_{yy} = -R_{xx} \qquad \text{at } p. \tag{121}$$

By this reason and by the axial symmetry of ω_λ the terms of order ρ^2, integrated, will vanish. Similarly, by symmetry, also the cubic ones will vanish, and therefore by (113) we deduce

$$\begin{aligned} \left|\int_{\{\rho\leq\rho_0\}} Ru^2\theta\wedge d\theta\right| &= \left|\int_{\{\rho\leq\rho_0\}} R\omega_\lambda^2\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta}\right| + O\left(\int_{\{\rho\leq\rho_0\}} \rho^6\omega_\lambda^2\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta}\right) \leq C\int_{\{\rho\leq\rho_0\}} \rho^4\omega_\lambda^2\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta} \\ &\leq C\int_0^{\rho_0} \frac{\lambda^2}{(1+\lambda^4\rho^4)}\rho^4 d\rho \leq \frac{C}{\lambda^3}\int_0^{\lambda\rho_0} \frac{\tilde{\rho}^4}{(1+\tilde{\rho})^4}d\tilde{\rho} \leq \frac{C\rho_0}{\lambda^2}. \end{aligned} \tag{122}$$

5.2.3 Estimate of the boundary term

From the Stokes theorem, for a smooth domain $\Omega \subseteq \mathbb{H}^1$ we get

$$\begin{aligned} \int_\Omega |\overset{\circ}{\nabla}_b u|^2\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta} &= \int_\Omega \overset{\circ}{Z}_1 u \overset{\circ}{Z}_{\overline{1}} u\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta} + \int_\Omega \overset{\circ}{Z}_{\overline{1}} u\overset{\circ}{Z}_1 u\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta} \\ &= i\oint_{\partial\Omega} u(\overset{\circ}{Z}_{\overline{1}}u)\overset{\circ}{\theta}{}^{\overline{1}}\wedge\overset{\circ}{\theta} - i\oint_{\partial\Omega} u(\overset{\circ}{Z}_1 u)\overset{\circ}{\theta}{}^1\wedge\overset{\circ}{\theta} - \int_\Omega u\overset{\circ}{\Delta}_b u\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta}. \end{aligned} \tag{123}$$

Next we take $\Omega = \{\rho < \rho_0\}$ and $u = \omega_\lambda$, focusing our attention to the boundary integral. From elementary computations we find

$$\overset{\circ}{Z}_1 u = -\frac{1}{\sqrt{2}}\frac{\overline{z}(1+\lambda^2|z|^2+it\lambda^2)\lambda^3}{[\lambda^4t^2+(1+\lambda^2|z|^2)^2]^{\frac{3}{2}}}; \qquad \overset{\circ}{Z}_{\overline{1}} u = -\frac{1}{\sqrt{2}}\frac{z(1+\lambda^2|z|^2-it\lambda^2)\lambda^3}{[\lambda^4t^2+(1+\lambda^2|z|^2)^2]^{\frac{3}{2}}},$$

hence after some manipulations the above boundary integral becomes

$$-i\oint_{S_{\rho_0}} \frac{z(1+\lambda^2|z|^2-it\lambda^2)\lambda^4}{[\lambda^4t^2+(1+\lambda^2|z|^2)^2]^2}d\overline{z}\wedge(dt - i\overline{z}dz) + \text{conj.}. \tag{124}$$

On the other hand, the function ω_λ satisfies (107), therefore from the above computations we get

$$\begin{aligned} \int_{\{\rho\leq\rho_0\}} |\overset{\circ}{\nabla}_b u|^2\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta} &= \int_{\{\rho\leq\rho_0\}} \omega_\lambda^4\overset{\circ}{\theta}\wedge d\overset{\circ}{\theta} \\ &- i\oint_{S_{\rho_0}} \frac{z(1+\lambda^2|z|^2-it\lambda^2)\lambda^4}{[\lambda^4t^2+(1+\lambda^2|z|^2)^2]^2}d\overline{z}\wedge(dt-i\overline{z}dz) + \text{conj.} \\ &= -2\oint_S \frac{\lambda^4(|z|^2+\lambda^2\rho^4)}{[\lambda^4t^2+(1+\lambda^2|z|^2)^2]^2}d\varphi\wedge dt. \end{aligned} \tag{125}$$

We next evaluate the integrals on $M \setminus \{\rho \leq \rho_0\}$. We have

$$\begin{aligned} &\int_{M\setminus\{\rho\leq\rho_0\}} \left(|\nabla_b u|^2 + \frac{1}{4}Ru^2\right)\theta\wedge d\theta = \varepsilon_0^2\int_{M\setminus\{\rho\leq\rho_0\}} \left(|\nabla_b\tilde{G}_p|^2 + \frac{1}{4}R\tilde{G}_p^2\right)\theta\wedge d\theta \\ &+ \frac{1}{\lambda^2}\int_{\{\rho\leq 2\rho_0\}\setminus\{\rho\leq\rho_0\}} |\nabla_b(\varphi\psi)|^2\theta\wedge d\theta + \frac{1}{4}\int_{\{\rho\leq 2\rho_0\}\setminus\{\rho\leq\rho_0\}} R(u^2 - \varepsilon_0^2\tilde{G}_p^2)\theta\wedge d\theta \\ &+ \varepsilon_0^2\int_{\{\rho\leq 2\rho_0\}\setminus\{\rho\leq\rho_0\}} \left(|\nabla_b(\psi\tilde{w})|^2 - 2\nabla_b\tilde{G}_p\cdot\nabla_b(\psi\tilde{w})\right)\theta\wedge d\theta \\ &+ 2\frac{\varepsilon_0}{\lambda}\int_{\{\rho\leq 2\rho_0\}\setminus\{\rho\leq\rho_0\}} \left(\nabla_b\tilde{G}_p\cdot\nabla_b(\varphi\psi) - \nabla_b(\psi\tilde{w})\cdot\nabla_b(\varphi\psi)\right)\theta\wedge d\theta. \end{aligned} \tag{126}$$

We derive now some estimates on the above terms. First of all we notice that we can take

$$\psi(z,t) = \psi_0\left(\frac{z}{\rho_0}, \frac{t}{\rho_0^2}\right), \tag{127}$$

for a smooth fixed ψ_0 which, using (114), implies

$$Z_1\psi = \frac{1}{\rho_0}\partial_z\psi_0\left(\frac{z}{\rho_0}, \frac{t}{\rho_0^2}\right) + i\frac{\overline{z}}{\rho_0^2}\partial_t\psi_0\left(\frac{z}{\rho_0}, \frac{t}{\rho_0^2}\right) + O(\rho_0^3) + O(\rho_0) = O\left(\frac{1}{\rho_0}\right).$$

A similar estimate holds true for $Z_{\overline{1}}\psi$ and therefore, since $\tilde{w}(z,t) = O(\rho)$ we have

$$|\nabla_b(\psi\tilde{w})| \leq C \qquad \text{in } \{\rho \leq 2\rho_0\} \setminus \{\rho \leq \rho_0\} \qquad \text{for some fixed } C > 0.$$

Using also the fact that $\lambda\rho_0 \gg 1$, from a Taylor expansion we find

$$\begin{aligned} \varphi &= \rho^{-2}\left[\left(1 + \frac{2|z|^2}{\lambda^2\rho^4} + \frac{1}{\lambda^4\rho^4}\right)^{-\frac{1}{2}} - 1\right] = \frac{1}{\rho^2}O\left(\frac{2|z|^2}{\lambda^2\rho^4} + \frac{1}{\lambda^4\rho^4}\right) \\ &= \frac{1}{\lambda^4\rho^6}O\left(1 + \lambda^2|z|^2\right) = O\left(\frac{1}{\lambda^2\rho^4}\right). \end{aligned} \tag{128}$$

By straightforward computations we also get

$$\overset{\circ}{Z}_1\varphi = \frac{1}{\sqrt{2}}\frac{\overline{z}\rho}{\lambda^2}\frac{\lambda^6\rho^6}{(\lambda^4t^2 + (1+\lambda^2|z|^2)^2)^{\frac{3}{2}}}\left\{\frac{\lambda^2(|z|^2 + it)}{\lambda^6\rho^6}\left[(\lambda^4t^2 + (1+\lambda^2|z|^2)^2)^{\frac{3}{2}} - \lambda^6\rho^6\right] - 1\right\},$$

and similarly

$$\overset{\circ}{Z}_{\overline{1}}\varphi = \frac{1}{\sqrt{2}}\frac{z\rho}{\lambda^2}\frac{\lambda^6\rho^6}{(\lambda^4t^2 + (1+\lambda^2|z|^2)^2)^{\frac{3}{2}}}\left\{\frac{\lambda^2(|z|^2 - it)}{\lambda^6\rho^6}\left[(\lambda^4t^2 + (1+\lambda^2|z|^2)^2)^{\frac{3}{2}} - \lambda^6\rho^6\right] - 1\right\}.$$

Using some Taylor expansions, the fact that $|\overset{\circ}{T}\varphi| = O\left(\frac{1}{\lambda^2\rho^6}\right)$ and (112) we then deduce

$$|\nabla_b\varphi| = O\left(\frac{1}{\lambda^2\rho_0^5}\right) \qquad \text{in } \{\rho \leq 2\rho_0\} \setminus \{\rho \leq \rho_0\}.$$

From the above estimates on ψ this implies

$$|\nabla_b(\varphi\psi)| = O\left(\frac{1}{\lambda^2\rho_0^5}\right) \qquad \text{in } \{\rho \leq 2\rho_0\} \setminus \{\rho \leq \rho_0\}. \tag{129}$$

It is also easy to see that

$$|\nabla_b\tilde{G}_p| = O\left(\frac{1}{\rho_0^3}\right) \qquad \text{in } \{\rho \leq 2\rho_0\} \setminus \{\rho \leq \rho_0\}. \tag{130}$$

Next, from (109), (110), the expression of $\tilde{G}_p$, $\tilde{w} = O(\rho)$, (128) and $\lambda\rho_0 \gg 1$ we get

$$|u^2 - \varepsilon_0^2\tilde{G}_p^2| \leq \varepsilon_0\rho_0^{-2}\left(\varepsilon_0\rho_0 + \frac{1}{\lambda^3\rho_0^4}\right) + \varepsilon_0^2\rho_0^2 + \frac{1}{\lambda^6\rho_0^8} \leq C\left(\frac{1}{\lambda^2\rho_0} + \frac{1}{\lambda^4\rho_0^6}\right).$$

This and (121) imply

$$\frac{1}{4}\int_{\{\rho\leq 2\rho_0\}\setminus\{\rho\leq\rho_0\}} R(u^2 - \varepsilon_0^2\tilde{G}_p^2)\theta\wedge d\theta \leq C\left(\frac{\rho_0^5}{\lambda^2} + \frac{1}{\lambda^4}\right).$$

Therefore, integrating and using the fact that the volume of $\{\rho < 2\rho_0\} \setminus \{\rho \le \rho_0\}$ is of order ρ_0^4, from (126) and the above estimates we obtain

$$\begin{aligned}\int_{M\setminus\{\rho\le\rho_0\}} \left(|\nabla_b u|^2 + \frac{1}{4}Ru^2\right)\theta\wedge d\theta &= \varepsilon_0^2 \int_{M\setminus\{\rho\le\rho_0\}} \left(|\nabla_b \tilde{G}_p|^2 + \frac{1}{4}R\tilde{G}_p^2\right)\theta\wedge d\theta \\ &+ O\left(\frac{1}{\lambda^6\rho_0^6} + \varepsilon_0^2\rho_0 + \frac{\varepsilon_0}{\lambda^3\rho_0^4}\right). \end{aligned} \tag{131}$$

The first term in this expression can be evaluated using an integration by parts, yielding a boundary term: recall that the Green's function satisfies $-\Delta_b\tilde{G}_p + \frac{1}{4}R\tilde{G}_p = 0$ outside the singularity. Therefore, as for (123) one finds

$$\int_{M\setminus\{\rho\le\rho_0\}} \left(|\nabla_b \tilde{G}_p|^2 + \frac{1}{4}R\tilde{G}_p^2\right)\theta\wedge d\theta = -i\oint_{S_{\rho_0}} \tilde{G}_p(Z_{\overline{1}}\tilde{G}_p)\theta^{\overline{1}}\wedge\theta + i\oint_{S_{\rho_0}} \tilde{G}_p(Z_1\tilde{G}_p)\theta^1\wedge\theta,$$

the minus sign coming from the fact that we are working in the exterior of $\{\rho \le \rho_0\}$.

By direct computations we have that

$$\begin{aligned} & -i\tilde{G}_p(Z_{\overline{1}}\tilde{G}_p)\theta^{\overline{1}}\wedge\theta + i\tilde{G}_p(Z_1\tilde{G}_p)\theta^1\wedge\theta \\ = \; & -i\tilde{G}_p\left[\frac{1}{\sqrt{2}}\frac{\overline{z}(|z|^2+it)}{\rho^6}\sqrt{2}dz\wedge(dt+izd\overline{z}) - \frac{1}{\sqrt{2}}\frac{z(|z|^2-it)}{\rho^6}\sqrt{2}d\overline{z}\wedge(dt-i\overline{z}dz) + O(\rho)d\varphi\wedge dt\right]. \end{aligned}$$

Using some cancelations we get

$$\int_{M\setminus\{\rho\le\rho_0\}} \left(|\nabla_b \tilde{G}_p|^2 + \frac{1}{4}R\tilde{G}_p^2\right)\theta\wedge d\theta = \oint_{S_{\rho_0}} \left(\frac{1}{\rho^2} + \tilde{A} + \tilde{w}\right)\left(\frac{2}{\rho^2} + O(\rho)\right)d\varphi\wedge dt, \tag{132}$$

therefore after integration we obtain

$$\int_{M\setminus\{\rho\le\rho_0\}} \left(|\nabla_b \tilde{G}_p|^2 + \frac{1}{4}R\tilde{G}_p^2\right)\theta\wedge d\theta = \oint_{S_{\rho_0}} \frac{2(1+\tilde{A}\rho^2)}{\rho^4}d\varphi\wedge dt + O(\rho_0^2). \tag{133}$$

Now, using the formula for ε_0 in (110) and some straightforward computations one finds that the contribution of the boundary term in (125) together with the one in the last formula becomes (there is cancelation of the two main terms after subtraction)

$$\oint_{S_{\rho_0}} 2\frac{3\lambda^6\rho^4|z|^2 + 1 + 4\lambda^4|z|^4 + 2\lambda^4\rho^4 + 4\lambda^2|z|^2 - \tilde{A}\lambda^8\rho^{10} - \tilde{A}\rho^6\lambda^6|z|^2}{\rho^4\lambda^{10}(1+\tilde{A}\rho^2)\left(\rho^4 + \frac{1}{\lambda^4} + 2\frac{|z|^2}{\lambda^2}\right)^2}d\varphi\wedge dt.$$

To get some asymptotics of the integrand (especially its sign) we can neglect the term $\tilde{A}\rho^2$ in the denominator, while in the second bracket of the denominator we can simply take $(\rho^4)^2$. For the numerator, we recall that $\lambda\rho_0 \gg 1$. In this way we have to find the asymptotics of

$$\oint_{S_{\rho_0}} 2\frac{3|z|^2 - \tilde{A}\lambda^2\rho^6}{\rho^8\lambda^4}d\varphi\wedge dt.$$

If we also choose λ and ρ_0 so that $\lambda^2\rho_0^4 \gg 1$ then the last term in the numerator dominates, and we are reduced to

$$-2\frac{\tilde{A}}{\rho_0^2\lambda^2}\oint_{S_{\rho_0}} d\varphi\wedge dt = -8\pi\frac{\tilde{A}}{\lambda^2}.$$

5.2.4 Final estimates

Collecting all the terms in (122), (125), (131), (132) and (133), and taking into account the previous computations, with our choices of ρ_0 and λ we find

$$\int_M \left(|\nabla_b u|^2 + \frac{1}{4} R u^2 \right) \theta \wedge d\theta = \int_{\{\rho \leq \rho_0\}} \omega_\lambda^4 \overset{\circ}{\theta} \wedge d\overset{\circ}{\theta} - 8\pi \frac{\tilde{A}}{\lambda^2} + O\left(\frac{1}{\lambda^6 \rho_0^6} \right) + O\left(\frac{\rho_0}{\lambda^2} \right) + O\left(\frac{1}{\lambda^4 \rho_0^4} \right). \tag{134}$$

From $\lambda \rho_0 \gg 1$ we get

$$\int_M \left(|\nabla_b u|^2 + \frac{1}{4} R u^2 \right) \theta \wedge d\theta = \int_{\{\rho \leq \rho_0\}} \omega_\lambda^4 \overset{\circ}{\theta} \wedge d\overset{\circ}{\theta} - (8\pi + o(1)) \frac{\tilde{A}}{\lambda^2}. \tag{135}$$

Finally, we estimate the denominator in (111). Clearly the contribution inside $\{\rho \leq \rho_0\}$ is just the same as the one of the bubble. In $\{\rho \leq 2\rho_0\} \setminus \{\rho \leq \rho_0\}$ we have that $|u| \leq \frac{C}{\lambda \rho_0^2}$ (by the expression of ε_0 and the asymptotics of $\tilde{G}_p$), so integrating we get

$$\int_{\{\rho \leq 2\rho_0\} \setminus \{\rho \leq \rho_0\}} |u|^4 \theta \wedge d\theta = O\left(\frac{1}{\lambda^4 \rho_0^4} \right) \ll \frac{1}{\lambda^2}.$$

Similarly we also find

$$\int_{M \setminus \{\rho \leq 2\rho_0\}} |u|^4 \theta \wedge d\theta \leq C \frac{1}{\lambda^4} \int_{\rho_0}^{\infty} \frac{\rho^3 d\rho}{\rho^8} = O\left(\frac{1}{\lambda^4 \rho_0^4} \right) \ll \frac{1}{\lambda^2}.$$

Moreover, from (113) and the expression of ω_λ we obtain

$$\int_{\{\rho \leq \rho_0\}} |u|^4 \theta \wedge d\theta = \int_{\{\rho \leq \rho_0\}} \omega_\lambda^4 \overset{\circ}{\theta} \wedge d\overset{\circ}{\theta} + O\left(\frac{1}{\lambda^4} \log(\lambda \rho_0) \right).$$

In conclusion, using (135) and the last three formulas, the CR Yamabe quotient (111) for the test function (109) becomes

$$\frac{\int_M |\nabla_b u|^2 \theta \wedge d\theta}{\left(\int_M |u|^4 \theta \wedge d\theta \right)^{\frac{1}{2}}} = \frac{\int_{\{\rho \leq \rho_0\}} \omega_\lambda^4 \overset{\circ}{\theta} \wedge d\overset{\circ}{\theta} - (C_1 + o(1)) \frac{\tilde{A}}{\lambda^2 \rho_0^2}}{\left(\int_{\{\rho \leq \rho_0\}} \omega_\lambda^4 \overset{\circ}{\theta} \wedge d\overset{\circ}{\theta} \right)^{\frac{1}{2}} + O\left(\frac{1}{\lambda^4 \rho_0^4} + O\left(\frac{1}{\lambda^4} \log(\lambda \rho_0) \right) \right)}.$$

Since $O\left(\frac{1}{\lambda^4 \rho_0^4} \right) + O\left(\frac{1}{\lambda^4} \log(\lambda \rho_0) \right) \ll \frac{1}{\lambda^2}$, from the last formula and (108) we find

$$\frac{\int_M |\nabla_b u|^2 \theta \wedge d\theta}{\left(\int_M |u|^4 \theta \wedge d\theta \right)^{\frac{1}{2}}} < \frac{\int_{\mathbb{H}^1} |\nabla_b \omega_l|^2 \overset{\circ}{\theta} \wedge d\overset{\circ}{\theta}}{\left(\int_{\mathbb{H}^1} |\omega_l|^4 \overset{\circ}{\theta} \wedge d\overset{\circ}{\theta} \right)^{\frac{1}{2}}} = \mathcal{Y}_0,$$

which is the desired inequality.

The proof of Theorem 1.2 then follows from [28] in the case when M is CR equivalent to the 3-sphere, and from the variational argument in [27] in the complementary case.

Remark 5.4 *Since the minimization procedure for the CR Yamabe quotient is related to the positivity of the mass, in view of Proposition 4.4 there might be examples of pseudohermitian manifolds of positive CR Yamabe invariant for which there is no minimizer. In this case, the use of variational or topological methods (as in [22], [23]) seems to be a necessary tool in order to find conformal structures of constant Tanaka-Webster curvature.*

A Appendix: useful facts in pseudohermitian geometry

In this appendix we collect some useful facts in pseudohermitian geometry: in particular we discuss the variations of some geometric quantities when the contact form or the CR structure vary, and then the CR normal coordinates introduced by Jerison and Lee in [29].

A.1 Variations of interesting quantities

Here we consider variations of some geometric quantities either under the conformal change of contact form (pp. 421-422 in [31]), or under the change of the pseudohermitian structure (pp. 231-232 in [18]).

A.1.1 Conformal changes of contact form

Consider a new contact form $\hat{\theta} = e^{2f}\theta$, for a given smooth function f. Then it turns out that

$$\hat{\theta}^1 = e^f \left(\theta^1 + 2if^1\theta\right); \qquad \hat{h}_{1\bar{1}} = h_{1\bar{1}} \equiv 1, \tag{136}$$

and that

$$\hat{Z}_1 = e^{-f} Z_1; \qquad \hat{T} = e^{-2f}\left(T + 2if^{\bar{1}} Z_{\bar{1}} - 2if^1 Z_1\right). \tag{137}$$

Moreover we also have

$$\hat{\omega}_1^1 = \omega_1^1 + 3\left(f_1\theta^1 - f_{\bar{1}}\theta^{\bar{1}}\right) + i\left(f_{\bar{1}1} + f_{1\bar{1}} + 8f_1 f_{\bar{1}}\right)\theta. \tag{138}$$

Furthermore, concerning the torsion and the Tanaka-Webster curvature one has

$$\hat{A}_{11} = e^{-2f}\left(A_{11} + 2if_{11} - 4if_1 f_1\right); \qquad \hat{R} = e^{-2f}\left(R - 4\Delta_b f - 8f_1 f_{\bar{1}}\right). \tag{139}$$

A.1.2 Deformation of J

Here we consider instead a variation of the CR structure $J(s)$ for which

$$\frac{d}{ds}_{|s=0} J(s) = \dot{J} = 2E = 2E_{11}\theta^1 \otimes Z_{\bar{1}} + 2E_{\bar{1}\bar{1}}\theta^{\bar{1}} \otimes Z_1.$$

This implies

$$\dot{Z}_1 = -iE_1^{\bar{1}} Z_{\bar{1}}; \qquad \dot{\theta}^1 = -iE_{\bar{1}}^1\theta^{\bar{1}}, \tag{140}$$

and

$$\dot{\omega}_1^1 = i\left(A_{11}E_{\bar{1}\bar{1}} + A_{\bar{1}\bar{1}}E_{11}\right)\theta - iE^1_{\bar{1},1}\theta^{\bar{1}} - iE^{\bar{1}}_{1,\bar{1}}\theta^1; \qquad \dot{A}^1_{\bar{1}} = -iE^1_{\bar{1},0}. \tag{141}$$

We also have

$$\dot{R} = i\left(E_{11,\bar{1}\bar{1}} - E_{\bar{1}\bar{1},11}\right) - \left(A_{11}E_{\bar{1}\bar{1}} + A_{\bar{1}\bar{1}}E_{11}\right). \tag{142}$$

It is useful to include the variation of $-\Delta_b$ as well: one has

$$\Delta_b = \left(Z_{\bar{1}}Z_1 - \omega_1^1(Z_{\bar{1}})Z_1\right) + \text{conj.}.$$

From this formula, differentiating with respect to s one finds

$$\begin{aligned}
-\dot{\Delta}_b &= -iE_{\bar{1}\bar{1}}Z_1Z_1 + iE_{11,\bar{1}}Z_{\bar{1}} + iE_{11}Z_{\bar{1}}Z_{\bar{1}} \\
&- iE_{\bar{1}\bar{1},1}Z_1 + iE_{\bar{1}\bar{1}}\omega_1^1(Z_1)Z_1 - iE_{11}\omega_1^1(Z_{\bar{1}})Z_{\bar{1}} + \text{conj.} \\
&= 2\left(-iE_{\bar{1}\bar{1}}Z_1Z_1 + iE_{11}Z_{\bar{1}}Z_{\bar{1}} + iE_{11,\bar{1}}Z_{\bar{1}} - iE_{\bar{1}\bar{1},1}Z_1\right) \\
&+ iE_{\bar{1}\bar{1}}\omega_1^1(Z_1)Z_1 - iE_{11}\omega_1^1(Z_{\bar{1}})Z_{\bar{1}} - iE_{11}\omega_{\bar{1}}^{\bar{1}}(Z_{\bar{1}})Z_{\bar{1}} + iE_{\bar{1}\bar{1}}\omega_{\bar{1}}^{\bar{1}}(Z_1)Z_1.
\end{aligned}$$

From the fact that ω_1^1 is purely imaginary we find

$$-\dot{\Delta}_b = 2i\left(E_{11}Z_{\bar{1}}Z_{\bar{1}} + E_{11,\bar{1}}Z_{\bar{1}}\right) + \text{conj.}.$$

To derive these formulas we have used the above transformation laws for J, Z_1 and ω_1^1.

If we differentiate once more we find that

$$(E_{11,\bar{1}})^{\cdot} = iE_{\bar{1}\bar{1}}E_{11,1} + 2iE_{\bar{1}\bar{1},1}E_{11} + (\dot{E}_{11})_{,\bar{1}},$$

and hence

$$\begin{aligned} -\ddot{\Delta}_b &= 2i\left(\dot{E}_{11}Z_{\bar{1}}Z_{\bar{1}} + E_{11}\dot{Z}_{\bar{1}}Z_{\bar{1}} + E_{11}Z_{\bar{1}}\dot{Z}_{\bar{1}} + (E_{11,\bar{1}})^{\cdot}Z_{\bar{1}} + E_{11,\bar{1}}\dot{Z}_{\bar{1}}\right) + \text{conj.} \\ &= 2i\dot{E}_{11}Z_{\bar{1}}Z_{\bar{1}} - 2i\dot{E}_{\bar{1}\bar{1}}Z_1Z_1 - 4|E_{11}|^2\Delta_b - \left(4E_{11}E_{\bar{1}\bar{1},\bar{1}} + 6E_{\bar{1}\bar{1}}E_{11,\bar{1}}\right)Z_1 \\ &\quad - \left(4E_{\bar{1}\bar{1}}E_{11,1} + 6E_{11}E_{\bar{1}\bar{1},1}\right)Z_{\bar{1}} + 2i(\dot{E}_{11})_{,\bar{1}}Z_{\bar{1}} - 2i(\dot{E}_{\bar{1}\bar{1}})_{,1}Z_1. \end{aligned} \tag{143}$$

Using similar formulas we can also deduce the expression of $\ddot{R}$.

A.2 CR normal coordinates

We recall the following result in [29] on page 313, Proposition 2.5. For a differential form η, let us denote by $\eta_{(m)}$ the part of its Taylor series that is homogeneous of degree m in terms of the parabolic dilations (see [29] for more details).

Proposition A.1 *Let $\tilde{Z}_1$ be a special frame dual to $\tilde{\theta}^1$ (such that $\tilde{h}_{1\bar{1}} = 2$). Let $\theta^1 = \sqrt{2}\tilde{\theta}^1$ be a unitary coframe (i.e., $h_{1\bar{1}} = 1$). Then in pseudohermitian normal coordinates (z,t) with respect to $\tilde{Z}_1$, $\tilde{\theta}^1$, we have*

(a) $\theta_{(2)} = \overset{\circ}{\theta}$; $\quad \theta_{(3)} = 0$; $\quad \theta_{(m)} = \frac{1}{m}\sqrt{2}\left(iz\theta^{\bar{1}} - i\bar{z}\theta^1\right)_{(m)}$, $\quad m \geq 4$;

(b) $\theta^1_{(1)} = \sqrt{2}dz$; $\quad \theta^1_{(2)} = 0$; $\quad \theta^1_{(m)} = \frac{1}{m}\left(\sqrt{2}z\omega_1^1 + 2tA_{\bar{1}\bar{1}}\theta^{\bar{1}} - \sqrt{2}\bar{z}A_{\bar{1}\bar{1}}\theta\right)_{(m)}$, $\quad m \geq 3$

(c) $(\omega_1^1)_{(1)} = 0$; $\quad (\omega_1^1)_{(m)} = \frac{1}{m}\left(\sqrt{2}R(z\theta^{\bar{1}} - \bar{z}\theta^1) + A_{11,\bar{1}}(\sqrt{2}z\theta - 2t\theta^1) - A_{\bar{1}\bar{1},1}(\sqrt{2}\bar{z}\theta - 2t\theta^{\bar{1}})\right)_{(m)}$, $m \geq 2$.

Definition A.2 *Given a three dimensional pseudohermitian manifold (M,θ) we define a real symmetric tensor Q as*

$$Q = Q_{jk}\theta^j \otimes \theta^k, \qquad j,k \in \{0,1,\bar{1}\}$$

with $\theta^0 := \theta$, whose components with respect to any admissible coframe are given by

$$Q_{11} = \overline{Q_{\bar{1}\bar{1}}} = 3iA_{11}; \qquad Q_{1\bar{1}} = Q_{\bar{1}1} = h_{1\bar{1}}R;$$

$$Q_{01} = Q_{10} = \overline{Q_{0\bar{1}}} = \overline{Q_{\bar{1}0}} = 4A_{11,}{}^{1} + iR_{,1}; \qquad Q_{00} = 16 Im\ A_{11,}{}^{11} - 2\Delta_b R.$$

We have then the following result, see page 315 in [29], Theorem 3.1.

Proposition A.3 *Suppose M is a strictly pseudoconvex pseudohermitian manifold of dimension 3 and let $q \in M$. Then for any integer $N \geq 2$ there exists a choice of contact form θ such that all symmetrized covariant derivatives of Q with total order less or equal than N vanish at q, that is*

$$Q_{\langle jk,L\rangle} = 0 \qquad \text{at } q \text{ if} \quad \mathbb{O}(jkL) \leq N. \tag{144}$$

By CR normal coordinates of order N we mean the pseudohermitian normal coordinates with θ chosen as in Proposition A.3.

Remark A.4 *We recall ([29]) that (a) For a multi index $L = (l_1, \ldots, l_s)$ we count its order as*

$$\mathbb{O}(J) = \mathbb{O}(j_1) + \cdots + \mathbb{O}(j_s),$$

where $\mathbb{O}(1) = \mathbb{O}(\bar{1}) = 1$ and where $\mathbb{O}(0) = 2$,

(b) The symmetrized covariant derivatives are defined by

$$Q_{\langle L \rangle} = \frac{1}{s!} \sum_{\sigma \in \mathbb{S}_s} Q_{\sigma L}; \qquad \sigma L = \left(l_{\sigma(1)}, \ldots, l_{\sigma(s)}\right).$$

Let us apply Proposition A.3 for $N = 4$ and derive some consequences. At order 2, at q we have

$$0 = Q_{11} = 3iA_{11}; \qquad 0 = Q_{1\bar{1}} = R.$$

At order 3 we have

$$0 = Q_{01} = 4A_{11,}{}^{1} + iR_{,1},$$

and

$$0 = 3! Q_{\langle 11, \bar{1} \rangle} = Q_{11,\bar{1}} + Q_{1\bar{1},1} + Q_{\bar{1}1,1} = 3iA_{11,\bar{1}} + R_{,1} + R_{,1} = 3iA_{11,\bar{1}} + 2R_{,1}.$$

These two equations imply that

$$A_{11,\bar{1}} = R_{,1} = 0 \qquad \text{at } q.$$

We also have

$$0 = Q_{\langle 11,1 \rangle} = Q_{11,1} = 3iA_{11,1}.$$

At order 4 we find

$$0 = Q_{00} = 16 \text{Im } A_{11,}{}^{11} - 2\Delta_b R$$

and

$$0 = Q_{1\bar{1},0} + Q_{01,\bar{1}} + Q_{0\bar{1},1} = R_{,0} + \left(4A_{11,}{}^{1} + iR_{,1}\right)_{,\bar{1}} + \left(4A_{\overline{11},}{}^{\bar{1}} - iR_{,\bar{1}}\right)_{,\bar{1}}.$$

This quantity is equal to

$$\begin{aligned} 0 &= R_{,0} + 4A_{11,\,\bar{1}}{}^{1} + iR_{,1\bar{1}} + 4A_{\overline{11},\,1}{}^{\bar{1}} - iR_{,\bar{1}1} \\ &= R_{,0} + 8 \text{Re } A_{11,}{}^{11} + i(iR_{,0}) = 8 \text{Re } A_{11,}{}^{11}. \end{aligned}$$

We also have that

$$0 = Q_{11,0} + Q_{10,1} + Q_{01,1} = 3iA_{11,0} + 2\left(4A_{11,}{}^{1} + iR_{,1}\right)_{,1} = 3iA_{11,0} + 8A_{11,\bar{1}}{}^{\bar{1}} + 2iR_{,11}; \tag{145}$$

$$0 = Q_{\langle 11, \overline{11} \rangle} = 4Q_{11,\overline{11}} + 4Q_{1\bar{1},1\bar{1}} + 4Q_{1\bar{1},\bar{1}1} + 4Q_{\overline{11},11} + 4Q_{\bar{1}1,\bar{1}1} + 4Q_{\bar{1}1,1\bar{1}},$$

namely

$$0 = 3iA_{11,\overline{11}} + R_{,1\bar{1}} + R_{,\bar{1}1} + \text{conj.} = -6 \text{Im } A_{11,\overline{11}} - 2\Delta_b R.$$

From these relations we deduce that

$$\text{Im } A_{11,}{}^{11} = \Delta_b R = 0,$$

and hence

$$A_{11,}{}^{11} = 0 \quad \Rightarrow \quad R_{,0} = 0 \quad \Rightarrow \quad \Box_b R = 0.$$

We also have

$$24 Q_{\langle 11, 1\bar{1} \rangle} = 6\left(Q_{11,1\bar{1}} + Q_{11,\bar{1}1} + Q_{1\bar{1},11} + Q_{\bar{1}1,11}\right) = 6\left(3i(A_{11,1\bar{1}} + A_{11,\bar{1}1}) + 2R_{,11}\right),$$

and

$$0 = 3i\left(A_{11,\bar{1}1} + iA_{11,0} + 2RA_{11} + A_{11,\bar{1}1}\right) + 2R_{,11} = -3A_{11,0} + 6iA_{11,\bar{1}1} + 2R_{,11}. \tag{146}$$

From (145), (146) and the definition of Cartan tensor $\mathfrak{Q}$ (see page 227 in [18]) we have that, at q

$$\begin{cases} 3iA_{11,0} + 8A_{11,\bar{1}1} + 2iR_{,11} = 0; \\ -3A_{11,0} + 6iA_{11,\bar{1}1} + 2R_{,11} = 0; \\ -6A_{11,0} - 4iA_{11,\bar{1}1} + R_{,11} = 6\mathfrak{Q}_{11}, \end{cases}$$

where

$$\mathfrak{Q}_{11} = \frac{1}{6}R_{,11} + \frac{i}{2}RA_{11} - A_{11,0} - \frac{2}{3}iA_{11,\bar{1}1}.$$

Therefore we deduce that, at q

$$A_{11,0} = -\frac{4}{5}\mathfrak{Q}_{11}; \qquad A_{11,\bar{1}1} = \frac{12}{35}i\mathfrak{Q}_{11}; \qquad R_{,11} = -\frac{6}{35}\mathfrak{Q}_{11}.$$

For $N = 4$, suppose we have chosen a contact form $\hat{\theta}$ such that (144) holds true. Then one can check that

$$\hat{\omega}_1^1{}_{(2)} = \hat{\omega}_1^1{}_{(3)} = 0; \qquad \hat{\theta}^1_{(3)} = \hat{\theta}^1_{(4)} = 0; \qquad \hat{\theta}_{(4)} = \hat{\theta}_{(5)} = 0.$$

For example we have

$$\begin{aligned} \hat{\omega}_1^1{}_{(2)} &= \frac{1}{2}\left(\sqrt{2}R(z\hat{\theta}^{\bar{1}} - \bar{z}\hat{\theta}^1) + A_{11,\bar{1}}(\sqrt{2}z\hat{\theta} - 2t\hat{\theta}^1) - A_{\bar{1}\bar{1},1}(\sqrt{2}\bar{z}\hat{\theta} - 2t\hat{\theta}^{\bar{1}})\right)_{(2)} \\ &= \frac{1}{2}\left(\sqrt{2}z(R\hat{\theta}^{\bar{1}})_{(1)} - \sqrt{2}\bar{z}(R\hat{\theta}^1)_{(1)} + \sqrt{2}z(A_{11,\bar{1}}\hat{\theta})_{(1)} - 2t(A_{11,\bar{1}}\hat{\theta}^1)_{(0)}\right. \\ &- \left.\sqrt{2}\bar{z}(A_{\bar{1}\bar{1},1}\hat{\theta})_{(1)} + 2t(A_{\bar{1}\bar{1},1}\hat{\theta}^{\bar{1}})_{(0)}\right) = 0, \end{aligned}$$

and similarly $\hat{\omega}_1^1{}_{(3)} = 0$. Now we have that

$$\begin{aligned} \hat{\omega}_1^1{}_{(4)} &= \frac{1}{4}\left(\sqrt{2}R(z\hat{\theta}^{\bar{1}} - \bar{z}\hat{\theta}^1) + A_{11,\bar{1}}(\sqrt{2}z\hat{\theta} - 2t\hat{\theta}^1) - A_{\bar{1}\bar{1},1}(\sqrt{2}\bar{z}\hat{\theta} - 2t\hat{\theta}^{\bar{1}})\right)_{(4)} \\ &= \frac{1}{4}\left(\sqrt{2}z(R\hat{\theta}^{\bar{1}})_{(3)} - \sqrt{2}\bar{z}(R\hat{\theta}^1)_{(3)} + \sqrt{2}z(A_{11,\bar{1}}\hat{\theta})_{(3)} - 2t(A_{11,\bar{1}}\hat{\theta}^1)_{(2)}\right. \\ &- \left.\sqrt{2}\bar{z}(A_{\bar{1}\bar{1},1}\hat{\theta})_{(3)} + 2t(A_{\bar{1}\bar{1},1}\hat{\theta}^{\bar{1}})_{(2)}\right) \\ &= \frac{1}{4}\left(2R_{(2)}zd\bar{z} - 2R_{(2)}\bar{z}dz + \sqrt{2}(A_{11,\bar{1}})_{(1)}z\mathring{\theta} - 2(A_{11,\bar{1}})_{(1)}t\sqrt{2}dz\right. \\ &- \left.\sqrt{2}(A_{\bar{1}\bar{1},1})_{(1)}\bar{z}\mathring{\theta} + 2(A_{\bar{1}\bar{1},1})_{(1)}t\sqrt{2}d\bar{z}\right) \\ &= \frac{1}{4}\left(-\sqrt{2}R_{(2)}\bar{z} - 2(A_{11,\bar{1}})_{(1)}t\right)\sqrt{2}dz + \frac{1}{4}\left(\sqrt{2}R_{(2)}z + 2(A_{\bar{1}\bar{1},1})_{(1)}t\right)\sqrt{2}d\bar{z} \\ &+ \frac{\sqrt{2}}{4}\left((A_{11,\bar{1}})_{(1)}z - (A_{\bar{1}\bar{1},1})_{(1)}\bar{z}\right)\mathring{\theta}, \end{aligned}$$

so we deduce

$$\begin{aligned} \hat{\omega}_1^1{}_{(4)} &= \left(-R_{,11}(q)z^2\bar{z} - R_{,\bar{1}\bar{1}}(q)\bar{z}^3 - A_{11,\bar{1}1}(q)zt\right)dz + \left(R_{,11}(q)z^3 + R_{,\bar{1}\bar{1}}(q)\bar{z}^2z + A_{\bar{1}\bar{1},1\bar{1}}(q)\bar{z}t\right)d\bar{z} \\ &+ \frac{1}{2}\left(A_{11,\bar{1}1}(q)z^2 - A_{\bar{1}\bar{1},1\bar{1}}(q)\bar{z}^2\right)\mathring{\theta}. \end{aligned}$$

Hence we conclude

$$\hat{\omega}_1^1 = O(\rho^3)dz + O(\rho^3)d\bar{z} + O(\rho^2)\mathring{\theta}.$$

We also have

$$\begin{aligned} \hat{\theta}^1_{(5)} &= \frac{1}{5}\left(\sqrt{2}z\hat{\omega}_1^1 + 2tA_{\bar{1}\bar{1}}\hat{\theta}^{\bar{1}} - \sqrt{2}\bar{z}A_{\bar{1}\bar{1}}\theta\right)_{(5)} = \frac{1}{5}\left(\sqrt{2}z(\hat{\omega}_1^1)_{(4)} + 2t(A_{\bar{1}\bar{1}}\hat{\theta}^{\bar{1}})_{(3)} - \sqrt{2}\bar{z}(A_{\bar{1}\bar{1}}\theta)_{(4)}\right) \\ &= \frac{1}{5}\left(\sqrt{2}z(\hat{\omega}_1^1)_{(4)} + 2t(A_{\bar{1}\bar{1}})_{(2)}\sqrt{2}d\bar{z} - \sqrt{2}\bar{z}(A_{\bar{1}\bar{1}})_{(2)}\mathring{\theta}\right), \end{aligned}$$

and therefore we get

$$\begin{aligned}
&\hat{\theta}^1_{(5)} = \frac{1}{20}\left(-4R_{,11}(q)z^3\overline{z} - 4R_{,\overline{1}\overline{1}}(q)\overline{z}^3 z - 4A_{11,\overline{1}1}(q)z^2 t\right)\sqrt{2}dz \\
+ \quad & \left[\frac{1}{5}\left(R_{,11}(q)z^4 + R_{,\overline{1}\overline{1}}(q)z^2\overline{z}^2 + A_{\overline{1}\overline{1},1\overline{1}}(q)z\overline{z}t\right) + \frac{2}{5}A_{\overline{1}\overline{1},0}(q)t^2 + \frac{4}{5}(2A_{\overline{1}\overline{1},1\overline{1}}(q) - iA_{\overline{1}\overline{1},0}(q))z\overline{z}t\right]\sqrt{2}d\overline{z} \\
+ \quad & \left[\frac{\sqrt{2}}{10}\left(A_{11,\overline{1}1}(q)z^3 - A_{\overline{1}\overline{1},1\overline{1}}(q)z\overline{z}^2\right) - \frac{\sqrt{2}}{5}A_{\overline{1}\overline{1},0}(q)\overline{z}t - \frac{2\sqrt{2}}{5}\left(2A_{\overline{1}\overline{1},1\overline{1}}(q) - iA_{\overline{1}\overline{1},0}(q)\right)z\overline{z}^2\right]\mathring{\theta},
\end{aligned}$$

which implies

$$\hat{\theta}^1 = \left(1 + O(\rho^4)\right)\sqrt{2}dz + O(\rho^4)d\overline{z} + O(\rho^3)\mathring{\theta}.$$

We also have

$$\hat{\theta}_{(6)} = \frac{1}{6}\left(\sqrt{2}iz\hat{\theta}^{\overline{1}} - \sqrt{2}i\overline{z}\hat{\theta}^1\right)_{(6)} = \frac{\sqrt{2}}{6}\left(iz\hat{\theta}^{\overline{1}}_{(5)} - i\overline{z}\hat{\theta}^1_{(5)}\right),$$

and hence

$$\hat{\theta} = \left(1 + O(\rho^4)\right)\mathring{\theta} + O(\rho^5)dz + O(\rho^5)d\overline{z}.$$

Let us now try to understand the behavior of the dual vectors. Let

$$\hat{W}_1 = (1+a)\mathring{Z}_1 + b\mathring{Z}_{\overline{1}} + c\frac{\partial}{\partial t},$$

where we recall $\mathring{Z}_1 = \frac{1}{\sqrt{2}}(\frac{\partial}{\partial z} + i\overline{z}\frac{\partial}{\partial t})$ (see (8)). From these formulas, if we set

$$\hat{\theta} = \mathring{\theta} + \sum_{m\geq 6}\hat{\theta}_{(m)}; \qquad \hat{\theta}^1 = \sqrt{2}dz + \sum_{n\geq 5}\hat{\theta}^1_{(n)}; \qquad \hat{\theta}^{\overline{1}} = \sqrt{2}d\overline{z} + \sum_{n\geq 5}\hat{\theta}^{\overline{1}}_{(n)},$$

we have that

$$\begin{aligned}
0 &= \hat{\theta}(\hat{W}_1) = \left(\mathring{\theta} + \sum_{m\geq 6}\hat{\theta}_{(m)}\right)\left((1+a)\mathring{Z}_1 + b\mathring{Z}_{\overline{1}} + c\frac{\partial}{\partial t}\right) \\
&= (1+a)\mathring{\theta}(\mathring{Z}_1) + b\mathring{\theta}(\mathring{Z}_{\overline{1}}) + c\mathring{\theta}(\frac{\partial}{\partial t}) + (1+a)\sum_{m\geq 6}\hat{\theta}_{(m)}(\mathring{Z}_1) + b\sum_{m\geq 6}\hat{\theta}_{(m)}(\mathring{Z}_{\overline{1}}) + c\sum_{m\geq 6}\hat{\theta}_{(m)}(\frac{\partial}{\partial t}) \\
&= c + O(\rho^5) + aO(\rho^5) + bO(\rho^5) + cO(\rho^4)
\end{aligned}$$

and hence we find that $c = O(\rho^5)$.

Similarly

$$1 = \hat{\theta}^1(\hat{W}_1) \quad \Rightarrow \quad a = O(\rho^4); \qquad\qquad 0 = \hat{\theta}^{\overline{1}}(\hat{W}_1) \quad \Rightarrow \quad b = O(\rho^4).$$

Also, if we set

$$\hat{T} = (1+a)\frac{\partial}{\partial t} + b\mathring{Z}_1 + c\mathring{Z}_{\overline{1}},$$

then from

$$1 = \hat{\theta}(\hat{T}); \qquad 0 = \hat{\theta}^1(\hat{T}); \qquad 0 = \hat{\theta}^{\overline{1}}(\hat{T})$$

we deduce that $a = O(\rho^4), b = O(\rho^3), c = O(\rho^3)$, and hence we obtain

$$\hat{T} = \left(1 + O(\rho^4)\right)\frac{\partial}{\partial t} + O(\rho^3)\mathring{Z}_1 + O(\rho^3)\mathring{Z}_{\overline{1}}.$$

In conclusion, we arrive to the following result.

Proposition A.5 *In CR normal coordinates of order $N = 4$, we have a contact form $\hat{\theta}$ such that*

$$\hat{\theta} = \left(1 + O(\rho^4)\right) \overset{\circ}{\theta} + O(\rho^5)dz + O(\rho^5)d\overline{z}; \qquad \hat{\theta}^1 = \left(1 + O(\rho^4)\right) \sqrt{2}dz + O(\rho^4)d\overline{z} + O(\rho^3)\overset{\circ}{\theta};$$

$$\hat{\omega}_1^1 = O(\rho^3)dz + O(\rho^3)d\overline{z} + O(\rho^2)\overset{\circ}{\theta};$$

$$\hat{W}_1 = \left(1 + O(\rho^4)\right) \overset{\circ}{Z}_1 + O(\rho^4)\overset{\circ}{Z}_{\overline{1}} + O(\rho^5)\frac{\partial}{\partial t}; \qquad \hat{T} = \left(1 + O(\rho^4)\right) \frac{\partial}{\partial t} + O(\rho^3)\overset{\circ}{Z}_1 + O(\rho^3)\overset{\circ}{Z}_{\overline{1}},$$

where we recall

$$\overset{\circ}{\theta} = dt + izd\overline{z} - i\overline{z}dz; \qquad \overset{\circ}{Z}_1 = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial z} + i\overline{z}\frac{\partial}{\partial t}\right); \qquad \rho^4 = t^2 + |z|^4.$$

The above computation concluding the proof of Proposition A.5 was first done by H.-L. Chiu in the summer of 2007 when he visited J.-H. Cheng.

References

[1] Andreotti, A., Siu, Y.-T., *Projective Embedding of Pseudoconcave Spaces*, Annali della Scuola Normale Sup. di Pisa 24 (1970) 231-278.

[2] Arnowitt, R., Deser, S., Misner, C., *Energy and the criteria for radiation in general relativity*, Phys. Rev., 118 (1960) 1100-1104.

[3] Arnowitt, R., Deser, S., Misner, C., *Coordinate invariance and energy expressions in general relativity*, Phys. Rev., 122 (1961) 997-1006.

[4] Aubin, T., *Équations différentielles non linéaires et probléme de Yamabe concernant la courboure scalaire*, J. Math. Pures Appl., 55 (1976) 269-296.

[5] Bahri, A., Brezis, H. *Non-linear elliptic equations on Riemannian manifolds with the Sobolev critical exponent*, Topics in geometry, 1-100, Progr. Nonlinear Differential Equations Appl., 20, Birkuser Boston, Boston, MA, 1996.

[6] Bland, J., *Contact geometry and CR structures on S^3*, Acta Math., 172 (1994) 1-49.

[7] Brendle, S., *Convergence of the Yamabe flow for arbitrary initial energy*, J. Differential Geom., 69 (2005), 217-278.

[8] Brendle, S., *Convergence of the Yamabe flow in dimension 6 and higher*, Invent. Math., 170 (2007) 541-576.

[9] Burns, D.M., Epstein, C.L. *Embeddability for three-dimensional CR-manifolds*, J. Amer. Math. Soc., 3 (1990) 809-841.

[10] Chang, S.-C., Cheng, J.-H., Chiu, H.-L. *A fourth order curvature flow on a CR 3-manifold*, Indiana Univ. Math. J., 56 (2007) 1793-1826.

[11] Chang, S.-C. and Chiu, H.-L., *Nonnegativity of CR Paneitz operator and its application to the CR Obata's theorem,* Math. Ann., 345 (2009) 33-51.

[12] Chanillo, S., Chiu, H.-L., Yang, P., *Embeddability for 3-dimensional Cauchy-Riemann manifolds and CR Yamabe invariants*, Duke Math. J., 161 (2012) 2909-2921.

[13] Case, J.S., Chanillo, S., Yang, P., *The CR Paneitz operator and the stability of CR pluriharmonic functions*, preprint, 2015.

[14] Chanillo, S., Manfredi, J., *Sharp Global Bounds for the Hessian on Pseudo-Hermitian Manifolds*, Recent developments in real and harmonic analysis, 159?172, Appl. Numer. Harmon. Anal., Birkhuser, 2010.

[15] Chen S.-C., Shaw M.-C., *Partial differential equations in several complex variables*, AMS, 2001.

[16] Cheng, J.-H., *Flows and a tangency condition for embeddable CR structures in dimension 3*, Methods and Applications of Analysis, 21 (2014) 337-356.

[17] Cheng, J.-H., Chiu, H.-L, Yang, P., *Uniformization of spherical CR manifolds*, Adv. in Math., 255 (2014) 182-216.

[18] Cheng, J.-H., Lee, John M., *The Burns-Epstein invariant and deformation of CR structures*, Duke Math. J., 60 (1990) 221-254.

[19] Cheng, J.-H., Lee, J.-M., *A local slice theorem for 3-dimensional CR structures*, Amer. J. Math., 117 (1995) 1249-1298.

[20] Chern, S.-S., Hamilton, R.-S., *On Riemannian metrics adapted to three-dimensional contact manifolds*, Springer Lecture Notes 1111, Springer-Verlag (1985) 279-308.

[21] Folland, G.B., Stein, E.M., *Estimates for the $\bar{\partial}_b$ complex and analysis on the Heisenberg group.* Comm. Pure Appl. Math. 27 (1974) 429-522.

[22] Gamara, N., *The CR Yamabe conjecture the case $n = 1$*, J. Eur. Math. Soc. 3 (2001), 105-137.

[23] Gamara, N., Jacoub, R., *CR Yamabe conjecture the conformally flat case*, Pacific J. Math. 201 (2001), 121-175.

[24] Graham, C. R., Lee, J.M., *Smooth solutions of degenerate Laplacians on strictly pseudoconvex domains*, Duke Math. J., 57 (1988) 697-720.

[25] Hirachi, K., *Scalar pseudo-hermitian invariants and the Szegö kernel on three-dimensional CR manifolds*, Lect. Notes in Pure and Appl. Math., 143 (1993) 67-76.

[26] Hsiao, C.-Y, Yung, P.-L., *Solving the Kohn Laplacian on asymptotically flat CR manifolds of dimension 3*, Advances in Math., 281 (2015) 734-822.

[27] Jerison, D., Lee, J.M., *The Yamabe problem on CR manifolds*, J. Diff. Geom., 25 (1987) 167-197.

[28] Jerison, D., Lee, J.M., *Extremals for the Sobolev inequality on the Heisenberg group and the CR Yamabe problem*, J. Amer. Math. Soc., 1 (1988) 1-13.

[29] Jerison, D., Lee, J.M., *Intrinsic CR normal coordinates and the CR Yamabe problem*, J. Diff. Geom., 29 (1989) 303-343.

[30] Khuri, M.A., Marques, F.C., Schoen, R., *A compactness theorem for the Yamabe problem*, J. Differential Geom. 81 (2009) 143-196.

[31] Lee, J., *The Fefferman metric and pseudohermitian invariants*, Trans. Amer. Math. Soc. 296 (1986) 411-429.

[32] Lee, J., *Pseudo-Einstein structures on CR manifolds*, Amer. J. Math., 110 (1988) 157-178.

[33] Lee, J., Parker, T., *The Yamabe problem*, Bull. Amer. Math. Soc. 17 (1987) 37-91.

[34] Parker, T., Taubes, C.H., *On Witten's proof of the positive energy theorem*, Commun.Math. Phys., 84 (1982) 223-238.

[35] Rossi, H., *Attaching analytic spaces to an analytic space along a pseudoconvex boundary*, Proc. Conf. Complex Manifold, Springer-Verlag, New York (1965) 242-256.

[36] Schoen, R., *Conformal deformation of a Riemannian metric to constant scalar curvature*, J. Diff. Geom. 20 (1984) 479-495.

[37] Schoen, R., Yau, S.-T., *On the proof of the positive mass conjecture in general relativity*, Commun. Math. Phys., 65 (1979) 45-76.

[38] Schoen, R., Yau, S.-T., *Positivity of the total mass in a general space-time*, Phys. Rev. Lett., 43 (1979) 1457-1459.

[39] Schoen, R., Yau, S.-T., *Proof of the positive mass theorem II*, Commun. Math. Phys., 79 (1981) 231-260.

[40] Schoen, R., Yau, S.-T., *The energy and the linear momentum of space-times in general relativity*, Commun. Math. Phys., 79 (1981) 47-51.

[41] N. Trudinger, *Remarks concerning the conformal deformation of Riemannian structures on compact maniflods*, Ann. Scuola Norm. Sup. Cl. Sci., 22 (1968) 265-274.

[42] Witten, E., *A new proof of the positive energy theorem*, Commun. Math. Phys., 80 (1981) 381-402.