A positive mass theorem in three dimensional Cauchy-Riemann geometry

Jih-Hsin Cheng\(^{(a)}\), Andrea Malchiodi\(^{(b)}\), and Paul Yang\(^{(c)}\)

\(^{(a)}\) Institute of Mathematics, Academia Sinica and NCTS, Taipei office
6F, Astronomy-Mathematics Building No. 1, Sec. 4 Roosevelt Road, Taipei 10617, TAIWAN

\(^{(b)}\) University of Warwick, Mathematics Institute - Zeeman Building Coventry CV4 7AL and SISSA, Via Bonomea 265, 34136 Trieste, ITALY

\(^{(c)}\) Princeton University, Department of Mathematics
Fine Hall, Washington Road, Princeton NJ 08544-1000 USA

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 Tanaka-Webster class 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, conformal geometry, Tanaka-Webster Yamabe problem

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

Table of Contents

1. Introduction and statement of the results
2. Asymptotically flat pseudohermitian manifolds and definition of the p-mass
3. Proof of Theorem 1.1
4. Some examples
5. Proof of Theorem 1.2
6. Appendix: useful facts in pseudohermitian geometry

\(^{1}\)E-mail address: cheng@math.sinica.edu.tw, A.Malchiodi@warwick.ac.uk, malchiod@sissa.it, yang@math.princeton.edu
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. [3], [4]. The total energy was called the \( \textit{ADM-mass} \) 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 ([38], [39], [40], [41]) and by Witten using the Dirac equation for spinors ([43]; a rigorous proof is given in [35]) in late 70’s and early 80’s. Since there is a strong analogy between CR geometry and conformal geometry, one may wonder about what happens in CR geometry correspondingly. This is the main goal of this paper.

We recall some well known definitions and facts, referring to [34] for more details. A Riemannian manifold \( N \) (of dimension \( n \)) with a smooth metric \( g \) is called \textit{asymptotically flat} of order \( \tau > 0 \) if \( N \) decomposes as \( N = N_0 \cup N_\infty \), where \( N_0 \) is compact and \( N_\infty \) is diffeomorphic to \( \mathbb{R}^n \setminus B_R(0) \) for some \( R > 0 \), and if \( g \) on \( N_\infty \) 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 \textit{asymptotic coordinates}. One then considers the Einstein-Hilbert action

\[
A(g) := -\int_N S_g dV_g,
\]

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

\[
\frac{d}{ds}|_{s=0} (S_g dV_g) = - \left( v^{ij} G_{ij} + \nabla^* \xi \right) dV_g,
\]

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

\[
m(g) = \lim_{R \to +\infty} \omega_n^{-1} \int_{\Sigma_R} \mu dV_g \quad \mu = (\partial_i g_{ij} - \partial_j g_{ij}) \partial_j, \quad \Sigma_R = \{|x| = R\}.
\]

By varying the metric it turns out that

\[
\frac{d}{ds} (A(g_s) + m(g_s)) = \int_N v^{ij} G_{ij} dV_g.
\]

The positive mass theorem was then used by Schoen in [37] to prove the Yamabe conjecture (finding conformal metrics with constant scalar curvature) in the cases left open in 1976 by T.Aubin ([5]), namely in dimension 3, 4, 5 or when the metric is locally conformally flat. As shown in [42], to solve the problem (in the \textit{positive case}, the most difficult one) it is sufficient to show that the Yamabe quotient of the manifold is smaller than the one of \( \mathbb{R}^n \). This was done both in [5] and in [37] using suitable test functions. In particular Schoen’s argument consists in gluing a \textit{standard bubble} near any \( p \in M \) to \( g_p \), the Green’s function of the conformal Laplacian with pole at \( p \). It turns out that the regular part of \( g_p \) coincides with the mass of \( (M \setminus \{p\}, G_p^{\infty} g) \), the \textit{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 [8], [9], [31].

The goal of this paper is to introduce a notion of asymptotically flat pseudohermitian manifold, define a \textit{pseudohermitian mass} and to prove its positivity under suitable conditions. We give then applications concerning existence of minimizers for the Tanaka-Webster quotient, which is useful to study the CR analogue of the Yamabe quotient.

We consider a compact three dimensional pseudohermitian manifold \( (M, J, \theta) \) (with no boundary) of \textit{positive Tanaka-Webster class}. This means that the first eigenvalue of the \textit{conformal sublaplacian}

\[
L_b := -4 \Delta_b + R,
\]
is strictly positive. Here $\Delta_b$ stands for the sublaplacian of $M$ and $R$ for the Tanaka-Webster curvature, see Subsection 1.1 for their definition. The conformal sublaplacian has the following covariance property under a conformal change of contact form

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

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

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

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

$$(3) \quad \mathcal{Y}(J) := \inf_{\hat{\theta}} \int_M R_{J,\hat{\theta}} \hat{\theta} \wedge d\hat{\theta} > 0,$$

where $\hat{\theta}$ is any contact form which annihilates $\xi$ (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 6.2) $G_p$ 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

$$(4) \quad N = (M \setminus \{p\}, J, \theta = G_p^2 \hat{\theta}),$$

where $\hat{\theta}$ is chosen so that near $p$ it has the behavior as described in Proposition 6.5. 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

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

where we have set $S_\Lambda = \{ \rho = \Lambda \}$, $\rho^4 = |z|^4 + t^2$, and where $\omega^1$ 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 (2), see 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 Subsection 2.3 we prove an integral formula for the p-mass, in the spirit of [43]. To state this formula we need to introduce another conformally covariant operator, the CR Paneitz operator

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

(where we are following the notation of Subsection 1.1). The operator $P$ satisfies the covariance property ([26])

$$(5) \quad P_{(J,\hat{\theta})} = u^{-4} P_{(J,\theta)}; \quad \hat{\theta} = u^2 \theta.$$
In Proposition 2.6 we prove then the following integral formula, which holds for an asymptotically flat pseudohermitian manifold $N$

$$2 \frac{m(J, \theta)}{3} = - \int_N |\nabla_b \beta|^2 \wedge d\theta + 2 \int_N |\beta|_{\mathcal{H}}^2 \wedge d\theta + 2 \int_N R|\beta|_{\mathcal{H}}^2 \wedge d\theta + \frac{1}{2} \int_N \beta P \beta \wedge d\theta. \quad (6)$$

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

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

with $\Box_b = -2\beta_{\mathcal{H}}$ and with $\beta_{-1}$ a suitable function with homogeneity $-1$ in $\rho$ (satisfying condition (39) below).

To explain the link between [43] and the $\Box_b$ operator, let us consider a general spin$^c$ structure on a contact bundle $\xi$ over an asymptotically flat pseudohermitian manifold $M$ of dimension $2n + 1$. Let $W$ denote the spinor bundle with a spin$^c$ connection $\nabla$ compatible with the pseudohermitian connection $\nabla_{\text{p.h.}}$. Let $e_1, ..., e_{2n}$ denote an orthonormal basis of $\xi$ with respect to the Levi metric. Denote the contact Dirac operator $D_\xi$ by

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

(summation convention) for a section $\psi$ of $W$, where $\Gamma$ denotes the Clifford multiplication. Let $T$ denote the Reeb vector field associated to the contact form $\theta$. Let $D_\xi^*, \nabla^*$ denote the adjoint operator of $D_\xi$, $\nabla$, resp.. We then have the following formula

$$D_\xi^2 D_\xi \psi = \sum_{a=1}^{2n} \nabla^*_{e_a} \nabla_{e_a} \psi - 2 \sum_{a=1}^{2n} \Gamma(e_a e_{n+a}) \nabla_T \psi$$

$$+ \sum_{a<b} \Gamma(e_a) \Gamma(e_b) R^\nabla(e_a, e_b) \psi \quad (7)$$

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

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

where, again, $R$ denotes the Tanaka-Webster scalar curvature. On the other hand, $2^{-n} tr_W R^\nabla_{ab} = F_A(e_a, e_b)$ in which the curvature 2-form $F_A := dA$ and $2A$ is the connection form of an associated line bundle $L_{\Theta}$ (det $W = L_{\text{det}}^{2^{n-1}}$). Therefore we can reduce (7) to

$$D_\xi^2 D_\xi \psi = \sum_{a=1}^{2n} \nabla^*_{e_a} \nabla_{e_a} \psi - 2 \sum_{a=1}^{2n} \Gamma(e_a e_{n+a}) \nabla_T \psi$$

$$+ \frac{1}{4} R \psi + \rho(F_A) \psi \quad (8)$$

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 (8), we consider the canonical spin$^c$ structure with $W = \Lambda^0,^*\Lambda$ the bundle of all $(0, q)$ forms. In particular, we take $\psi = \partial_u u = u_{,\beta} \theta^\beta$ (summation convention throughout the remaining part), a $(0, 1)$ form with components being derivatives of a complex function $u$. Then we have

$$D_\xi \psi = (\partial_u + \partial_u^\Theta) \circ \partial_u = \partial_u^\Theta \circ \partial_u = \Box_u$$
where $\Box_b := \bar{\partial}_b \circ \bar{\partial}_b^* + \bar{\partial}_b^* \circ \bar{\partial}_b$ is Kohn’s Laplacian. Note that $\bar{\partial}_b^* u = 0$. To solve the contact Dirac equation $D_\xi \psi = 0$ for $\psi$ 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 $2n + 1 \geq 5$), $P$ is non-negative (for closed $M$ and open $M$ with suitably decaying test functions) (see [12], [25]). 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). 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 three dimensional 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 $\theta$ be a blow-up of contact form as in (4). 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).

We prove this theorem in Section 3. The assumptions we give here are conformally invariant, and are needed to ensure the positivity of the right-hand side in (6). By the result in [13], 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 (6) vanish): we first find an approximate solution through the expansion of $\Box_b \mathcal{T}$ 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 [27]. The positivity of the CR Paneitz operator is used instead to control the last term in the right-hand side of (6), 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 3.4. More comments on the relation between the embeddability and the non-negativity of $P$ for manifolds of positive Tanaka-Webster class 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 $\theta$ be a blow-up of contact form as in (4). Then the same conclusions of Theorem 1.1 hold.

In Section 4 we construct some examples of structures using the deformation formulas in Subsection 6.1. 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 [13]). 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 Tanaka-Webster class and negative mass (when the blow-up is done at suitable points), see Proposition 4.4. This is in striking contrast with respect to 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 $\mathbb{H}^3 \setminus \{0\}$.

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 [21]), 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 [28] one always has
\[
(9) \quad \mathcal{Y}(J) \leq \mathcal{Y}_0,
\]
and if strict inequality holds, then the problem is solvable. The strict inequality is needed to ensure compactness of the minimizing sequences in (3). This condition was verified in [30] for (real) dimension greater or equal to five, and for non-spherical structures, in the spirit of [5] 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 \( p \):
\[
(10) \quad G_p = c_n \rho^{-2n} + A + O(\rho),
\]
where \( \rho \) 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 (10) holds for \( n = 1 \) (dimension 3 case) and for \( N \) being spherical of all dimensions.

For such manifolds of dimension greater or equal to 5 (some extra technical condition in dimension 5) with positive CR Yamabe or Tanaka-Webster class, one can prove a positive mass theorem for \( A \) (and hence find solutions of the CR Yamabe problem with minimal energy) through another approach ([18]).

Our next result gives the strict Webster-Sobolev inequality 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.

\textbf{Theorem 1.2} Suppose we are under the assumptions of Theorem 1.1. 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 Tanaka-Webster 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 [23] and [24] respectively (we also refer to [21] and [18]). While the proof in these papers relies on topological arguments and may not provide energy extremals, in the spirit of [6], 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 [37], 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 [30]. 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.

\textbf{1.1 Notation and preliminaries}

We collect here some useful material: throughout this paper, we will mostly use notations taken from [32]. Consider a three-dimensional CR manifold endowed with a contact structure \( \xi \) and a CR structure \( J : \xi \to \xi \) such that \( J^2 = -1 \). We assume that there exists a global choice of contact form \( \theta \) which annihilates \( \xi \) and for which \( \theta \wedge d\theta \) is always nonzero. We define the \textit{Reeb vector field} as the unique vector field \( T \) for which
\[
\theta(T) = 1; \quad T \perp d\theta.
\]
Given \( J \) as above, we have a local choice of a vector field \( Z_1 \) such that
\[
(11) \quad JZ_1 = iZ_1; \quad JZ_{\tau} = -iZ_{\tau}, \quad \text{where} \quad Z_{\tau} = \overline{(Z_1)}.
\]
We also define \((\theta, \theta^1, \theta^\top)\) as the dual triple to \((T, Z_1, Z_\top)\), so that
\[
d\theta = i h \theta^1 \wedge \theta^\top \quad \text{for some } h > 0 \quad (\text{possibly replacing } \theta \text{ by } -\theta).
\]
In the following we will always assume that \(h = 1\).

The connection 1-form \(\omega_1^1\) and the torsion are uniquely determined by the equations
\[
\begin{align*}
d\theta^1 &= \theta^1 \wedge \omega_1^1 + A^2_1 \theta \wedge \theta^\top; \\
\omega_1^1 + \omega_\top^1 &= 0.
\end{align*}
\]

The Tanaka-Webster curvature is then defined by the formula
\[
d\omega_1^1 = R \theta^1 \wedge \theta^\top \quad (\text{mod } \theta).
\]

In the (3-dimensional) Heisenberg group \(\mathbb{H}^1\) standard choices for the dual forms are
\[
\begin{align*}
\check{\theta} &= dt + i dz - i \overline{d}z; \\
\check{\theta}^1 &= \sqrt{2} dz; \\
\check{\theta}^\top &= \sqrt{2} \overline{d}z,
\end{align*}
\]
while for the vector fields we can take
\[
\begin{align*}
\check{T} &= \frac{\partial}{\partial t}; \\
\check{Z}_1 &= \frac{1}{\sqrt{2}} \left( \frac{\partial}{\partial z} + i \frac{\partial}{\partial \overline{z}} \right); \\
\check{Z}_\top &= \frac{1}{\sqrt{2}} \left( \frac{\partial}{\partial \overline{z}} - i \frac{\partial}{\partial z} \right).
\end{align*}
\]
(12)

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

We recall the rules for the covariant differentiation with respect to \(\omega_1^1\). For a complex function \(f\) we set
\[
f_1 = f, \check{1} = Z_1 f; \quad f_\perp = Z_\perp Z_1 f - \omega_1^1(Z_\perp) Z_1 f; \quad f_0 = T f, \ldots
\]
We also define the operators
\[
\Delta_b f = f_{\perp 1} + f_{\perp \top} = f_{\perp 1} + f_{\top 1}; \quad \Box_b f = -\Delta_b f + i T f,
\]
where we have used \(h = h_\perp = 1\) to raise or lower the indices. We also recall the commutation relations
(13)
\[
\begin{align*}
c_{1} - c_{\perp 1} &= i c_{0} + kcR; \\
c_{1} - c_{\top 0} &= c_1 A_{\perp 1} - kc A_{\perp 1}; \\
c_{0} - c_{\top 0} &= c_1 A_{\perp 1} + kc A_{\perp 1}.
\end{align*}
\]
(see Lemma 2.3 in [33]; here we are considering the \(n = 1\) case) where \(c\) is a tensor with 1 or \(\perp\) as subindices, \(k\) is the number of 1-subindices of \(c\) minus the number of \(\perp\)-subindices of \(c\) and where we recall, we are assuming that \(h_\perp = 1\) (so \(A_{\perp 1} = A_1^\perp\) and \(A_{\perp 1}\) is the complex conjugate of \(A_{\perp 1}\)).

The CR Paneitz operator \(P\) is defined by
\[
P\varphi := 4(\varphi_{\perp 1}^1 + i A_{\perp 1} \varphi^1)^1.
\]
(14)

Let \(\tilde{P}_3 \varphi := \varphi_{\perp 1}^1 + i A_{\perp 1} \varphi^1\). The CR pluriharmonic functions are characterized by \(\tilde{P}_3 \varphi = 0\) ([33]) while \(P\) is identified with the compatibility operator for solving a certain degenerate Laplace equation (see [25]).
The operator $P$ is also a CR analogue of the Paneitz operator in conformal geometry (see [26] for the relation to a CR analogue of the $Q$-curvature and the log-term coefficient in the Szegő kernel expansion). On a compact pseudohermitian 3-dimensional manifold $(M, J, \theta)$, we call $P$ non-negative if

$$\int_M \varphi P\varphi \theta \wedge d\theta \geq 0$$

for all real ($C^\infty$) smooth functions $\varphi$. When we want to emphasize the dependence of $\theta$, we write $P_\theta$ instead of $P$. $P$ is pseudohermitian covariant in the sense that

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

for the contact form change $\theta = e^{2f} \hat{\theta}$ ([26]). The CR Paneitz operator enters in the assumptions of the following embeddability theorem.

**Theorem 1.3** ([13]) 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 [13]) the non-negativity of $P$ implies the embeddability of the structure. A partial converse is shown in [14], where non-negativity of the CR Paneitz operator is shown to be preserved under embedded analytic deformations. The non-negativity of $P$ is also used in [15] 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 1.3 in [13]) 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

$$\rho^4 = |z|^4 + t^2.$$
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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 Tanaka-Webster invariant. For these, the conformal 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 6.2) 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 1 in Section 10 of [27]: 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 6.5 (which relies on results by D.Jerison and J.Lee from [30]), we can find a contact form $\hat{\theta}$ near $p$ and local coordinates $(z,t)$ such that

$$\hat{\theta} = (1 + O(\rho^4)) \theta_0 + O(\rho^5)dz + O(\rho^5)d\bar{z};$$

$$\hat{\theta}^1 = \sqrt{2} (1 + O(\rho^4)) dz + O(\rho^4)d\bar{z} + O(\rho^3)\theta_0,$$

where we have set

$$\theta_0 = dt + izd\bar{z} - izdz.$$

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

$$(18) \quad (M \setminus \{p\}, J, \theta \equiv G_p^2 \hat{\theta}),$$

where we made a conformal change as in Subsection 6.1.1, taking $f = \log G_p$. Then by (135) we also have

$$(19) \quad \theta^1 = G_p \left( \hat{\theta}^1 + 2i (\log G_p)_\Sigma \hat{\theta} \right).$$

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

$$(20) \quad G_p = \frac{1}{2\pi \rho^2} + A + O(\rho) \quad \text{near } p.$$

Hence, from Proposition 6.5 we have that

$$\theta = G_p^2 \hat{\theta} = \left( \frac{1}{2\pi} \rho^{-2} + A + O(\rho) \right)^2 \left[ (1 + O(\rho^4)) \theta_0 + O(\rho^5)dz + O(\rho^5)d\bar{z} \right]$$

$$= \left( \frac{1}{(2\pi)^2} \rho^{-4} + 2\frac{1}{2\pi} A \rho^{-2} + O(\rho^{-1}) \right) \left[ (1 + O(\rho^4)) \theta_0 + O(\rho^5)dz + O(\rho^5)d\bar{z} \right]$$

$$= \left( \frac{1}{(2\pi)^2} \rho^{-4} + 2\frac{1}{2\pi} A \rho^{-2} + O(\rho^{-1}) \right) \theta_0 + O(\rho)dz + O(\rho)d\bar{z}.$$
Recall also the second equation in (19), which we rewrite as
\[
\theta^1 = G_p \left[ \hat{\theta}^1 + 2i \left( \frac{G_p}{G_p} \right)_T \hat{\theta}^1 \right] = G_p \hat{\theta}^1 + 2i (G_p)_T \hat{\theta}^1.
\]
Using the fact that
\[
(\rho^{-2})_T = \frac{1}{\sqrt{2}} \frac{i z v}{\rho^2} + O(\rho),
\]
where \( v = t + i |z|^2 \), we get
\[
(22) \quad (G_p)_T = \frac{1}{2 \pi} \frac{i z v}{\sqrt{2} \rho^2} + O(1),
\]
from which we deduce
\[
\theta^1 = G_p \hat{\theta}^1 + 2i (G_p)_T \hat{\theta}^1
\]
\[
= \left( \frac{1}{2 \pi} \rho^{-2} + A + O(\rho) \right) \left( \sqrt{2} (1 + O(\rho^4)) \, dz + O(\rho^4) \, dz + O(\rho^3) \, d\bar{z} \right)
\]
\[
+ 2i \left( \frac{1}{2 \pi} \frac{i z v}{\sqrt{2} \rho^2} + O(1) \right) \left( (1 + O(\rho^4)) \, \theta_0 + O(\rho^5) \, dz + O(\rho^5) \, d\bar{z} \right)
\]
\[
= \left( \frac{1}{2 \pi} \rho^{-2} + A + O(\rho) \right) \sqrt{2} dz + O(\rho^2) \, d\bar{z} + \left( -\frac{1}{\sqrt{2}} \rho^{-2} + O(\rho) \right) \theta_0.
\]
Using (137), the new connection form becomes
\[
(24) \quad \omega^1_1 = \hat{\omega}^1_1 + 3 (\log G_p)_1 \hat{\theta}^1 - 3 (\log G_p)_T \hat{\theta}^1 + i \left( \Delta_b (\log G_p) + 8 (\log G_p)_1 (\log G_p)_T \right) \hat{\theta}.
\]
From (22) we find
\[
(\log G_p)_T = \frac{(G_p)_T}{G_p} = \frac{1}{2 \pi} \frac{i z v}{\sqrt{2} \rho^2} + O(1) = \frac{1}{2 \pi} \frac{i z v}{\rho^2} + O(\rho^2)
\]
which implies
\[
3 (\log G_p)_1 \hat{\theta}^1 - 3 (\log G_p)_T \hat{\theta}^1
\]
\[
(25) = \left( -\frac{3i z v}{\sqrt{2} \rho^2} + 3 \sqrt{2} \pi A \frac{z v}{\rho^2} + O(\rho^2) \right) \left( \sqrt{2} dz + O(\rho^4) \, dz + O(\rho^4) \, d\bar{z} + O(\rho^3) \, d\bar{z} \right)
\]
\[
+ \left( -\frac{3i z v}{\sqrt{2} \rho^2} + 3 \sqrt{2} \pi A \frac{z v}{\rho^2} + O(\rho^2) \right) \left( \sqrt{2} d\bar{z} + O(\rho^4) \, dz + O(\rho^4) \, d\bar{z} + O(\rho^3) \, d\bar{z} \right).
\]
On the other hand, we also have that
\[
\Delta_b (\log G_p) + 8 (\log G_p)_1 (\log G_p)_T = \left( \frac{(G_p)_1}{G_p} \right)_T + \left( \frac{(G_p)_1}{G_p} \right)_T \left( \frac{(G_p)_T}{G_p} \right)_1 + 8 \left( \frac{(G_p)_1}{G_p} \right) \left( \frac{(G_p)_T}{G_p} \right)
\]
\[
= \Delta_b G_p + 6 \left( \frac{(G_p)_T (G_p)_1}{G_p^2} \right).
\]
Letting \( \tilde{\Delta}_b \) denote the standard sublaplacian in the Heisenberg group, from the choice of CR normal coordinates we find
\[
\Delta_b = \tilde{\Delta}_b + O(\rho^4) \tilde{Z}_1 \tilde{Z}_1 + O(\rho^4) \tilde{Z}_1 \tilde{Z}_1 + O(\rho^4) \tilde{Z}_1 \tilde{Z}_1 + O(\rho^4) \tilde{Z}_1 \tilde{Z}_1 + O(\rho^4) \tilde{Z}_1 \tilde{Z}_1 + O(\rho^4) \tilde{Z}_1 \tilde{Z}_1 + O(\rho^4) \tilde{Z}_1 \tilde{Z}_1 + O(\rho^4) \tilde{Z}_1 \tilde{Z}_1.
\]
Using this expansion and the fact that $\Delta_{\theta} \rho^{-2} = 0$ in $\mathbb{H}^3$ we obtain

$$\Delta_{\theta} \frac{G_p}{G_p} = \frac{\Delta_{\theta} \left( \frac{1}{2\pi \rho} + A + O(\rho) \right)}{\frac{1}{2\pi \rho} + A + O(\rho)} = O(\rho) \quad (\rho \text{ small}),$$

and

$$6 \frac{(G_p)_{\tau}(G_p)_{\tau}}{G_p^2} = 6 \left( \frac{1}{\sqrt{2}} - \frac{\sqrt{2}}{\rho} + O(1) \right) \left( \frac{1}{\sqrt{2}} + \frac{\sqrt{2}}{\rho} + O(1) \right)$$

$$= 6 \left( \frac{1}{\sqrt{2}} - \frac{\sqrt{2}}{\rho} + O(1) \right) \left( \frac{\sqrt{2}}{\rho} + O(\rho^2) \right) \left( \frac{1}{\sqrt{2}} + 2\pi \rho^2 + O(\rho^3) \right)^2 = 3 \frac{|z|^2}{\rho^4} - \frac{3}{\rho} \frac{|z|^2}{\rho^4} 4\pi A \rho^2 + O(\rho).$$

Therefore we get

$$\Delta_{\theta} (\log G_p) + 8 (\log G_p)_{\tau} (\log G_p)_{\tau} 1 = 3 \frac{|z|^2}{\rho^4} - 12 \frac{|z|^2}{\rho^4} \pi A + O(\rho).$$

From (25) and (26), taking Proposition 6.5 into account then one finds

$$\omega_1 = -3 \frac{\sqrt{2}}{\rho^4} dz - 3 \frac{z \sqrt{2}}{\rho^4} dz + 3 \frac{|z|^2}{\rho^4} \rho \theta_0$$

$$+ \left( 3 \sqrt{2} \pi Ai \frac{z}{\rho^2} + O(\rho^2) \right) \sqrt{2} dz + \left( 3 \sqrt{2} \pi Ai \frac{z}{\rho^2} + O(\rho^2) \right) \sqrt{2} d\tau$$

$$+ \left( -12 \pi Ai \frac{|z|^2}{\rho^2} + O(\rho) \right) \theta_0.$$

### 2.2 CR inversion

Next we want to express $\theta$ and $\theta^1$ 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

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

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

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

which imply

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

We can write that

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

so using elementary computations one finds

$$\frac{\partial z}{\partial z_*} = -\frac{t_*}{v_*^2}; \quad \frac{\partial z}{\partial \overline{z}_*} = \frac{z_*^2}{v_*^2}; \quad \frac{\partial z}{\partial t_*} = \frac{z_*}{v_*^2}.$$
Now from (21) we have that
\[ \theta = (\theta_0)_* = (\rho_0)_*^4; \quad \rho = \frac{1}{\rho_*}, \quad (\rho_*)^4 = (t_*)^2 + |z_*|^4, \]
where \((\theta_0)_* = dt_* + iz_*d\bar{z}_* - i\bar{z}_*dz_*, \) and also
\[ dz = -t_*dz_* + iz_*^2d\bar{z}_* + z_*dt_* = \frac{z_*(\theta_0)_* - \bar{\tau}_*dz_*}{v_*^2}. \]

Now from (21) we have that
\[ \theta = G^2_\rho^2 \theta = \frac{1}{(2\pi)^2} \rho^{-4} + 2\frac{1}{2\pi} A \rho^{-2} + O(\rho^{-1}) \theta_0 + O(\rho)dz + O(\rho)d\bar{z} \]
\[ = \frac{1}{(2\pi)^2} \rho_*^{-4} + 2\frac{1}{2\pi} A \rho_*^{-2} + O(\rho_*^{-1}) (\theta_0)_* + O(\rho_*^{-1}) \frac{\bar{\tau}_*(\theta_0)_* - \bar{\tau}_*dz_*}{(v_*^2)^2} + O(\rho_*^{-1}) \frac{\bar{\tau}_*(\theta_0)_* - v_*d\bar{z}_*}{(v_*^2)^2} \]
\[ = \frac{1}{(2\pi)^2} + \frac{1}{\rho_*^2} + O(\rho_*^{-3}) (\theta_0)_* + O(\rho_*^{-3})dz_* + O(\rho_*^{-3})d\bar{z}_*. \]

Similarly from (23) we deduce
\[ \theta_1 = \frac{1}{2\pi} \rho_*^{-2} + A + O(\rho) \sqrt{2}dz + O(\rho^2)d\bar{z} + \left( -\frac{1}{\rho_*} \frac{1}{\sqrt{2}} \frac{z_*}{\rho_*^2} + O(\rho) \right) \theta_0 \]
\[ = \frac{1}{2\pi} \rho_*^2 + A + O(\rho_*^{-1}) \sqrt{2} \left( \frac{z_*(\theta_0)_* - \bar{\tau}_*dz_*}{(v_*^2)^2} \right) + O(\rho_*^{-2}) \left( \frac{\bar{\tau}_*(\theta_0)_* - v_*d\bar{z}_*}{(v_*^2)^2} \right) \]
\[ = \frac{1}{2\pi} \rho_*^2 + A - \frac{1}{\sqrt{2}} \frac{z_*}{(v_*^2)^2} + O(\rho_*^{-1}) \frac{\theta_0)_*}{\rho_*^2} + O(\rho_*^{-3})dz_* + O(\rho_*^{-3})d\bar{z}_*. \]

It is irrelevant to multiply the form \(\theta_1\) by a complex unitary factor, which we can choose to be \(-\frac{v_*}{\rho_*} := e^{i\varphi}\). In this way the new \(\theta_1\), which we will denote as \(\theta_n^1\) is given by
\[ \theta_n^1 = \left( -\frac{1}{\sqrt{2}} \frac{A z_* v_*}{\rho_*^6} + O(\rho_*^{-5}) \right) (\theta_0)_* + O(\rho_*^{-1})dz_* + \left( \frac{1}{\sqrt{2}} + A \frac{\bar{\tau}_*^2}{v_*^2} + O(\rho_*^{-3}) \right) dz_* + O(\rho_*^{-3})d\bar{z}_*. \]

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 \(\varphi\) is defined by
\[ i\varphi = \log \left( -\frac{\rho_*^2 \bar{\tau}_*}{v_*^2} \right) = \log (\rho^{-2}v^2\bar{\tau}^{-1}) = 2\log v - 2\log \rho - \log \bar{\tau}. \]

By elementary computations one finds
\[ \frac{i}{\bar{\tau}} \varphi = \frac{1}{\sqrt{2}} \frac{3 \bar{\tau}}{\rho_*^2}; \quad \partial_\varphi \varphi = -\frac{2}{\rho_*^4} |z_*|^2 \text{.} \]

Hence, using Proposition 6.5 one has
\[ d\varphi = \varphi_1 \theta^1 + \varphi \theta^2 + \varphi_0 \theta^3 \]
\[ = \frac{1}{\sqrt{2}} \frac{3 \bar{\tau}}{\rho_*^2} \sqrt{2}dz + 1 \frac{3z_* v_*}{\rho_*^4} \sqrt{2}d\bar{z} - 3 |z_*|^2 \rho_*^2 \theta_0 + O(\rho^3)dz + O(\rho^3)d\bar{z} + O(\rho^3) \theta_0. \]
By (27) and (31) we then obtain

\[ (\omega_n^1)_n = 6\pi Ai \frac{\overline{\tau}}{\rho^2} dz + 6\pi Ai \frac{z}{\rho^2} d\overline{\tau} - 12\pi Ai \frac{|z|^2}{\rho^2} \theta_0 + O(\rho)^2 dz + O(\rho^2) d\overline{\tau} + O(\rho) \theta_0. \]

From (28) and (30) one then gets

\[ 6\pi Ai \frac{\overline{\tau}}{\rho^2} dz + 6\pi Ai \frac{z}{\rho^2} d\overline{\tau} = -6\pi A \frac{z_s}{\rho_0^6} (|z_s|^2 + iz_s) dz_s - 6\pi A \frac{z_s}{\rho_0^6} (-|z_s|^2 + iz_s) d\overline{\tau}_s + 12i\pi A \frac{|z_s|^2}{\rho_0^6} (\theta_0)_s, \]

and the coefficient of \((\theta_0)_s\) cancels with

\[ -12\pi Ai \frac{|z|^2}{\rho^2} \theta_0 = -12\pi Ai \frac{|z_s|^2}{\rho_0^6} (\theta_0)_s. \]

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

\[ (\omega_n^1)_n = \left[ -6\pi A \frac{z_s}{\rho_0^6} (|z_s|^2 + iz_s) + O(\rho^{-4}) \right] dz_s + \left[ -6\pi A \frac{z_s}{\rho_0^6} (-|z_s|^2 + iz_s) + O(\rho^{-4}) \right] d\overline{\tau}_s + O(\rho^{-5})(\theta_0)_s. \]

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

\[ \theta = (1 + 4\pi A \rho^{-2} + O(\rho^{-3})) (\theta_0)_s + O(\rho^{-3}) dz_s + O(\rho^{-5}) d\overline{\tau}_s; \]

\[ \theta^1 = \left( -2\sqrt{2\pi} A \frac{z_s}{\rho_0^6} + O(\rho^{-5}) \right) (\theta_0)_s + O(\rho^{-4}) d\overline{\tau}_s + (1 + 2\pi A \rho^{-2} + O(\rho^{-3})) \sqrt{2} dz_s. \]

Notice that by (137) 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 (34), (35), 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 \((J_0, \theta_0 = \theta)\). Let \(B_{\rho_0}\) denote the Heisenberg ball of radius \(\rho_0\).

**Definition 2.1** A three dimensional pseudohermitian manifold \((N, J, \theta)\) is said to be asymptotically flat pseudohermitian if \(N = N_0 \cup N_{\infty}\), with \(N_0\) compact and \(N_{\infty}\) diffeomorphic to \(\mathbb{H}^1 \setminus B_{\rho_0}\), in which \((J, \theta)\) is close to \((J_0, \theta_0)\) in the sense that

\[ \theta = (1 + 4\pi A \rho^{-2} + O(\rho^{-3})) \theta_0 + O(\rho^{-3}) dz + O(\rho^{-5}) d\overline{\tau}; \]

\[ \theta^1 = O(\rho^{-3}) \theta_0 + O(\rho^{-4}) d\overline{\tau} + (1 + 2\pi A \rho^{-2} + O(\rho^{-3})) \sqrt{2} dz, \]

for some unitary coframe \(\theta^1\) 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

\[ \theta^1 = \left( -2\sqrt{2\pi} A \frac{z_s}{\rho_0^6} + O(\rho^{-4}) \right) \theta_0 + O(\rho^{-4}) d\overline{\tau} + (1 + 2\pi A \rho^{-2} + O(\rho^{-3})) \sqrt{2} dz; \]

and

\[ \omega^1 = \left[ -6\pi A \frac{z_s}{\rho_0^6} (|z|^2 + it) + O(\rho^{-4}) \right] dz + \left[ -6\pi A \frac{-|z|^2 + it}{\rho_0^6} + O(\rho^{-4}) \right] d\overline{\tau} + O(\rho^{-5}) \theta_0. \]
We look for an expansion of the vector field $Z_1$ of the type 

$$Z_1 = (1 + a) \mathring{Z}_1 + b \mathring{Z}_T + c \mathring{T}$$

(recall the notation in (12)). From the three relations 

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

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

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

we deduce that 

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

Similarly we obtain 

$$T = (1 - 4\pi A\rho^{-2} + O(\rho^{-3})) \mathring{T} + \left(2\sqrt{2}\pi A \frac{zv}{\rho^6} + O(\rho^{-4})\right) \mathring{Z}_1 + \left(2\sqrt{2}\pi A \frac{zv}{\rho^6} + O(\rho^{-4})\right) \mathring{Z}_T.$$

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

$$A_{11} = O(\rho^{-4}); \quad R = Z_1(\omega^1_1(Z_T)) - Z_T(\omega^1_1(Z_1)) + i\omega^1_1(T) + 2\omega^1_1(Z_1)\omega^1_1(Z_T).$$

Note that if we use $1 + O(\rho^{-2})$ as the $\sqrt{2}dz$-coefficient of $\theta^1$ in Definition 2.1, then only the real part of $O(\rho^{-2})$ (namely, $2\pi A\rho^{-2}$) is determined. But then the $\theta_0$-coefficient of $\omega^1_1$ 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 (2). Considering a one-parameter family of CR structures $J(s)$ and using the notation of Subsection 6.1.2, we have that 

$$\dot{J} = 2E = 2E_{11}\theta^1 \otimes Z_T + 2E_{TT}\theta^T \otimes Z_T.$$ 

Denoting by $R(s)$ the corresponding Tanaka-Webster curvature and using (140)-(141) we then find 

$$\frac{d}{ds}_{|s=0} \int_N R(s) \theta \wedge d\theta = \int_N R \theta \wedge d\theta$$

$$= \int_N \left[i (E_{11,TT} - E_{11,TT}) \right] \theta \wedge d\theta$$

$$= \int_N \left[i \left(E_{11,TT} - A_{11}E_{TT} + A_{TT}E_{11}\right)\right] \theta \wedge d\theta$$

$$= \int_N \left[i \left(E_{11,TT} - A_{11}E_{TT} + A_{TT}E_{11}\right)\right] \theta \wedge d\theta$$

$$= \int_N \left[i \omega^1_1 \wedge \theta - \int_N (A_{11}E_{TT} + \text{conj.}) \theta \wedge d\theta\right].$$

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 $(N, J, \theta)$ as

$$m(J, \theta) := i \int_{S_\Lambda} \omega^1_1 \wedge \theta := \lim_{\Lambda \to +\infty} i \int_{S_\Lambda} \omega^1_1 \wedge \theta,$$

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

14
Remark 2.4  By the above computations one finds
\[ \frac{d}{ds}_{|s=0} \left( \int_N R(s) \theta \wedge d\theta + m(J(s), \theta) \right) = \int_N (A_{11} E_{\overline{11}} + A_{\overline{11}} E_{11}) \theta \wedge d\theta, \]
which is the counterpart of (2), as desired. Apparently the definition of the p-mass depends on a choice of asymptotic coordinates and a (co)frame \( \theta \). 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 (20), then
\[ m(J, \theta) = 48 \pi^2 A. \]

**Proof.**  By (33) and some elementary estimates one finds
\[ m(J, \theta) = \oint_{\infty} i \omega_1 \wedge = -3i2\pi A \int_{\infty}^{\rho} [(|z|^2 \overline{\tau} + i\tau t) dz - (|z|^2 z - izt) d\overline{\tau}] \wedge \theta_0 - 6i\pi A \int_{S} (i\tau t dz + iztd\overline{\tau}) \wedge \theta_0, \]
where we have set \( S = \{ \rho = 1 \} \).

Using the relations
\[ (36) \quad z = r e^{i\varphi}; \quad dz = e^{i\varphi} (dr + ird\varphi); \quad \overline{z} dz - z d\overline{\tau} = 2ir^2 d\varphi, \]
we get
\[ m(J, \theta) = -6i\pi A \oint_{S} \left[ 2ir^2 d\varphi + 2tr dr \right] \wedge \theta_0 = 12 \pi A \oint_{S} \left[ r^4 d\varphi \wedge dt + tr (dr \wedge dt + 2r^2 dr \wedge d\varphi) \right] \]
\[ = 12 \pi A \oint_{S} \left( r^4 d\varphi \wedge dt + tr dr \wedge dt + 2tr^3 dr \wedge d\varphi \right). \]

On \( S \) we have \( 4r^3 dr + 2t dt = 0 \), so the last formula becomes
\[ m(J, \theta) = 12 \pi A \oint_{S} \left( r^4 d\varphi \wedge dt - r^2 dt \wedge d\varphi \right) = 12 \pi A \oint_{S} d\varphi \wedge dt = 48 \pi^2 A. \]

Therefore we obtain the conclusion. 

Let \( N \) be a three dimensional asymptotically flat pseudohermitian manifold: we derive next an integral formula for the p-mass.

**Proposition 2.6**  Let \( (N, J, \theta) \) be an asymptotically flat pseudohermitian manifold. Let \( \beta : N \rightarrow \mathbb{C} \) be such that
\[ (37) \quad \beta = \overline{\tau} + \beta_{-1} + O(\rho^{-2+\varepsilon}) \quad \text{near } \infty, \]
and
\[ (38) \quad \Box_b \beta = O(\rho^{-4}), \]
where \( \beta_{-1} \) is a term with the homogeneity of \( \rho^{-1} \) satisfying
\[ (39) \quad (\beta_{-1})_{\overline{T}} = -2\sqrt{2} \pi A \frac{1}{\rho^2} = \frac{\sqrt{2} A}{|\overline{z}|^2 + it}. \]
near infinity, where $\varepsilon \in (0, 1)$. Then one has

$$m(J, \theta) = -\int_N |\Box_b \beta|^2 \theta \land d\theta + 2 \int_N |\beta|_{\mathcal{P}}^2 \theta \land d\theta + 2 \int_N R|\beta|_{\mathcal{P}}^2 \theta \land d\theta + \frac{1}{2} \int_N P\beta \theta \land d\theta,$$

where

$$P\beta := \Box_b \Box_b \beta + 4i(A_{11}\beta)_{111}$$

is the CR Paneitz operator.

**Remark 2.7** We will show in Section 3 that it is indeed possible to find a solution of (38) satisfying (37) and condition (39).

**Proof.** By the commutation rules (13) we have that

$$\beta_{111} = \beta_{11} + i\beta_{10} - R\beta_{11}$$

Multiply by $\beta_{11}$ to obtain

$$\beta_{111} + R\beta_{11} = \beta_{111} + i\beta_{10} + (\beta_{11} - \beta_{111}) + i(\beta_{10} - i\beta_{101})$$

Integrating by parts we get

$$\int_N (\beta_{11} + R\beta_{111}) \beta_{11} \theta \land d\theta + \text{conj.} = i \int_N (Z_{11}) \beta_{11} \beta \land \theta \land d\theta + \text{conj.}.\int_N \omega_1^1(Z_{11}) \beta_{11} \beta \land \theta \land d\theta + \text{conj.}$$

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

$$i \int_N (Z_{11}) \beta_{11} \beta \land \theta \land d\theta + \text{conj.} = i \int_N Z_{11} \beta_{11} \beta \land (dt - 1zdz) + \text{conj.},$$

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

$$i \int_N \omega_1^1(Z_{11}) \beta_{11} \beta \land \theta \land d\theta + \text{conj.} = \frac{1}{2} m(J, \theta).$$

For the second divergence term in (41) and recalling the asymptotics of $\omega_1^1$ in Definition 2.1 we get

$$\int_N i(\beta_{11} + R\beta_{111}) \beta_{11} \theta \land d\theta + \text{conj.} = -\int_N \beta_{10} \beta \land \theta \land d\theta + \text{conj.}$$

$$\int_N i(\beta_{11} + R\beta_{111}) \beta_{11} \theta \land d\theta + \text{conj.} = -\int_N (T\beta_{11} + iA_{11}\beta_{111}) \beta \land \theta \land d\theta + \text{conj.}$$

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

$$-\int_N \frac{1}{4} (P\beta) \beta \land d\theta + \text{conj.} = -\int_N (\beta_{111} + iA_{11}\beta_{111}) \beta \land d\theta + \text{conj.}$$

and (from (13) and the identity $i\beta_{101} = \beta_{11} - \beta_{111}$)

$$-i \int_N \beta_{10} \beta \land d\theta + \text{conj.} = -i \int_N \beta_{111} \beta \land d\theta + \text{conj.}$$

16
We will show next the following two identities

\[
(43) \quad i \oint_{\infty} Z T^{\beta,T} \partial \tau \wedge (dt - i \partial \tau dz) + \text{conj.} = \frac{7}{12} m(J, \theta);
\]

\[
(44) \quad - \oint_{\infty} (T^{\beta,T} \bar{z} \sqrt{2} \partial \tau \wedge (dt - i \partial \tau dz) + \text{conj.} = -\frac{5}{12} m(J, \theta).
\]

To prove (43) we notice that (modulo \(O(\rho^{-3+\varepsilon})\))

\[
\beta^{T} = (1 - 2\pi A \rho^{-2}) \hat{\beta}^{T} (\tau) + (\beta_{-1})^{T} = \frac{1}{\sqrt{2}} - \sqrt{2} \pi A \rho^{-2} - 2 \sqrt{2} \pi A \frac{1}{\rho^{2}} - \frac{\sqrt{2} A}{|z|^{2} + it}
\]

By elementary computations one finds

\[
Z T^{\beta,T} = -3 \pi A z \frac{(it - |z|^{2})}{\rho^{6}} + \frac{2 A z (|z|^{2} - it)^{2}}{\rho^{8}} = \pi A z \tilde{\mathfrak{g}} + \frac{2 A z (|z|^{2} - it)^{2}}{\rho^{8}}
\]

where we have set

\[
\tilde{\mathfrak{g}} = 3 |z|^{2}; \quad \mathfrak{G} = -3.
\]

Then, by a scaling argument, we obtain

\[
i \oint_{\infty} Z T^{\beta,T} \partial \tau \wedge (dt - i \partial \tau dz) + \text{conj.} = \pi A \int_{S} \tilde{\mathfrak{g}} (|z|^{2} - it)^{2} d\phi \wedge dt
\]

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

\[
(45) \quad zd\tau + \partial \tau dz = 2r dr; \quad dz \wedge d\tau = 2ir d\phi \wedge dr
\]

we find

\[
i \oint_{\infty} Z T^{\beta,T} \partial \tau \wedge (dt - i \partial \tau dz) + \text{conj.} = 2 \pi A \int_{S} \tilde{\mathfrak{g}} (|z|^{2} - it)^{2} d\phi \wedge dt - 2 \pi A \int_{S} \mathfrak{G} t^{2} d\phi \wedge dt
\]

\[
+ 8 \pi A \int_{-1}^{1} \sqrt{1 - t^{2}} dt.
\]

Substituting for \(\tilde{\mathfrak{g}}\) and \(\mathfrak{G}\) we then get

\[
i \oint_{\infty} Z T^{\beta,T} \partial \tau \wedge (dt - i \partial \tau dz) + \text{conj.} = 24 \pi A + 8 \pi A \int_{-1}^{1} \sqrt{1 - t^{2}} dt = 28 \pi^{2} A = \frac{7}{12} m(J, \theta),
\]

which is (43).

To prove (44) instead we use the following formula, which can be obtained from the expansion of \(T\) in Remark 2.2

\[
T^{\beta,T} = 3 \sqrt{2} \pi A \frac{t}{\rho^{2}} + \frac{i A \sqrt{2}}{(|z|^{2} + it)^{2}} + O(\rho^{-5+\varepsilon})
\]

\[
= - \sqrt{2} \pi A \frac{t}{\rho^{2}} + \frac{i A \sqrt{2} (|z|^{2} - it)^{2}}{\rho^{8}} + O(\rho^{-5+\varepsilon}),
\]

17
where, using a notation similar to the previous one,
\[ \tilde{\mathbf{F}} = 0; \quad \tilde{\mathbf{G}} = 3. \]

Using again a scaling and elementary computations (some of which similar to those for the proof of (43)) one gets
\[
- \int_{\infty} \left( T_{\mathbf{\beta}} \mathbf{\tau} z \sqrt{2} d\mathbf{\tau} \wedge (dt - i \mathbf{\tau} dz) + \text{conj.} \right) = 2\pi A \int_S \left( \tilde{\mathbf{F}} t \mathbf{\tau} z \sqrt{2} d\mathbf{\tau} \wedge (dt - i \mathbf{\tau} dz) - \frac{1}{12} m(J, \theta) \right). \]

Exactly as for (45) and (47) we deduce
\[
- \int_{\infty} \left( T_{\mathbf{\beta}} \mathbf{\tau} z \sqrt{2} d\mathbf{\tau} \wedge (dt - i \mathbf{\tau} dz) + \text{conj.} \right) = 4\pi A \int_S \tilde{\mathbf{F}} |z|^2 d\varphi \wedge dt - 4\pi A \int_S \tilde{\mathbf{G}} t^2 d\varphi \wedge dt - \frac{1}{12} m(J, \theta), \]

which proves also (44).

Using all the above formulas and the fact that \( P \) is real we then obtain
\[
-2 \int |\beta_{1,1}|^2 \theta \wedge d\theta + 2 \int_N R|\beta_{1,1}|^2 \theta \wedge d\theta = \frac{2}{3} m(J, \theta) - 2 \int_N |\beta_{1,1}|^2 \theta \wedge d\theta + 2 \int_N |\beta_{1,1}|^2 \theta \wedge d\theta - \frac{1}{2} \int_N \beta(P\beta) \theta \wedge d\theta. \]

Since \( \square_{b} = -2\beta_{1,1} \), we finally get the conclusion.

### 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
\[
(f_1 \ast f_2)(Z) = \int_{\mathbb{H}^1} f_1(ZW^{-1})f_2(W)dW = \int_{\mathbb{H}^1} f_1(W)f_2(W^{-1}Z)dW; \quad Z = (z, t), \quad W = (w, s), \]

with
\[
W^{-1}Z = (z - w, t - s - 2 \text{ Im } \mathbf{\tau} w); \quad dW = \left( \mathbf{\theta} \wedge d\mathbf{\tau} \right)(W), \]

see the notation in Subsection 1.1.

By the solvability theory of \( \square_{b} \) in \( \mathbb{H}^1 \) (see Chapter 10 in [16]) we have that
\[
(48) \quad \square_{b} K = K \square_{b} = I d - \mathcal{S} \quad \text{ on } L^2(\mathbb{H}^1), \]

where \( \mathcal{S} \) is the Szegö projection
\[
\mathcal{S} h = \lim_{\epsilon \to 0} \frac{1}{4\pi^2} h * \eta_{\epsilon}^{-2}; \quad \eta_{\epsilon} = |z|^2 + \epsilon^2 - it, \]

and where
\[
\mathcal{K} h = h * \Phi; \quad \Phi = \frac{1}{8\pi^2} \log \left( \frac{|z|^2 - it}{|z|^2 + it} \right) (|z|^2 - it)^{-1}. \]
Define now

\[ f = 4\pi A \frac{|z|^2 + it}{\rho^6}, \]

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

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

Our next goal is to find a function \( \beta_{-1} \) which has the homogeneity of \( \rho^{-1} \) near infinity and such that

\[ \Box_b \beta_{-1} = -\chi f \quad \text{near infinity}. \]

This function will be useful to solve (38) and to determine the asymptotics of a function \( \beta \) as in Proposition 2.6. We can exhibit indeed two functions \( \hat{g} \) and \( \tilde{g} \) which satisfy

\[ \Box_b g = -4\pi A \frac{|z|^2 + it}{\rho^6} \quad \text{in } \mathbb{H}^1 \]

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

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

and

\[ \tilde{g}(z,t) = -4i\pi A \frac{\rho^2}{vz} \quad \text{for } z \neq 0, \]

where we have set

\[ v = v(z,t) = t + i|z|^2. \]

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 solution \( \beta \) of

\[ \Box_b \beta = O(\rho^{-1}) \quad \text{on } N \]

satisfying (37). More precisely, if \( \varepsilon \in (0,1) \) and if \( f \) is as in (49), we can choose \( \beta_{-1} \) so that

\[ \beta_{-1} = \mathcal{K}(-\chi f) + O(\rho^{-2+\varepsilon}) \quad \text{for } \rho \text{ large}, \]

and

\[ (\beta_{-1})_T = -2\sqrt{2} \pi A \frac{1}{\rho^2} - \frac{\sqrt{2} A}{|z|^2 + it} \]

near infinity. Moreover, if \( N \) is the blow-up of an embeddable compact three dimensional CR manifold with \( \mathcal{V}(J) > 0 \), then there exists a \( C^\infty \)-smooth solution \( \beta \) of \( \Box_b \beta = 0 \) satisfying (37).

The proof of Proposition 3.1 is given in the next three subsections.
3.1 Expansion of \( \Box_b \mathcal{F} \) near infinity

To study equation (38), we begin finding a correction to \( \mathcal{F} \) by evaluating first \( \Box_b \) on \( \mathcal{F} \). The following asymptotic expansion holds.

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

\[
\Box_b \mathcal{F} = 4 \pi A \frac{\mathcal{F}}{\rho^6} (|z|^2 + i t) + O(\rho^{-4}) \quad \text{near infinity.}
\]

**Proof.** We want to express \( Z_1 \) in asymptotic coordinates, recalling that

\[
\frac{\partial}{\partial z_{1}} \left( \frac{\partial}{\partial \rho} \right) = \frac{1}{\sqrt{2}} \left( \frac{\partial}{\partial \rho} + iz \frac{\partial}{\partial t} \right) \quad \text{and} \quad \omega_1 = 0.
\]

Recall also that, from the expansions in Section 2

\[
\theta = (1 + 4 \pi A \rho^{-2} + O(\rho^{-3})) \theta_0 + O(\rho^{-3}) dz + O(\rho^{-3}) d\tau,
\]

\[
\theta_1 = \left( 2 \sqrt{2} \pi A \frac{\mathcal{F}}{\rho^6} + O(\rho^{-5}) \right) \theta_0 + O(\rho^{-4}) d\tau + (1 + 2 \pi A \rho^{-2} + O(\rho^{-3})) \sqrt{2} dz.
\]

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

\[
Z_1 Z_T + \omega_1 (Z_1) Z_T = \left[ (1 + a) \frac{\partial}{\partial z_{1}} + b \frac{\partial}{\partial \rho} + c \frac{\partial}{\partial \tau} \right] \left[ (1 + a) \frac{\partial}{\partial z_{1}} + b \frac{\partial}{\partial \rho} + c \frac{\partial}{\partial \tau} \right] + \omega_1 (Z_1) Z_T
\]

\[
= \hat{Z}_1 \hat{Z}_T + (\hat{Z}_1 a) \hat{Z}_T + 2a \hat{Z}_1 \hat{Z}_T + \omega_1 (Z_1) Z_T + R_{\Box_b},
\]

where the remainder term \( R_{\Box_b} \) satisfies

\[
R_{\Box_b} = O(\rho^{-4}) \frac{\partial}{\partial z_{1}} + O(\rho^{-4}) \frac{\partial^2}{\partial \rho^2} + O(\rho^{-4}) \frac{\partial}{\partial \rho} + O(\rho^{-5}) \frac{\partial^2}{\partial \rho \partial \tau} + O(\rho^{-5}) \frac{\partial^2}{\partial \tau^2}.
\]

Recall that, by Definition 2.1 one has

\[
\omega_1 = \left[ -\frac{\pi A \sqrt{2}}{\rho^6} + O(\rho^{-4}) \right] dz + \left[ \frac{\sqrt{2}}{\rho^6} + O(\rho^{-4}) \right] d\tau + O(\rho^{-5}) \theta_0,
\]

where

\[
g_{-3} = \frac{\pi A \sqrt{2}}{\rho^6} (|z|^2 - 3i t).
\]

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

\[
\frac{\partial}{\partial z_{1}} a + O(\rho^{-4}) = -2 \pi A \frac{\partial}{\partial \rho} - \frac{1}{\sqrt{2}} \frac{\partial}{\partial \tau} + O(\rho^{-4}) = 2 \pi A \frac{1}{\sqrt{2}} \frac{\partial}{\partial \rho} + O(\rho^{-4}),
\]

we obtain the expansion

\[
\mathcal{E} = -4a \hat{Z}_1 \hat{Z}_T - 2(\hat{Z}_1 a) \hat{Z}_T + 2g_{-3} \hat{Z}_T - 2R_{\Box_b}
\]

\[
= 8 \pi A \rho^{-2} \hat{Z}_1 \hat{Z}_T - 4 \pi A \frac{1}{\sqrt{2}} \frac{\partial}{\partial \rho} \hat{Z}_T + 2g_{-3} \hat{Z}_T - 2R_{\Box_b}
\]

\[
= 8 \pi A \rho^{-2} \hat{Z}_1 \hat{Z}_T + 2 \sqrt{2} \pi A \frac{\mathcal{F}}{\rho^6} (|z|^2 + i t) \hat{Z}_T - 2R_{\Box_b}
\]

\[
= 8 \pi A \rho^{-2} \hat{Z}_1 \hat{Z}_T + 4 \sqrt{2} \pi A \frac{\mathcal{F}}{\rho^6} (|z|^2 + i t) \hat{Z}_T - 2R_{\Box_b}.
\]

Applying this operator to the function \( \mathcal{F} \) we have that

\[
(57) \quad \mathcal{E} \mathcal{F} = 8 \pi A \rho^{-2} \hat{Z}_1 (1 + 4 \pi A \frac{\mathcal{F}}{\rho^6} (|z|^2 + i t) + O(\rho^{-4}) = 4 \pi A \frac{\mathcal{F}}{\rho^6} (|z|^2 + i t) + O(\rho^{-4}),
\]

which gives the desired conclusion. \( \blacksquare \)
3.2 Existence of a solution to $\Box_b \beta = 0$ and proof of (55)

In this Section we will prove the existence part under the stronger assumption that $N$ is a blow-up as in the statement. For the general situation, see Remark 3.8.

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

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

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

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

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

Since

$$\hat{Z}_T \left( \frac{1}{z} \right) = 0; \quad \hat{Z}_T \left( \frac{\rho^2}{u z} \right) = \rho^{-2}$$

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

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

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

We then compute

$$-(S\hat{f})(Z) = -\frac{1}{4\pi^3} \lim_{\epsilon \to 0} \int_{\mathbb{H}^1} \hat{f}(W) \eta^{-2}_e (W^{-1} Z) dW = -\frac{1}{2\pi^2} \lim_{\epsilon \to 0} \int_{\mathbb{H}^1} (\chi \hat{g})_\tau (W) \eta^{-2}_e (W^{-1} Z) dW$$

$$= -\frac{1}{2\pi^2} \lim_{\epsilon \to 0} \int_{\mathbb{H}^1} ((\chi \hat{g})_\tau (W) \eta^{-2}_e (W^{-1} Z))_1 dW + \frac{1}{2\pi^2} \lim_{\epsilon \to 0} \int_{\mathbb{H}^1} (\chi \hat{g})_\tau (W) (\eta^{-2}_e (W^{-1} Z))_1 dW$$

$$= -\frac{1}{2\pi^2} \lim_{\epsilon \to 0} \int_{\mathbb{H}^1} ((\chi \hat{g})_\tau (W) \eta^{-2}_e (W^{-1} Z))_1 dW.$$

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

$$\int_{\mathbb{H}^1} \hat{\Box}_b (\chi \hat{g}) \eta^{-2}_e (W^{-1} Z) dW$$

$$= i \frac{1}{2\pi^2} \lim_{\epsilon \to 0} \left[ \int_{t=0}^{\epsilon} (\hat{g})_\tau (W) \eta^{-2}_e (W^{-1} Z) (\theta \wedge \theta^\tau)(W) - \int_{t=0}^{\epsilon} (\hat{g})_\tau (W) \eta^{-2}_e (W^{-1} Z) (\theta \wedge \theta^\tau)(W) \right]$$

$$= \frac{1}{2\pi^2} \lim_{\epsilon \to 0} \left[ \int_{t=0}^{\epsilon} (\hat{g})_\tau (W) \eta^{-2}_e (W^{-1} Z) \frac{\overline{\tau}}{\sqrt{2}} dW \wedge d\overline{w} - \int_{t=0}^{\epsilon} (\hat{g})_\tau (W) \eta^{-2}_e (W^{-1} Z) \frac{\tau}{\sqrt{2}} dW \wedge d\overline{w} \right].$$

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

$$\eta^{-2}_e (W^{-1} Z) = O(\rho^{-4}) (Z) \quad \text{for } W \text{ in any given compact set of } \mathbb{H}^1.$$  

The last two formulas then imply

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

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

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

which is the desired conclusion. ■
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 \( \alpha \) is a multi-index and \( \mathcal{Z}^{(\alpha)} \) is a composition of \( Z_1 \) and \( Z_T \) derivatives of order \( |\alpha| \), and where \( C_{\alpha,u} \) is a positive constant depending on \( \alpha \) and \( u \). The main tool to prove the existence part in Proposition 3.1 is the next result (notice that in [27] a different convention for \( \theta \) is used). Define

\[
\square_{b,1} := G_p^2 \square_b; \quad m_1 := G_p^{-2} \theta \wedge d\theta.
\]

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

**Theorem 3.4** (Theorem 1.3 and Theorem 1.4 in [27]) Suppose \( N \) is the blow-up of an embeddable compact three dimensional CR manifold with \( \mathcal{Y}(J) > 0 \). Then

\[
\square_{b,1} : \text{Dom}(\square_{b,1}) \subseteq L^2(m_1) \rightarrow L^2(m_1)
\]

has closed range, and the following decomposition holds

\[
\square_{b,1} K_N + \mathcal{S}_N = \text{Id} \quad \text{on } L^2(m_1),
\]

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

\[
K_N : \mathcal{E}(\rho^{2-\varepsilon}) \rightarrow \mathcal{E}(\rho^{-\varepsilon}); \quad \mathcal{S}_N : \mathcal{E}(\rho^{2-\varepsilon}) \rightarrow \mathcal{E}(\rho^{2-\varepsilon})
\]

and hence there holds

\[
\square_{b,1} K_N + \mathcal{S}_N = \text{Id} \quad \text{on } \mathcal{E}(\rho^{2-\varepsilon}).
\]

**Remark 3.5** Note that \( \square_b \) may not have \( L^2 \) closed range with respect to the volume form \( \theta \wedge d\theta \). This causes difficulty to solve the \( \square_b \) equation directly. In [27] the authors introduce the above weighted Kohn Laplacian \( \square_{b,1} \) and show that \( \square_{b,1} \) has \( L^2 \) closed range with respect to the weighted volume form \( m_1 \).

We apply Theorem 3.4 with

\[
h = -\square_{b,1}(\chi^\square + \mathcal{K}(-\chi f)).
\]

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 \( h \in \mathcal{E}(\rho^\mu) \) and hence we can find \( u = K_N h \in \mathcal{E}(\rho^{-2+\varepsilon}) \) such that \( \square_{b,1} u = h \) (note that \( \mathcal{S}_N h = 0 \), see Theorem 1.5 in [27]). Therefore the function

\[
\beta = \chi^\square + \mathcal{K}(-\chi f) + u
\]

is a solution of \( \square_{b,1} \beta = 0 \), hence \( \square_b \beta = 0 \) (see also the deduction in the introduction of [27]). By scaling arguments, one finds that \( \mathcal{K}(\chi f) \) is the sum of a function with the homogeneity of \( \rho^{-1} \) and a function of order \( \rho^{-2+\varepsilon} \), and therefore we deduce (55).

### 3.3 Proof of (56)

Since

\[
(\tilde{g})_\square = -2\sqrt{2}\pi A \frac{1}{\rho^\mu} \quad (z \neq 0)
\]

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

\[
(\mathcal{K}(-\chi f))_\square + \frac{\sqrt{2}A}{|z|^2 + \varepsilon} = (\tilde{g})_\square + O(\rho^{-3}) \quad \text{for } z \neq 0 \text{ and } \rho \text{ large}.
\]

\[
(\mathcal{K}(-\chi f))_\square + \frac{\sqrt{2}A}{|z|^2 + \varepsilon} = (\tilde{g})_\square + O(\rho^{-3}) \quad \text{for } z \neq 0 \text{ and } \rho \text{ large}.
\]
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

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

for any test function $\varphi \in C_0^\infty(\mathbb{H}^1)$. We have now the following result.

**Lemma 3.6** If $\tilde{g}$ is defined as in (53) then one has

$$(59) \quad \Box_b \tilde{g} = -\tilde{f} - 4\sqrt{2} i \pi^2 A \frac{\rho^2}{v} Z_1 \delta_{\{z = 0\}} \quad \text{in the distributional sense of } \mathbb{H}^1 \setminus \{0\}.$$

**Proof.** We have

$$(60) \quad Z_1 \tilde{g} = -4i \pi A Z_1 \left( \frac{\rho^2}{v} \right) \frac{1}{z} - 4i \pi A \frac{\rho^2}{v} Z_1 \left( \frac{1}{z} \right).$$

We next notice that, for any function $\varphi \in C_0^\infty(\mathbb{H}^1)$

$$(Z_1 \frac{1}{z}, \varphi) = \langle \frac{1}{z}, Z_1 \varphi \rangle = \langle \frac{1}{z}, -Z_1 \varphi \rangle = \frac{1}{\sqrt{2}} \int_{\mathbb{H}^1} \log |z|^2 \left| \partial \varphi + iz \partial t \varphi \right| \wedge \frac{\partial z}{\partial \theta} = \frac{1}{\sqrt{2}} \int_{\mathbb{H}^1} \log |z|^2 \langle \partial \varphi, \varphi \rangle$$

$$= \frac{1}{\sqrt{2}} \cdot 4 \pi \langle \delta_{\{z = 0\}}, \varphi \rangle = \pi \frac{1}{\sqrt{2}} \langle \delta_{\{z = 0\}}, \varphi \rangle.$$

Therefore by (60) we have

$$Z_1 \tilde{g} = -4i \pi A Z_1 \left( \frac{\rho^2}{v} \right) \frac{1}{z} + 4 \pi \langle \delta_{\{z = 0\}}, \varphi \rangle = \frac{1}{\sqrt{2}} \frac{i \pi}{2} Z_1 \delta_{\{z = 0\}} (z, t \neq (0, 0)).$$

Using the (distributional) formulas

$$Z_1 \frac{1}{z} = \frac{1}{\sqrt{2}} \frac{1}{z^2}, \quad Z_1 \left( \frac{\rho^2}{v} \right) = -\frac{i}{\sqrt{2}} \frac{z(t - i |z|^2)}{\rho^0}$$

and the fact that $\pi \delta_{\{z = 0\}} = 0$ we find

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

$$= -\tilde{f} - 4\sqrt{2} i \pi^2 A \frac{\rho^2}{v} Z_1 \delta_{\{z = 0\}} (z, t \neq (0, 0)),$$

which is the desired conclusion. 

The previous lemma implies clearly that

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

where $\tau$ is a distribution with compact support $A_\tau$.

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

$$\chi_j(\rho) = 1 \quad \text{for } \rho \leq j; \quad \chi_j(\rho) = 0 \quad \text{for } \rho \geq j + 1,$$
and another sequence of nondecreasing cutoff functions \( \tilde{\chi}_j = \tilde{\chi}_j(|z|) \) satisfying
\[
\tilde{\chi}_j(|z|) = 1 \quad \text{for} \quad |z| \geq \frac{1}{j}; \quad \tilde{\chi}_j(|z|) = 0 \quad \text{for} \quad |z| \leq \frac{1}{2j}.
\]
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
\[
\hat{\rho}_b \tilde{g}_j = -\chi_j\hat{\rho} + \zeta_j + \xi_j,
\]
where \( \zeta_j \) is a sequence of functions supported in \( \{|1 \leq \rho \leq j + 1\} \cap \{|z| \leq 1/j\} \) satisfying
\[
\zeta_j \xrightarrow{D^*} -4\sqrt{2}it A\rho^2 \delta_{\{z=0\}},
\]
on every open bounded set of \( \mathbb{H}^1 \) which does not intersect \( \{\rho \geq 2\} \), and where \( \xi_j \) 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
\[
\left(\frac{Z}{T}\right)(\mathcal{K}(\hat{\rho}_b \tilde{g}_j))(Z) = \int_{\mathbb{H}^1} (\hat{\rho}_b \tilde{g}_j)(W) \left(\frac{Z}{T}\right) \Phi(W^{-1}Z)dW = \int_{\mathbb{H}^1} (\chi_j\hat{\rho})(W) \left(\frac{Z}{T}\right) \Phi(W^{-1}Z)dW
\]
\[
+ \int_{\mathbb{H}^1} \zeta_j(W) \left(\frac{Z}{T}\right) \Phi(W^{-1}Z)dW + \int_{\mathbb{H}^1} \xi_j(W) \left(\frac{Z}{T}\right) \Phi(W^{-1}Z)dW.
\]

**Lemma 3.7** The following three formulas hold
\[
\int_{\mathbb{H}^1} (\chi_j\hat{\rho})(W) \left(\frac{Z}{T}\right) \Phi(W^{-1}Z)dW = Z\mathcal{K}(\chi)(Z) + o_j(1)O(\rho^{-3});
\]
\[
\int_{\mathbb{H}^1} \zeta_j(W) \left(\frac{Z}{T}\right) \Phi(W^{-1}Z)dW = \frac{\sqrt{2}A}{|z|^2 + it} + O(\rho^{-3}) + o_j(1);
\]
\[
\int_{\mathbb{H}^1} \xi_j(W) \left(\frac{Z}{T}\right) \Phi(W^{-1}Z)dW = O(\rho^{-3}) + o_j(1).
\]

**Proof.** To prove (64) we notice that clearly
\[
\left(\frac{Z}{T}\right)(\mathcal{K}(\chi_j\hat{\rho}_b \tilde{g}_j))(Z) = \int_{\mathbb{H}^1} (\chi_j\hat{\rho})(W) \left(\frac{Z}{T}\right) \Phi(W^{-1}Z)dW
\]
\[
+ \int_{\mathbb{H}^1} ((1 - \chi_j)\hat{\rho})(W) \left(\frac{Z}{T}\right) \Phi(W^{-1}Z)dW,
\]
so it is sufficient to show
\[
\int_{\mathbb{H}^1} ((1 - \chi_j)\hat{\rho})(W) \left(\frac{Z}{T}\right) \Phi(W^{-1}Z)dW = o_j(1)O(\rho^{-3}).
\]
We first notice that
\[
\left(\frac{Z}{T}\right) \Phi(W^{-1}Z) = \frac{\sqrt{2}}{8\pi^2} \frac{w - z}{(\rho(W^{-1}Z))^3} = O(\rho^{-3}(W^{-1}Z)),
\]
which implies
\[
\left| \int_{\mathbb{H}^1} ((1 - \chi_j)\hat{\rho})(W) \left(\frac{Z}{T}\right) \Phi(W^{-1}Z) \right| \leq C \int_{\rho(W) \geq j} (\rho(W))^{-3}(\rho(W^{-1}Z))^{-3}dW.
\]
By a scaling argument one shows that
\[
\int_{\{\rho(W) \geq \varepsilon\}} (\rho(W))^{-3} (\rho(W^{-1}Z)^{-3} dW \leq C(\rho(Z))^{-2} \int_{\{\rho(W) \geq \frac{1}{\pi^2}\}} (\rho(W))^{-6} dW \leq \frac{C}{j} (\rho(Z))^{-3},
\]
giving (64). Recalling the properties of the support of \(\zeta_j\), we can write that
\[
\int_{\mathbb{H}^1} \xi_j(W) \frac{Z}{Z} \Phi(W^{-1}Z) dW = \int_{\{1 \leq \rho(W) \leq 2\}} \xi_j(W) \frac{Z}{Z} \Phi(W^{-1}Z) dW + \int_{\{2 \leq \rho(W) \leq 2\}} \xi_j(W) \frac{Z}{Z} \Phi(W^{-1}Z) dW.
\]
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
\[
\left| \int_{\{1 \leq \rho(W) \leq 2\}} \xi_j(W) \frac{Z}{Z} \Phi(W^{-1}Z) dW \right| \leq C \int_{\{1 \leq \rho(W) \leq 2\}} (\rho(W^{-1}Z)^{-3} dW = O((\rho(Z))^{-3}),
\]
which gives (66).

It remains to show (65). In this case, we divide the integral into the three regions
\[\mathcal{A}_1 = \{1 \leq \rho \leq 4\}; \quad \mathcal{A}_2 = \{4 \leq \rho \leq j\}; \quad \mathcal{A}_3 = \{j \leq \rho \leq j + 1\}.
\]
Using scaling arguments similar to the previous ones, (62), and the fact that
\[
\frac{(W)}{Z} \frac{(Z)}{Z} \Phi(W^{-1}Z) = -\frac{1}{8\pi^2 (\rho(w)^2 + i(t - s - 2\text{Im}(w)))^2},
\]
we easily obtain
\[
\left| \int_{\mathcal{A}_1} \zeta_j(W) \frac{Z}{Z} \Phi(W^{-1}Z) dW \right| = O((\rho(Z))^{-3}); \quad \left| \int_{\mathcal{A}_2} \zeta_j(W) \frac{Z}{Z} \Phi(W^{-1}Z) dW \right| = o_j(1).
\]
On the other hand, from (62) and some elementary estimates one finds
\[
\int_{\mathcal{A}_2} \zeta_j(W) \frac{Z}{Z} \Phi(W^{-1}Z) dW = -4\sqrt{2}i\pi^2 A \int_{\mathcal{A}_2} \frac{\rho^2}{w} \frac{(W)}{Z} \frac{(Z)}{Z} \Phi(W^{-1}Z) dW + o_j(1).
\]
Using the facts that
\[
Z_1 \left( \frac{\rho^2}{s + i|w|^2} \right) = -i \frac{1}{\sqrt{2}} \frac{\text{Im}(s - i|w|^2)}{\rho^6} = 0; \quad \frac{\rho^2}{s + i|w|^2} = \begin{cases} 1, & \text{for } s > 0; \\ -1, & \text{for } s < 0, \end{cases}
\]
if \(w = 0\),
we deduce
\[
\int_{\mathcal{A}_2} \zeta_j(W) \frac{Z}{Z} \Phi(W^{-1}Z) dW = -4\sqrt{2}i\pi^2 A \int_{\mathcal{A}_2} \frac{\rho^2(W)}{s + i|w|^2} \left( \frac{(W)}{Z} \frac{(Z)}{Z} \Phi(W^{-1}Z) \right) dW + o_j(1)
\]
\[
= 4\sqrt{2}i\pi^2 A \int_{\mathcal{A}_2} \delta_{w=0} \left\{ \frac{s}{|s|} \frac{(W)}{Z} \frac{(Z)}{Z} (\Phi(W^{-1}Z)) \right\} dW + o_j(1).
\]
Using also the identity
\[
\frac{(W)}{Z} \frac{(Z)}{Z} \Phi(W^{-1}Z) = -\frac{1}{8\pi^2 (|z|^2 + i(t - s))^2},
\]
for \(w = 0\),
we then find

\[
\int_{A_2} \zeta_j(W) \overline{Z} \Phi(W^{-1} Z) dW = -\frac{\sqrt{2}}{2} i A \int_1^j \frac{1}{(|z|^2 + i(t-s))^2} ds + \frac{\sqrt{2}}{2} i A \int_{-j}^{-4} \frac{1}{(|z|^2 + i(t-s))^2} ds + o_j(1)
\]

which gives (65). □

Summing up, by (63) and Lemma 3.7 we obtained that

\[
Z_1(\mathcal{K}(\tilde{\beta} \tilde{g}_j)) = Z_1(\mathcal{K}(-\chi f)) + \frac{\sqrt{2} A}{|z| + i t} + O(\rho^{-3}) + o_j(1).
\]

Since \( \mathcal{K} \tilde{\beta} = Id - S \) on distributions with compact support and since the image of the Szegő projection consists of CR functions, by Lemma 3.3 we deduce that for \( z \neq 0 \)

\[
Z_1(\tilde{g}_j) = Z_1(\mathcal{K}(-\chi f)) + \frac{\sqrt{2} A}{|z| + i t} + O(\rho^{-3}) + o_j(1).
\]

Letting \( j \to +\infty \), this means

\[
Z_1(\tilde{g}) = Z_1(\mathcal{K}(\chi f)) + \frac{\sqrt{2} A}{|z| + i t} + O(\rho^{-3}) \quad \text{for } z \neq 0 \text{ and } \rho \text{ large}.
\]

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

**Remark 3.8** Under the more general assumption of Proposition 3.1, it is sufficient to apply all the above arguments except for Theorem 3.4, which allows to pass from a solution of \( \square_b = O(\rho^{-4}) \) to a solution of \( \square_b \beta = 0 \).

### 3.4 The role of positivity of the Paneitz operator

We prove here that the positivity of \( P \) on the compact manifold implies positivity of the last term in (40) 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 [27].

**Proposition 3.9** Let \( N \) be the blow-up of a three dimensional CR manifold with positive Tanaka-Webster invariant and non-negative CR Paneitz operator. Let \( \beta \) be as in Proposition 2.6: then one has

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

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

\[
\frac{4}{3} m(J, \theta) \geq -\int_N |\square_b \beta|^2 \wedge d\theta + 2 \int_N |\beta_{-1} + \beta_{-2+\varepsilon} + \overline{\theta}|^2 \wedge d\theta + 2 \int_N R|\beta_1|^2 \wedge d\theta.
\]

Moreover, if \( \theta \) is chosen as in (4) and \( \beta \) is chosen so that \( \square_b \beta = 0 \) (this can be achieved by Proposition 3.1), then \( R = 0 \) and the above inequality is reduced to

\[
\frac{4}{3} m(J, \theta) \geq 2 \int_N |\beta_{-1}|^2 \wedge d\theta \geq 0.
\]
We write the Paneitz operator $P\psi = 4(\psi_{111} + iA_{111}\psi_{1})_{\Gamma}$ as

$$P = P_{3} \circ \overline{\partial}_{b} \quad \text{or} \quad P = \partial_{\theta}^{*} \circ \tilde{P}_{3},$$

where

$$P_{3}(a_{1}\theta^{i}) = 4(a_{1,11} + iA_{11}a_{1})_{\overline{i}},$$

and

$$\tilde{P}_{3}(\psi) = 4(\psi_{111} + iA_{111}\psi_{1})\theta^{1}.$$ 

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

$$\int_{N} [(\overline{\beta} - \overline{\eta}) + \beta_{1} + \beta_{2+\varepsilon}] P(\beta_{-1} + \beta_{2+\varepsilon} + u) \theta \wedge d\theta$$

$$= \int_{N} [(z - u) + \overline{\beta}_{-1} + \overline{\beta}_{2+\varepsilon} + u] P(\beta_{-1} + \beta_{2+\varepsilon} + u) \theta \wedge d\theta. $$

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

$$\int_{N} [(\overline{\beta} - \overline{\eta}) + \beta_{-1} + \beta_{2+\varepsilon} + u] P(\beta_{-1} + \beta_{2+\varepsilon} + u) \theta \wedge d\theta$$

$$= - \int_{N} (\beta_{-1} + \beta_{2+\varepsilon} + u)_{\overline{T}} \tilde{P}_{3}(\beta_{-1} + \beta_{2+\varepsilon} + u) \theta \wedge d\theta + \int_{\infty} z \tilde{P}_{3}\beta_{1} \theta \wedge \theta^{1}. $$

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

$$\int_{\infty} z \tilde{P}_{3}\beta_{1} \theta \wedge \theta^{1} = \int_{\infty} z \tilde{P}_{3}\beta_{1} \theta \wedge \theta^{1} = \int_{\infty} z \tilde{P}_{3}\beta_{1} \theta \wedge \theta^{1}. $$

Using the Stokes theorem again, we find

$$\int_{\infty} z \tilde{P}_{3}\beta_{1} \theta \wedge \theta^{1} = \int_{N} (z - u) + \overline{\beta}_{-1} + \overline{\beta}_{2+\varepsilon} + u) P(\beta_{-1} + \beta_{2+\varepsilon} + u) \theta \wedge d\theta$$

$$+ \int_{N} (\overline{\beta}_{-1} + \overline{\beta}_{2+\varepsilon} + u)_{\overline{T}} \tilde{P}_{3}(\beta_{-1} + \beta_{2+\varepsilon} + u) \theta \wedge d\theta. $$

From the last formulas we deduce

$$\int_{N} \beta P \overline{\theta} \wedge d\theta = \int_{N} (\overline{\beta}_{-1} + \overline{\beta}_{2+\varepsilon} + u) P(\beta_{-1} + \beta_{2+\varepsilon} + u) \theta \wedge d\theta$$

$$+ \int_{\infty} z \tilde{P}_{3}\beta_{1} (dt - i\overline{\theta}dz + izd\overline{\theta}) \wedge \sqrt{2}dz. $$

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

$$\int_{\infty} \tilde{P}_{3}\beta_{1} \cdot z (dt - i\overline{\theta}dz + izd\overline{\theta}) \wedge \sqrt{2}dz = \int_{\infty} 4(\beta_{-1})_{\overline{T}1}(i\sqrt{2}zdz \wedge dz - \sqrt{2}z^{2}d\overline{\theta} \wedge dz). $$

27
By our choice of $\beta_{-1}$ we have that

$$-2(\beta_{-1})_{\Pi_1} = \bar{\beta}_{-1} = -4\pi A \frac{\bar{\theta}}{\rho^6} \{ |z|^2 + it \} + O(\rho^{-4}),$$

and moreover

$$(\partial_z + i \bar{\tau} \mathcal{D}_t) \left[ \frac{\bar{\theta}}{\rho^6} \{ |z|^2 + it \} \right] = -3\bar{\tau}^2 (|z|^2 + it)^2 \rho^{-6},$$

so we find

$$4(\beta_{-1})_{\Pi_1} = -12\sqrt{2} A \bar{\tau}^2 \{ |z|^2 + it \}^2 \rho^{10}. $$

Inserting this expression into the boundary formula we get

$$4 \oint_{\infty} (\beta_{-1})_{\Pi_1} (i \sqrt{2} z dt \wedge dz - \sqrt{2} \bar{z}^2 d\bar{\tau} \wedge dz) = -12\sqrt{2} \oint_{\infty} \pi A \{ |z|^4 - t^2 + 2it|z|^2 \} \rho^{-10} \bar{\tau}^2 (i \sqrt{2} z dt \wedge dz - \sqrt{2} \bar{z}^2 d\bar{\tau} \wedge dz) = -24\pi A \int_S \{ |z|^4 - t^2 + 2it|z|^2 \} \bar{\tau}^2 (iz dt \wedge dz - z^2 d\tau \wedge dz).$$

Using the fact that $r^4 + t^2 = 1$ on $S$ and the relations

$$dz \wedge d\bar{z} = -2i r dr \wedge d\phi; \quad dt \wedge dz = ire^{i\varphi} dt \wedge d\varphi,$$

one finds

$$4 \oint_{\infty} (\beta_{-1})_{\Pi_1} (i \sqrt{2} z dt \wedge dz - \sqrt{2} \bar{z}^2 d\bar{\tau} \wedge dz) = -24\pi A \int_S \{ |z|^4 - t^2 + 2it|z|^2 \} r^2 (-r^2 dt \wedge d\varphi - 2ir^3 dr \wedge d\phi) = -24\pi A \int_S \{ |z|^4 - t^2 + 2it|z|^2 \} (r^2 d\varphi \wedge dt + 2ir^5 d\varphi \wedge dr) = -24\pi A \int_S \{ |z|^4 - t^2 + 2it|z|^2 \} (r^4 d\varphi \wedge dt - ir^2 td\varphi \wedge dt).$$

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 (40), (70), (71) and the last formula we find

$$\frac{2}{3} m(J, \theta) = - \int_N |\Delta_0(\beta)|^2 \theta \wedge d\theta + 2 \int_N |\beta_{\Pi_1}|^2 \theta \wedge d\theta + \frac{1}{2} \int_N \bar{\beta} P \beta \theta \wedge d\theta = - \int_N |\Delta_0(\beta)|^2 \theta \wedge d\theta + 2 \int_N |\beta_{\Pi_1}|^2 \theta \wedge d\theta$$

$$+ \frac{1}{2} \int_N (\bar{\beta}_{-1} + \bar{\beta}_{-2+\varepsilon} + u) P(\beta_{-1} + \beta_{-2+\varepsilon} + \bar{\tau}) \theta \wedge d\theta - \frac{2}{3} m(J, \theta).$$

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

$$\int_N (\bar{\beta}_{-1} + \bar{\beta}_{-2+\varepsilon} + u) P(\beta_{-1} + \beta_{-2+\varepsilon} + \bar{\tau}) \theta \wedge d\theta = \int_{M \setminus \{p\}} (\bar{\beta}_{-1} + \bar{\beta}_{-2+\varepsilon} + u) P(\beta_{-1} + \beta_{-2+\varepsilon} + \bar{\tau}) \theta \wedge d\theta \geq 0.$$
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 $vP_\beta\tau$ for $v$ of class $\mathcal{C}^{2,2}(M)$.

Summing up we then obtain

$$\frac{4}{3}m(J, \theta) = -\int_N [\Box_b(\beta)]^2\theta d\theta + 2\int_N |\beta_{TT}|^2 \theta d\theta + 2\int_N R|\beta_T|^2 \theta d\theta + \frac{1}{2}\int_{M\setminus\{p\}} (\beta_{-1} - \beta_{-2+\epsilon} + u)P_\beta(\beta_{-1} + \beta_{-2+\epsilon} + \tau) \hat{\theta} \wedge d\hat{\theta},$$

which implies (68). Formula (69) then follows immediately. ■

### 3.5 Conclusion of the proof of Theorem 1.1

The first statement of the theorem follows immediately from Proposition 3.9.

Suppose now that $m(J, \theta) = 0$. Then, from (69), Proposition 3.1 and (67) we have the following identities

$$\beta_{TT} \equiv 0; \quad \beta_T \equiv 0; \quad P\beta \equiv 0.$$ (72)

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

$$R \equiv 0.$$ (74)

From $P\beta = 0$ we also deduce that $A_{11, T} \equiv 0$. Let us now show that the torsion vanishes identically; in order to do this, we follow the arguments of Section 3 in [38]. Since the ideas here require rather straightforward modifications, we will be rather sketchy in this part.

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

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

where $A_{j,\theta} = -iA_{11}\theta^1 \otimes z_T^1$-conj.. By the variation formulas (140), (141) we have that

$$\frac{d}{ds}R_{J_{(s)}, \theta} = -2|A_{11}|^2 + i(A_{11, TT} - A_{TT, 11}); \quad \frac{d}{ds}(A_{11})_{J_{(s)}, \theta} = iA_{11, t, 0}.$$ (73)

Since for an asymptotically flat manifold we have $A_{11} = O(\rho^{-4})$ at infinity (see Remark 2.2) and since $A_{11, T} \equiv 0$ at $s = 0$, from the second equation in (73) we derive that

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

Then the first equation in (73) implies that for $s$ small

$$R_{J_{(s)}, \theta} \geq \begin{cases} -Cs & \text{everywhere on } N; \\ -C\frac{s}{\rho} & \text{at infinity.} \end{cases}$$ (74)

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 [38] one has the Sobolev type inequality

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

This implies that

$$\int_N (4|\nabla_b u|^2 + R_{J_{(s)}, \theta} u^2) \theta \wedge d\theta \geq 4\int_N |\nabla_b u|^2 \theta \wedge d\theta - \left(\int_N R^2_{J_{(s)}, \theta} \theta \wedge d\theta\right)^{\frac{1}{2}} \left(\int_N u^4 \theta \wedge d\theta\right)^{\frac{1}{2}} \geq (4 + o_s(1))\int_N |\nabla_b u|^2 \theta \wedge d\theta \quad \text{as } s \to 0.$$
Therefore, the operator $-4\Delta_\tilde{s} + R_{J(s),\theta}$ is coercive for $s$ small. Estimates similar to (74) imply that $|R_{J(s),\theta}| \leq C\rho^{-8}$ at infinity, and hence we can find a solution $v_s$ of

$$-4\Delta_\tilde{s}v_s + R_{J(s),\theta}v_s = R_{J(s),\theta}$$

on $N$, which decays to zero at infinity. More precisely, using estimates similar to those of Lemma 3.2 in [38], together with Lemma 5.1 one finds that

$$v_s = \frac{1}{32\pi \rho^2} \int_N (R_{J(s),\theta} - R_{J(s),\theta}u_s) \theta \, d\theta + O(\rho^{-3})$$

at infinity.

The function $u_s = 1 - v_s$ then satisfies

$$-4\Delta_\tilde{s}u_s + R_{J(s),\theta}u_s = 0$$

on $N$, 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

$$u_s = 1 - \frac{1}{32\pi \rho^2} \int_N R_{J(s),\theta}u_s \theta \, d\theta + O(\rho^{-3})$$

at infinity,

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

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

Differentiating the last formula in $s$ and using the fact that $u_0 = 1$, together with (73), we find

$$\frac{d}{ds}_{s=0} m(J(s), u_s^2 \theta) = \frac{3}{2} \int_N |A_{11}|^2 \theta \, d\theta > 0$$

in case $A_{11} \neq 0$ 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 $(G_p)^{-2} \left[ \hat{T} + 2i(\log G_p)_1 \hat{Z}_1 - 2i(\log G_p)_7 \hat{Z}_7 \right]$, where $G_p$ is the Green’s function of $L_\theta$ on $M$ for $s = 0$, and $\hat{T}$ the corresponding Reeb vector field. Letting $\hat{J}_s(s)$ denote $(\hat{\varphi}_s)^* \hat{J}$, then one has clearly that $(G_p(s))_p = u_s G_p$ (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. The Tanaka-Webster class of $(M, \hat{J}_s)$ is indeed clearly positive, since it is a perturbation of a structure with positive class. Concerning the Paneitz operator, notice that we are pulling back the structure via the contact diffeomorphisms $\hat{\varphi}_s$, so the positivity of $P_{J(s),\theta}$ follows 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 (72) we find that

$$d(\beta_T \theta^T) = \beta_T \theta^1 \wedge \theta^T + \beta_T \theta^0 \wedge \theta^T = 0,$$

which implies that $\beta_{11} = \beta_{111} = 0$, $\beta_{11} = 0$, $|\beta_1|^2 = \text{constant} = 0$, and hence $d\beta = \beta_T \theta^T$. Taking $z = \overline{\beta}$ we have

$$d(\theta - izd\overline{z} + izdz) = i\theta^1 \wedge \theta^T - 2idz \wedge d\overline{z} = 0.$$
Note that $dz \wedge d\zeta = |\beta_1|^2 \theta^1 \wedge \theta^\ast$ and $|\beta_1|^2 = \frac{1}{2}$ 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 $d\tilde{t} = \theta - izd\zeta + rzdz$.

So we get a pseudohermitian isomorphism between $\mathcal{U}$ and its image in $\mathbb{H}_1$, $\mathcal{V}$, if we send $q \in \mathbb{R}$ into $q \mapsto (z(q), t(q)) = \left( \beta(q), \int_0^q d\tilde{t} \right)$, 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: next, we want to extend $\Psi$ globally on $\mathbb{H}_1$. Taking $q_0 \in \mathcal{V}$ and $q \in \mathbb{H}_1$ arbitrary, we can find a curve

$$\Gamma : [0, 1] \to \mathbb{H}_1, \quad \Gamma(0) = q_0, \quad \Gamma(1) = q.$$ 

We can then consider the curve $\tilde{\Gamma} : [0, 1] \to N$ obtained composing $\Gamma$ with $\Psi$ initially, and then prolonging it through the local pseudohermitian isomorphisms obtained before. In fact, given any such flat structure $(\mathcal{M}, J, \theta)$, any point $p \in \mathcal{M}$, and any unit contact vector $e_1$ at $p$, there exists a unique local pseudohermitian isomorphism mapping a neighborhood of the origin in $\mathbb{H}_1$ carrying 0 to $p$, and $\partial_x$ to $e_1$ (hence $\partial_y$ to $e_2 = Je_1$, and $\partial_z$ to $T$) onto a neighborhood of $p$ in $\mathcal{M}$. Then using the group structure, the same is true if we substitute 0 above by any point $q$ in the Heisenberg group, and $\partial_x$, by any unit contact vector at $q$.

We show that this procedure defines a map $\tilde{\Psi} : \mathbb{H}_1 \to N$, showing that $\tilde{\Gamma}(1)$ is independent of the choice of $\Gamma$ (once $q$ is fixed). In fact, if we choose two different curves $\Gamma_0, \Gamma_1$, we can then consider the new closed curve $\Gamma_2 = \Gamma_1^{-1} * \Gamma_0 : [0, 1] \to \mathbb{H}_1$, with $\Gamma_2(0) = \Gamma_2(1) = q_0$. We are done if we show that $\tilde{\Gamma}_2(1) = \tilde{\Gamma}_2(0)$.

By the simple connectedness of $\mathbb{H}_1$, there is a homotopy $\Gamma : [0, 1] \times [0, 1] \to \mathbb{H}_1$ such that $\Gamma(t, 0) = q_0$, $\Gamma(t, 1) = \Gamma_2(t)$ and such that $\Gamma(0, s) = \Gamma(1, s) = q_0$ for all $s$. We call $\Gamma(\cdot, s)$ the curve constructed with the above procedure starting from $\Gamma(\cdot, s)$. To prove the claim, it is sufficient to show that $\Gamma(1, s) = \tilde{\Gamma}(0) = \tilde{\Psi}(q_0)$ for all $s \in [0, 1]$.

This is clearly true for $s$ close to 0, since we have a local pseudohermitian isomorphism between a neighborhood of $q_0$ and a neighborhood of $\tilde{\Psi}(q_0)$, and since $\Gamma(\cdot, s)$ is contained in the first neighborhood for $s$ small. We call

$$I = \left\{ r \in (0, 1) : \tilde{\Gamma}(1, s) = \tilde{\Gamma}(0) \text{ for every } s \in [0, r] \right\}; \quad \bar{s} = \sup I.$$ 

Our goal is equivalent to prove that $\bar{s} = 1$. It is clear that $\bar{s} \in I$, so we obtain the claim if we show that $I$ is open in $[0, 1]$. Assume by contradiction that $\bar{s} < 1$: we can find infinitely many $t_i$'s

$$0 = t_0 < t_1 < \cdots < t_{k-1} < t_k = 1$$

such that in each interval $[t_{i-1}, t_{i+1}]$ a neighborhood $\mathcal{V}_i$ of $\Gamma(\cdot, \bar{s})$ is mapped homeomorphically onto a neighborhood $\mathcal{U}_i$ of $\Gamma(\cdot, \bar{s})$, for $i = 1, \ldots, k - 1$. We can then find $\varepsilon$ so small that

$$\Gamma(t, s) \in \mathcal{V}_i \quad \text{for } t \in [t_{i-1}, t_{i+1}], s \in [\bar{s}, \bar{s} + \varepsilon] \text{ and } i = 1, \ldots, k - 1.$$ 

Since $\tilde{\Psi}(q_0) \in \mathcal{U}_{k-1}$ and since all curves $\tilde{\Gamma}(\cdot, s) \in \mathcal{V}_{k-1}$ for $t \in [t_{k-1}, 1]$ and $s \in [\bar{s}, \bar{s} + \varepsilon]$, all ending in $q_0$, we have also that $\tilde{\Gamma}(1, s) = \tilde{\Psi}(q_0)$ for $s \in [\bar{s}, \bar{s} + \varepsilon]$, so we obtain the desired claim, namely the well definiteness of $\tilde{\Psi}$ as a local pseudohermitian isomorphism, and therefore as a covering map.

If $\mathcal{V}$ is as above, and if $q \in \mathcal{V}$, then we can connect $q_0$ to $q$ with a curve $\Gamma$ inside $\mathcal{V}$. This implies that $\tilde{\Psi}$ coincides with $\Psi$ on $\mathcal{V}$, and hence extends it. By construction, $\tilde{\Psi}$ is also proper, and hence by Corollary 1.4 in [1], Chapter 3, it is also injective. It is indeed easy to prove its surjectivity: given any
point \( \tilde{p} \in N \), we can find a curve \( \tilde{\Gamma} : [0, 1] \to N \) such that \( \tilde{\Gamma}(0) = \Psi(q_0) \) and such that \( \tilde{\Gamma}(1) = \tilde{p} \). Then, if we consider the curve \( \Gamma : [0, 1] \to \mathbb{H}^1 \) inverting \( \Psi \) along \( \tilde{\Gamma} \) (see Lemma 1.11 in Chapter 3 of [1]), we have that \( \Psi(\Gamma(1)) = \tilde{\Gamma}(1) = \tilde{p} \). Note that \( \mathbb{H}^1 \setminus \mathcal{V} \) is compact. In conclusion, we have shown that \( \Psi \) realizes a pseudohermitian isomorphism between \( \mathbb{H}^1 \) and \( N \). This concludes the proof.

**Remark 3.10** If \( J \) is spherical we have a different proof of the vanishing of \( A_{11} \). In fact, if \( \Omega \) stands for the Cartan tensor (see Subsection 6.2), for spherical structures one has

\[
0 = \Omega_{11} = \frac{1}{6} R_{11} + \frac{i}{2} R A_{11} - A_{11,0} - \frac{2}{3} i A_{11,T_1}.
\]

Then (see Section 6), since \( A_{11,T} = 0 \) and \( R = 0 \) we find that

\[
0 = i A_{11,0} = A_{11,1T} - A_{11,T_1} - 2 A_{11} R,
\]

which implies \( A_{11,1T} = 0 \). By integration we obtain

\[
0 = - \int_N A_{11,1T} A_{11T} \theta \wedge d\theta = \int_N A_{11,1} A_{11T,T_1} \theta \wedge d\theta = \int_N |A_{11,1}|^2 \theta \wedge d\theta,
\]

which implies \( A_{11,1} = 0 \). Differentiating we get \( |A_{11}|^2 = \text{const.} \) 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 \( S \times S^1 \) with non-negative Paneitz operator.

#### 4.1 Three dimensional CR manifolds with nonpositive Paneitz operator

Recall that from the commutation rules (13) one has

\[
\Box_b u = - \Delta_b u + i T u = - (u_{1T} + u_{1T_1}) + i u_{0} = -2 u_{1T_1} = -2 Z_1(Z_T u) - 2 Z_1^2(Z_1) Z_T u.
\]

Recall also that, along a deformation \( J_{1s} \) of the CR structure the following relations hold (see Subsection 6.1.2)

\[
\dot{Z}_1 = - i E_{11} Z_T, \quad \dot{\theta}_1 = - i E_{11} \theta^T,
\]

\[
\dot{\omega}_1 = i (A_{11} E_{11T} + A_{11T} E_{11}) \theta - i (E_{11,1} \theta^T + E_{11,1} \theta^T); \quad \dot{A}_{11} = i E_{11,0}.
\]

\[
- \dot{\Delta}_b = 2i (E_{11} Z_T Z_T + E_{11.T} Z_T) + \text{conj.}
\]

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

\[
P \psi := \Box_b \Box_b \psi + 4i (A_{11} \psi)_1
\]

for a smooth real function \( \psi \). By (77) the expression (81) is equivalent to

\[
P \psi = 4(\psi_{111} + i A_{11} \psi_{1})_1 \quad \text{or} \quad P \psi = \Delta^2 \psi + T^2 \psi + 4 \text{Im} (A_{11} \psi)_1.
\]

32
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

\[
\frac{d}{ds}(P_{(s)}\psi, \psi) = 2(\Delta_{\psi}, \Delta_{\psi}) - 4\text{Im} \int_M \hat{A}_{1\bar{1}}(\psi,1)^2 \theta \wedge d\theta - 8\text{Im} \int_M \hat{A}_{1\bar{1}}(\hat{\psi},1) \theta \wedge d\theta
\]

by (82). From (78) we have

\[
(\hat{\psi},1) = -iE_{1\bar{1}}\psi,\bar{1}.
\]

Substituting (79), (80), and (84) into (83), we obtain

\[
\frac{d}{ds}(P_{(s)}\psi, \psi) = 4\int_M E_{1\bar{1}}\psi,1(-i\psi,\bar{1}11 - i\psi,\bar{1}11 - \psi,\bar{1}10 + A_{11}\psi,\bar{1}) \theta \wedge d\theta + \text{conj.}
\]

\[
= -8i\int_M E_{1\bar{1}}\psi,1(\psi,\bar{1}11 + iA_{11}\psi,\bar{1}) \theta \wedge d\theta + \text{conj.}
\]

using an integration by parts and the commutation relations (13). Take \( \psi \in \text{Ker}P_{(0)} \), i.e.

\[
4(\psi,\bar{1}11 + iA_{11}\psi,\bar{1}) = 0.
\]

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 [33]). By the transformation law (5) we have that \( \text{Ker}P_{(0)} \) 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 (86) to get \( \psi,\bar{1}11 = 0 \). Multiplying this by \( \psi,\bar{1}1 \) and integrating, we get

\[
0 = \int_M \psi,\bar{1}11 \psi,\bar{1}1\theta_{(0)} \wedge d\theta_{(0)} - \int_M \psi,\bar{1}11 \psi,\bar{1}1\theta_{(0)} \wedge d\theta_{(0)}
\]

\[
= -\int_M |\psi,\bar{1}11|^2 \theta_{(0)} \wedge d\theta_{(0)}
\]

using an integration by parts and the fact that \( \psi \) is real. It follows that \( \psi,\bar{1}11 = 0 \), so from (85) we have

\[
\frac{d}{ds}|_{s=0}(P_{(s)}\psi, \psi) = 0
\]

for \( \psi \in \text{Ker}P_{(0)} \) 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, \( \psi \in \text{Ker}P_{(0)} \) implies that \( \psi \) is CR-pluriharmonic if \( J_{(0)} \) has transverse symmetry. So by Proposition 3.4 in [33], we have

\[
\psi,\bar{1}11 + iA_{11}\psi,\bar{1} = 0
\]

with respect to \( J_{(0)} \) coupled with any contact form. Starting with (85) we compute

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

by (88). From (78) and (79) we obtain

\[
\frac{d}{ds}\psi,\bar{1}1 = i[(E_{1\bar{1}}\psi,1)_{,1} - (E_{1\bar{1}}\psi,1)_{,\bar{1}}].
\]

We then have

\[
\frac{d}{ds}\psi,\bar{1}11 = \left(\frac{d}{ds}Z_1\right)(\psi,\bar{1}1) + Z_1\left(\frac{d}{ds}\psi,\bar{1}\right) = -iE_{1\bar{1}}\psi,\bar{1}11 + i(E_{1\bar{1}}\psi,1)_{,11} - i(E_{1\bar{1}}\psi,1)_{,\bar{1}}
\]

33
by (78) and (90). Substituting (91), the conjugate of (84), and \( \hat{A}_{11} = iE_{11,0} \) into (89) we get

\[
\frac{d^2}{ds^2}(P(s)\psi, \psi)|_{s=0} = 8 \int_{S^3} E_{11,1} \left[ \left( E_{11,1} \right)_{,11} - \left( E_{11,1} \right)_{,11} \right] \\
- E_{11,1,1111} + iE_{11,0} \psi_{,1} + iA_{11} E_{11,1} \theta(0) \wedge d\theta(0) + \text{conj.}
\]

In view of the conjugate of (88) and the commutation relations (13), we compute

\[
\psi_{,1111} = \psi_{,111} - i\psi_{,00} = iA_{11} \psi_{,1} - i\dot{\psi}_{,0} - i\dot{\psi}_{,1} A_{11} = -i\dot{\psi}_{,0}.
\]

Substituting (93) into (92), integrating by parts, and making use of the first commutation relation in (13):

\[
i(\dot{E}_{11,1})_{,0} = (E_{11,1})_{,11} - (E_{11,1})_{,11} + (E_{11,1})R,
\]

hence we obtain

\[
\frac{d^2}{ds^2}(P(s)\psi, \psi)|_{s=0} = 8 \int_{S^3} (4|E_{11,1}|^2 - |E_{11,1}|^2 - |E_{11,1}|^2 - |E_{11,1}|^2) \\
- 2|E_{11,1}|^2 - 2R|E_{11,1}|^2 \theta(0) \wedge d\theta(0).
\]

In the last equality of (94) we have used \( A_{11} = 0 \). We now choose \( E_{11} \neq 0 \) such that

\[
E_{11,1} = 0
\]

Assuming (95), we reduce (94) to

\[
\frac{d^2}{ds^2}(P(s)\psi, \psi)|_{s=0} = 8 \int_{S^3} (4|E_{11,1}|^2 - |E_{11,1}|^2 - |E_{11,1}|^2 - |E_{11,1}|^2) \\
- 2|E_{11,1}|^2 - 2R|E_{11,1}|^2 \theta(0) \wedge d\theta(0).
\]

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

\[
\hat{\theta} = i(\overline{J} - J)(|z_1|^2 + |z_2|^2)
\]

is the standard contact form on \( (S^3, \hat{J}) \), we have that \( R \) is a positive constant. Note also that \( Z_1 = 1/\sqrt{2} (\hat{z}_2 \overline{\partial}_{\overline{z}_1} - \hat{z}_1 \overline{\partial}_{\overline{z}_2}) \), \( \overline{Z}_1 = 1/\sqrt{2} \left( z_2 \overline{\partial}_{z_1} - z_1 \overline{\partial}_{z_2} \right) \). To make (96) negative, we choose \( \psi = z_1 + \hat{z}_1 \) where \( (z_1, \hat{z}_1) \in S^3 \subseteq \mathbb{C}^2 \). It follows that

\[
\psi_{,1} = \frac{1}{\sqrt{2}} \hat{z}_2; \quad \psi_{,11} = 0; \quad \psi_{,111} = -\frac{1}{2} \hat{z}_1; \quad \psi_{,111} = \psi_{,111} = 0.
\]

Observing that the first three terms of the integrand in (96) vanish due to the fact that \( \psi_{,11} = 0 \) by (98), we have

\[
\frac{d^2}{ds^2}(P(s)\psi, \psi)|_{s=0} = 8 \int_{S^3} \left( - |E_{11,1} \hat{z}_2 - E_{11,1} \frac{1}{\sqrt{2}} \hat{z}_1 |^2 - R |E_{11,1} \hat{z}_2|^2 \right) \hat{\theta} \wedge d\hat{\theta} < 0.
\]

For example, we can take \( E_{11} \) to be a nonzero constant in (99), which satisfies (95). In view of (99), (87), 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.
Differentiating this formula twice in $u$ of $J$ we consider a deformation $b$ as in (11). Recall the variation formulas for $\Delta H$ the variation of the mass. We begin with a deformation in $\mathbb{H}^1$, namely such that $J(0)$ is as in (11). Recall the variation formulas for $\Delta s$ and $R$ in Subsection 6.1.2. Assuming the deformation of $J$ decays sufficiently fast near infinity, we can find a scalar flat conformal contact form $\theta_s = u_s^2 \hat{\theta}$, with $u_s$ satisfying (73), as in Subsection 3.5. Then the mass $m(J(s), u_s^2 \theta)$ will be still given by formula (76). Differentiating this formula twice in $s$, taking into account that $u \equiv 1$ and $R \equiv 0$ for $s = 0$ we obtain, at $s = 0$

\begin{equation}
\tilde{m}(J, \theta) = -\frac{3}{4} \int_{\mathbb{H}^1} \hat{R} \hat{\theta} \wedge d \hat{\theta} - \frac{3}{2} \int_{\mathbb{H}^1} \hat{R} \hat{\theta} \wedge d \hat{\theta}.
\end{equation}

We choose a deformation $J(s)$ so that $E_{11}$ (see the notation in Subsection 6.1.2) is a CR function, namely $E_{11, T} = 0$. We can take for example

\begin{equation}
E_{11}(z, \tau; t) = \frac{1}{(t + i(|z|^2 + 1))^k},
\end{equation}

with $k$ integer and large (to have a fast decay). By (141) we have then $\hat{R} = 0$, which by (101) implies

\begin{equation}
\tilde{m}(J, \theta) = -\frac{3}{4} \int_{\mathbb{H}^1} \hat{R} \hat{\theta} \wedge d \hat{\theta}.
\end{equation}

Reasoning as for (142), one can check that on $\mathbb{H}^1$

\begin{align*}
\hat{R} &= -6|E_{11, i}|^2 - 2|E_{11, 0}|^2 - 3E_{11, 1}E_{TT} - 3E_{TT, i}E_{11} - E_{11}E_{TT, i} - E_{TT}E_{11, T} \\
&\quad - iE_{11, 0}E_{TT} + iE_{TT, 0}E_{11}.
\end{align*}
Therefore, by our choice of \( E_{11} \) one has
\[
\dot{R} = -2 |E_{11,1}|^2 - E_{11} E_{\overline{1},1} - \frac{E_{11} E_{\overline{1},1} - i E_{11,0} E_{\overline{1},0} + i E_{\overline{1},0} E_{11}}{2}.
\]
Using the commutation rules (13) and again the fact that \( E_{11} \) is a CR function we obtain
\[
\dot{R} = -2 |E_{11,1}|^2 - 2 E_{11} E_{\overline{1},1} - 2 E_{\overline{1},0} E_{11,1}.
\]
Then the above formula (102) implies
\[
\dot{m}(J, \theta) = \frac{3}{2} \int_{\mathbb{H}^1} (|E_{11,1}|^2 + E_{11} E_{\overline{1},1} + E_{\overline{1},0} E_{11,1}) \dot{\theta} \wedge d \theta,
\]
so integrating by parts we obtain
\[
\dot{m}(J, \theta) = -\frac{3}{2} \int_{\mathbb{H}^1} |E_{11,1}|^2 \dot{\theta} \wedge d \theta < 0.
\]
We can transport the latter example on \( S^3 \) using the Cayley transform \( \varphi : S^3 \setminus p \to \mathbb{H}^1 \), \( p = (0, 1) \in \mathbb{C}^2 \), defined as
\[
\varphi(z_1, z_2) = \left( \frac{z_1}{1 + z_2}, \text{Re} \left( \frac{i - z_2}{1 + z_2} \right) \right),
\]
where \((z_1, z_2)\) are standard coordinates in \( \mathbb{C}^2 \). It turns out that
\[
G_p(z_1, z_2) = \frac{1}{\pi} \left( \frac{(1 + z_2)(1 + \overline{z_2})}{|z_1|^2 - (z_2 - \overline{z_2})^2} \right) \frac{1}{\pi}.
\]
As in Subsection 3.5, we can obtain \((\mathbb{H}^1, J,(s), u^2 \theta)\) as blow up of the structure \((S^3, \dot{J}_s, \dot{\theta})\) at the point \( p \) through the Green’s function \((G_p)_s = (u_s \circ \varphi)G_p\). 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 (18) at proper points, the resulting asymptotically flat pseudohermitian manifold has negative mass.

**Remark 4.5** For an arbitrary variation \( E_{11} \) we have
\[
\dot{R} = i (E_{11,1} - E_{\overline{1},1,1}),
\]
and
\[
\dot{m}(J, \theta) = -\frac{3}{4} \int_{\mathbb{H}^1} \dot{R} \dot{\theta} \wedge d \theta = -\frac{3}{4} \int_{\mathbb{H}^1} (E_{11,1} - E_{\overline{1},1,1}) \dot{\theta} \wedge d \theta.
\]
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
\[
\dot{\theta} = \rho^{-2} \tilde{\theta},
\]
the transformation \((z, t) \mapsto (2z, 4t)\) defines a pseudohermitian isomorphism. Introducing then the equivalence relation
\[
(z_1, t_1) \sim (z_2, t_2) \quad \text{if and only if} \quad z_1 = 2^k z_2 \text{ and } t_1 = 2^{2k} t_2 \text{ for some } k \in \mathbb{Z},
\]

36
we obtain a pseudohermitian structure on $S^2 \times S^1$. Using (138), one finds that
\[ \hat{A}_{11} = i|z|^2 (|z|^2 + it)^2 \rho^{-6}, \]
so the torsion of $(S^2 \times S^1, J_0, \hat{\theta})$ is non-zero. Given any smooth function $\varphi$ we would like to prove the non-negativity of $\int_{S^2 \times S^1} \varphi P_{(J_0, \hat{\theta})} \varphi \hat{\theta} \wedge d \hat{\theta}$.

Using the conformal covariance of $P$, see (5), we obtain
\[ \int_{S^2 \times S^1} \varphi P_{(J_0, \hat{\theta})} \varphi \hat{\theta} \wedge d \hat{\theta} = \int_{\{\rho \in [1,2]\}} \varphi P_{(J_0, \hat{\theta})} \varphi \hat{\theta} \wedge d \hat{\theta}. \]

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

We next consider a smooth cut-off function $\chi$, depending only on $\rho$, such that
\[ \begin{cases} \chi(\rho) = 0 & \text{for } \rho \leq \frac{\delta}{n+1}; \\ \chi(\rho) = 1 & \text{for } \rho \geq \frac{\delta}{n+1}, \end{cases} \]
and define the function $\tilde{\varphi}_n : \mathbb{H} \to \mathbb{R}$ as
\[ \tilde{\varphi}_n := \chi(\rho) \left[ 1 - \chi \left( 2^{-(n+1)} \rho \right) \right] \tilde{\varphi}. \]

By the non-negativity of $P_{(J_0, \hat{\theta})}$ (notice that the torsion vanishes identically) then we clearly have
\[ 0 \leq \int_{\mathbb{H}^1} \tilde{\varphi}_n P_{(J_0, \hat{\theta})} \tilde{\varphi}_n \hat{\theta} \wedge d \hat{\theta} = \int_{\{\rho \in [1,2^n]\}} \tilde{\varphi} P_{(J_0, \hat{\theta})} \tilde{\varphi} \hat{\theta} \wedge d \hat{\theta} + \int_{\{\rho \in [1/2,1]\}} \tilde{\varphi}_n P_{(J_0, \hat{\theta})} \tilde{\varphi}_n \hat{\theta} \wedge d \hat{\theta} + \int_{\{\rho \in [2^n, 2^{n+1}]\}} \tilde{\varphi}_n P_{(J_0, \hat{\theta})} \tilde{\varphi}_n \hat{\theta} \wedge d \hat{\theta}. \]

By dilation invariance the last two terms in the above formula are uniformly bounded: therefore by (103), (104) we obtain that
\[ \int_{S^2 \times S^1} \varphi P_{(J_0, \hat{\theta})} \varphi \hat{\theta} \wedge d \hat{\theta} = \lim_{n \to +\infty} \frac{1}{n} \int_{\mathbb{H}^1} \tilde{\varphi}_n P_{(J_0, \hat{\theta})} \tilde{\varphi}_n \hat{\theta} \wedge d \hat{\theta} \geq 0, \]
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 Tanaka-Webster quotient

Given a compact CR manifold $M$ of positive Tanaka-Webster class and a point $p \in M$, let us consider the equation
\[ -4\Delta_b G_p + RG_p = 16\delta_p, \]
where $\delta_p$ is the Dirac delta at the point $p$. We will use the classical method of the parametrix to construct the Green’s kernel.
Lemma 5.1 In the Heisenberg group one has
\[ \Delta_b \frac{1}{\rho^2} = -8\pi\delta_0. \]

Proof. One can easily check that \( \Delta_b \frac{1}{\rho^2} = 0 \) outside of the origin of \( \mathbb{H}^1 \). We compute then the flux of the subgradient of \( \frac{1}{\rho^2} \) on the boundary of any open set containing the origin. We can take for example the set \[ \{ \rho \leq 1 \}, \quad \text{with boundary } S = \{ \rho = 1 \}. \]

Let \( f = \frac{1}{\rho^2} \): since \( \Delta_b f = f_1T + f_1\overline{T} \), integrating by parts we get
\[ \int_{\{\rho \leq 1\}} \Delta_b f \, \theta \wedge d\overline{\theta} = \int_{\{\rho \leq 1\}} f_1T \theta \wedge d\overline{\theta} + \text{conj.} = -i \int_S f_1 \theta^1 \wedge \overline{\theta} + \text{conj.}. \]

By elementary computations one finds
\[ f_1 = -\frac{1}{\sqrt{2}} \frac{|z|^2 + it}{\rho^3}; \quad f_{1\overline{T}} = -\frac{1}{\sqrt{2}} \frac{|z|^2 - it}{\rho^3}, \]
which implies
\[ \int_{\{\rho \leq 1\}} \Delta_b f \, \theta \wedge d\overline{\theta} = \frac{i}{\sqrt{2}} \int_S (|z|^2 + it)\sqrt{2}\pi dz \wedge (dt + izd\overline{z}) + \text{conj.} \]
\[ = i \oint_S [(|z|^2 + it)\overline{z} dz \wedge (dt + izd\overline{z}) - (|z|^2 - it)z d\overline{z} \wedge (dt - i\overline{z} dz)] \]
\[ = i \oint_S \{|z|^2 [(\overline{z} dz - z d\overline{z})] \wedge dt\} + 2i|z|^2 dz \wedge d\overline{z}. \]

Using (36) and (46) we then deduce
\[ \int_{\{\rho \leq 1\}} \Delta_b f \, \theta \wedge d\overline{\theta} = -2 \oint_S (|z|^4 d\varphi \wedge dt + t^2 d\varphi \wedge dt) = -2 \oint_S d\varphi \wedge dt = -8\pi, \]
so we obtain the conclusion. \( \square \)

To find a solution of (105), using CR normal coordinates at \( p \), we are going to consider a function \( G_p \) of the form
\[ G_p = \frac{1}{2\pi} \rho^{-2} + w; \quad \rho^4 = |z|^4 + t^2, \]
where \( w \) has to be suitably chosen. First of all, we evaluate \( \Delta_b \) on \( \rho^{-2} \). Using the fact that
\[ |Z_1 \rho^i| \leq C_i \rho^{i-1}, \quad |T \rho^i| \leq C_i \rho^{i-2}; \quad i \in \mathbb{Z}, i < 0, \]
together with (111), we obtain
\[ \Delta_b (\rho^{-2}) = -8\pi \delta_p + g; \quad g = O(1). \]
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 6.2) it follows that \( R = O(\rho^2) \), which implies that \( w \) satisfies
\[ -4\Delta_b w + Rw = \tilde{g}; \quad \tilde{g} = O(1). \]
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 [22] then implies that \( w \in \mathcal{S}^{2,q}(M) \) 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 Tanaka-Webster class, and that $p \in M$. Then the conformal 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. Then the following expansion holds

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

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

To find suitable test functions we follow Schoen’s idea, see [37], and glue the Green’s function to a standard bubble, which for the Heisenberg group is given by

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

This function satisfies

$$-\Delta_b \omega_\lambda = \omega_\lambda^3$$

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

$$\int_{\mathbb{H}^1} |\nabla_b \omega_\lambda|^2 \theta \wedge d\theta = \inf_{v \in C^\infty_c(\mathbb{H}^1)} \left( \int_{\mathbb{H}^1} |\nabla_b v|^2 \theta \wedge d\theta \right)^{\frac{1}{2}} = Y_0.$$

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

$$\psi(z,t) = 1 \quad \text{in} \quad \{ \rho \leq \rho_0 \}; \quad \psi(z,t) = 0 \quad \text{in} \quad \mathbb{H}^1 \setminus \{ \rho \geq 2\rho_0 \}.$$

Next, consider the following test function

$$u(z,t) = \begin{cases} 
\omega_\lambda(z,t) 
& \text{in} \ \{ \rho \leq \rho_0 \}; \\
\varepsilon_0 \left( \tilde{G}_p(z,t) - \psi \tilde{w}(z,t) \right) + \psi(z,t) \frac{1}{\lambda} \phi(z,t) 
& \text{in} \ \{ \rho \leq 2\rho_0 \} \setminus \{ \rho \leq \rho_0 \}; \\
\varepsilon_0 \tilde{G}_p(z,t) 
& \text{in} \ \mathbb{H} \setminus \{ \rho \leq 2\rho_0 \},
\end{cases}$$

where we have set

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

The constant $\varepsilon_0$ has to be chosen so that the function $u$ is continuous, namely so that

$$\varepsilon_0 = \frac{1}{\lambda(1 + \tilde{A} \rho_0^2)}; \quad \tilde{A} = 2\pi A.$$
5.2 Estimates on the Tanaka-Webster quotient $\mathcal{Y}(J)$

We now evaluate the Sobolev-type quotient

\[(Q) \quad \frac{\int_M (|\nabla_b u|^2 + \frac{1}{4} Ru^2) \theta \wedge d\theta}{(\int_M |u|^4 \theta \wedge d\theta)^{\frac{3}{2}}}\]

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

Recall from Subsection 2.1 that for CR normal coordinates one has

\[(111) \quad \begin{cases} 
\theta = (1 + O(\rho^4)) \theta_0 + O(\rho^5) dz + O(\rho^6) d\bar{z}; \\
\theta^1 = \sqrt{2} (1 + O(\rho^4)) dz + O(\rho^4) d\bar{z} + O(\rho^3) d\theta_0,
\end{cases}\]

which implies

\[(112) \quad \theta \wedge d\theta = (1 + O(\rho^4)) \hat{\theta} \wedge d\hat{\theta},\]

and

\[(113) \quad \begin{cases} 
Z_1 = (1 + O(\rho^4)) \tilde{Z}_1 + O(\rho^4) \tilde{Z}_T + O(\rho^5) \tilde{T}; \\
T = (1 + O(\rho^4)) \tilde{T} + O(\rho^3) \tilde{Z}_1 + O(\rho^3) \tilde{Z}_T.
\end{cases}\]

Since $u$ is real, its squared subgradient is given by

\[|\nabla_b u|^2 = 2(Z_1 u)(\tilde{Z}_T u).\]

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

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

\[(114) \quad \int_{\{\rho \leq \rho_0\}} |\nabla_b u|^2 \theta \wedge d\theta = 2 \int_{\{\rho \leq \rho_0\}} (\tilde{Z}_1 u)(\tilde{Z}_T u) \theta \wedge d\theta + \int_{\{\rho \leq \rho_0\}} ((Z_1 u)(\tilde{Z}_T u) - (\tilde{Z}_1 u)(\tilde{Z}_T u)) \theta \wedge d\theta + 2 \int_{\{\rho \leq \rho_0\}} (\tilde{Z}_1 u)(\tilde{Z}_T u)(\theta \wedge d\theta - \theta \wedge d\hat{\theta}).\]

To evaluate the last term in the above expression we use (112), and the fact that

\[(115) \quad 2(\tilde{Z}_1 u)(\tilde{Z}_T u) = \frac{|z|^2 \lambda^6}{((1 + \lambda^2 |z|^2)^2 + \lambda^4 t^2)^2},\]

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

\[(116) \quad \left| \int_{\{\rho \leq \rho_0\}} (\tilde{Z}_1 u)(\tilde{Z}_T u)(\theta \wedge d\theta - \theta \wedge d\hat{\theta}) \right| \leq C \int_0^{\rho_0} \frac{\rho^2 \lambda^6 \rho^4}{(1 + \lambda^4 |z|^2)^2} \tilde{\rho}^2 d\tilde{\rho} \leq C \int_0^{\lambda \rho_0} \tilde{\rho}^2 d\tilde{\rho} \leq C \frac{\rho_0^3}{\lambda^2}.\]

To evaluate instead the second term in the right hand side of (114), we use (111) to find

\[(117) \quad \int_{\{\rho \leq \rho_0\}} [(Z_1 u)(\tilde{Z}_T u) - (\tilde{Z}_1 u)(\tilde{Z}_T u)] \theta \wedge d\theta \leq C \int_{\{\rho \leq \rho_0\}} |\nabla_b \omega_\lambda| (\rho^4 |\nabla_b \omega_\lambda| + \rho^5 |\tilde{T} \omega_\lambda|) \theta \wedge d\hat{\theta} + C \int_{\{\rho \leq \rho_0\}} \left( \rho^8 |\nabla_b \omega_\lambda|^2 + \rho^{10} |\tilde{T} \omega_\lambda|^2 \right) \theta \wedge d\hat{\theta}.\]
The first terms in the right hand side of the first line in (117) and in the second line in (117) can be treated exactly as for (116). For the remaining ones, we use the explicit expression

\[ \frac{\partial}{\partial t} \omega_\lambda = - \frac{t \lambda^5}{((1 + \lambda^2 |z|^2) + \lambda^4 t^2)^{3/2}} \]

to find

\[ \int_{\{\rho \leq \rho_0\}} |\nabla_b \omega_\lambda| \rho^5 \omega_\lambda \frac{\partial \omega_\lambda}{\partial \rho} \rho \wedge d \theta \leq C \int_0^{\rho_0} \frac{\rho^8 \lambda^8}{(1 + \lambda^4 \rho^4)^{3/2}} \rho^3 d \rho \leq \frac{C \int_0^{\rho_0} \lambda^8 \rho^3 d \rho}{(1 + \rho^4)^{3/2}} \leq \frac{C \rho_0^5}{\lambda^2} \]

\[ \int_{\{\rho \leq \rho_0\}} |\nabla_b \omega_\lambda| \rho^{10} \omega_\lambda \frac{\partial \omega_\lambda}{\partial \rho} \rho \wedge d \theta \leq C \int_0^{\rho_0} \frac{\rho^{14} \lambda^{10}}{(1 + \lambda^4 \rho^4)^{3/2}} \rho^3 d \rho \leq \frac{C \int_0^{\rho_0} \lambda^8 \rho^3 d \rho}{(1 + \rho^4)^{3/2}} \leq \frac{C \rho_0^5}{\lambda^2} \]

In conclusion, using (114), (116), (117) and the last two formulas we obtain that

\[ (118) \quad \left| \int_{\{\rho \leq \rho_0\}} |\nabla_b u|^2 \omega_\lambda \wedge d \theta - \int_{\{\rho \leq \rho_0\}} |\nabla_b u|^2 \delta \wedge d \theta \right| \leq C \frac{\rho_0^2}{\lambda^2}. \]

### 5.2.2 Integral estimate of $Ru^2$

We estimate next the term $\int_{\{\rho \leq \rho_0\}} Ru^2 \omega_\lambda \wedge d \theta$. For doing this, we first expand in Taylor series the Tanaka-Webster curvature $R$, using real CR normal coordinates. From the relations (see Subsection 6.2)

\[ (119) \quad R = 0; \quad R_{11} = 0; \quad \Delta_b R = R_{\omega \theta} + R_{\omega \theta} = 0; \quad R_{00} = 0, \]

and the fact that for a smooth function $f$ one has

\[ \Delta_b f = f_{xx} + f_{yy} + 2y f_{xt} - 2x f_{yt} + 4 |z|^2 f_{tt} \quad \text{at} \quad p, \]

we can write

\[ (120) \quad R(z, t) = \frac{1}{2} \left( R_{xx} x^2 + R_{yy} y^2 + 2 R_{xy} x y \right) + O(\rho^3), \quad \text{with} \quad R_{yy} = -R_{xx}. \]

By this reason and by the axial symmetry of $\omega_\lambda$ the terms of order $\rho^2$, integrated, will vanish. Similarly, by symmetry, also the cubic ones will vanish, and therefore by (112) we deduce

\[ (121) \quad \left| \int_{\{\rho \leq \rho_0\}} Ru^2 \wedge d \theta \right| = \int_{\{\rho \leq \rho_0\}} R \omega_\lambda \frac{\partial \omega_\lambda}{\partial \rho} \rho^4 \wedge d \theta + O \left( \int_{\{\rho \leq \rho_0\}} \rho^6 \omega_\lambda \frac{\partial \omega_\lambda}{\partial \rho} \rho^4 \wedge d \theta \right) \leq C \int_{\{\rho \leq \rho_0\}} \rho^4 \omega_\lambda \frac{\partial \omega_\lambda}{\partial \rho} \rho^4 \wedge d \theta \leq C \frac{\rho_0^5}{\lambda^2}. \]

### 5.2.3 Estimate of the boundary term

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

\[ \int_{\Omega} \left| \nabla_b u \right|^2 \omega_\lambda \wedge d \theta = \int_{\Omega} \partial_1 \left( \partial_1 u \right) \partial_1 \wedge d \theta + \int_{\Omega} \partial_1 \left( \partial_1 u \right) \partial_1 \wedge d \theta \]

\[ = i \int_{\partial \Omega} u \frac{\partial}{\partial \nu} \left( \partial_1 u \right) \wedge d \theta - i \int_{\partial \Omega} \left( \partial_1 u \right) \frac{\partial}{\partial \nu} \wedge d \theta - \int_{\Omega} \Delta_b u \partial_1 \wedge d \theta. \]

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

\[ \partial_1 \omega_\lambda = \frac{-1}{\sqrt{2}} \frac{(1 + \lambda^2 |z|^2 + it \lambda^2) \lambda^2}{[\lambda^4 t^2 + (1 + \lambda^2 |z|^2) t^2]^{3/2}} \quad \text{and} \quad \partial_1 \omega_\lambda = \frac{-1}{\sqrt{2}} \frac{z(1 + \lambda^2 |z|^2 - it \lambda^2) \lambda^2}{[\lambda^4 t^2 + (1 + \lambda^2 |z|^2) t^2]^{3/2}} \]
Using also the fact that \( \lambda \rho \) and similarly \( A \) similar estimate holds true for \( Z_\psi \). We derive now some estimates on the above terms. First of all we notice that we can take

\[
\psi(z,t) = \psi_0 \left( \frac{z}{\rho_0}, \frac{t}{\rho_0^3} \right),
\]

for a smooth fixed \( \psi_0 \) which, using (113), implies

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

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

\[
|\nabla_\psi(\tilde{w})| \leq C \quad \text{ in } \{ \rho \leq 2\rho_0 \} \setminus \{ \rho \leq \rho_0 \} \quad \text{ for some fixed } C > 0.
\]

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

\[
\varphi = \rho^{-2} \left[ \left( 1 + \frac{2|z|^2}{\lambda^2 \rho^4} + \frac{1}{\lambda^4 \rho^4} \right)^{-\frac{1}{2}} - 1 \right] = \frac{1}{\lambda^4 \rho^6} O \left( \frac{1}{\lambda^2 \rho^4} \right).
\]

(127)

By straightforward computations we also get

\[
\frac{\partial}{\partial t} \varphi = \frac{1}{\sqrt{2} \lambda^2} \left( \varphi - \varphi^3 \right) \left[ \frac{\varphi^2 - \varphi^4}{\lambda^2 \rho^6} \right] \left[ \frac{\varphi^2 + \varphi^4}{\lambda^2 \rho^6} \right] \left[ \frac{\varphi^2 - \varphi^4}{\lambda^2 \rho^6} \right] \left[ \frac{\varphi^2 + \varphi^4}{\lambda^2 \rho^6} \right] - 1\right),
\]

and similarly

\[
\frac{\partial}{\partial z} \varphi = \frac{1}{\sqrt{2} \lambda^2} \left( \varphi - \varphi^3 \right) \left[ \frac{\varphi^2 - \varphi^4}{\lambda^2 \rho^6} \right] \left[ \frac{\varphi^2 + \varphi^4}{\lambda^2 \rho^6} \right] \left[ \frac{\varphi^2 - \varphi^4}{\lambda^2 \rho^6} \right] \left[ \frac{\varphi^2 + \varphi^4}{\lambda^2 \rho^6} \right] - 1\right).
\]
Using some Taylor expansions, the fact that $|\tilde{T}\varphi| = O\left(\frac{1}{\lambda^2}\right)$ and (111) we then deduce

$$|\nabla_b\varphi| = O\left(\frac{1}{\lambda^2}\right)$$

in $\{\rho \leq 2\rho_0\} \setminus \{\rho \leq \rho_0\}$.

From the above estimates on $\psi$ this implies

$$|\nabla_b(\varphi\psi)| = O\left(\frac{1}{\lambda^2\rho_0}\right)$$

in $\{\rho \leq 2\rho_0\} \setminus \{\rho \leq \rho_0\}$.

It is also easy to see that

$$|\nabla_b\tilde{G}_p| = O\left(\frac{1}{\rho_0}\right)$$

in $\{\rho \leq 2\rho_0\} \setminus \{\rho \leq \rho_0\}$.

Next, from (109), (110), the expression of $\tilde{G}_p$, $\tilde{w} = O(\rho)$, (127) and $\lambda\rho_0 \gg 1$ we get

$$|u^2 - \varepsilon_0^2G_p^2| \leq \varepsilon_0\rho_0^{-2}\left(\varepsilon_0\rho_0 + \frac{1}{\lambda^2\rho_0^2}\right) + \varepsilon_0^2\rho_0^2 + \frac{1}{\lambda^2\rho_0^2} \leq C\left(\frac{1}{\lambda^2\rho_0} + \frac{1}{\lambda^4\rho_0^4}\right).$$

This and (120) imply

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

Therefore, integrating and using the fact that the volume of $B_{2\rho_0} \setminus \{\rho \leq \rho_0\}$ is of order $\rho_0^4$, from (125) and the above estimates we obtain

$$\int_{M \setminus \{\rho \leq \rho_0\}} \left(|\nabla_bu|^2 + \frac{1}{4}Ru^2\right) \theta \wedge d\theta = \varepsilon_0^2\int_{M \setminus \{\rho \leq \rho_0\}} \left(|\nabla_b\tilde{G}_p|^2 + \frac{1}{4}R\tilde{G}_p^2\right) \theta \wedge d\theta + O\left(\frac{\rho_0^4}{\lambda^2} + \frac{\varepsilon_0^2\rho_0^2}{\lambda^4\rho_0^4}\right).$$

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 (122) one finds

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

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

By direct computations we have that

$$-i\tilde{G}_p(Z_{\tilde{T}}\tilde{G}_p)\theta^\top \wedge \theta + i\tilde{G}_p(Z_1\tilde{G}_p)\theta^1 \wedge \theta = -i\tilde{G}_p\left(\frac{1}{\sqrt{2}}\frac{\bar{\varphi}(|z|^2 + i\bar{\varphi})}{\rho^6} \sqrt{2}\overline{dz \wedge (dt + i\overline{dz})} - \frac{1}{\sqrt{2}}\frac{\varphi(|z|^2 - i\varphi)}{\rho^6} \sqrt{2}\overline{d\varphi \wedge (dt - i\overline{d\varphi})} + O(\rho)d\varphi \wedge dt\right).$$

Using some cancellations we get

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

therefore after integration we obtain

$$\int_{M \setminus \{\rho \leq \rho_0\}} \left(|\nabla_b\tilde{G}_p|^2 + \frac{1}{4}R\tilde{G}_p^2\right) \theta \wedge d\theta = \oint_{S_{\rho_0}} \frac{2(1 + \tilde{A}\rho^2)}{\rho^4} d\varphi \wedge dt + O(\rho_0^2).$$
Now, using the formula for $\varepsilon_0$ in (110) and some straightforward computations one finds that the contribution of the boundary term in (124) together with the one in the last formula becomes (there is cancelation of the two main terms after subtraction)

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

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

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

If we also choose $\lambda$ and $\rho_0$ so that $\lambda^2 \rho_0^3 \gg 1$ then the last term in the numerator dominates, and we are reduced to

$$
-2\frac{\tilde{A}}{\rho_0^3 \lambda^2} \int_{S_{\rho_0}} d\varphi \wedge dt = -8\pi \frac{\tilde{A}}{\lambda^2}.
$$

5.2.4 Final estimates

Collecting all the terms in (121), (124), (130), (131) and (132), and taking into account the previous computations, with our choices of $\rho_0$ and $\lambda$ we find

$$
\int_M \left( |\nabla_k u|^2 + \frac{1}{4} Ru^2 \right) \theta \wedge d\theta = \int_{\{\rho \leq \rho_0\}} \omega^4 \theta \wedge d\theta - 8\pi \frac{\tilde{A}}{\lambda^2} + O \left( \frac{1}{\lambda^6 \rho_0^2} \right)
$$

(133)

$$
+ O \left( \frac{\rho_0}{\lambda^2} \right) + O \left( \frac{1}{\lambda^4 \rho_0^3} \right).
$$

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

$$
\int_M \left( |\nabla_k u|^2 + \frac{1}{4} Ru^2 \right) \theta \wedge d\theta = \int_{\{\rho \leq \rho_0\}} \omega^4 \theta \wedge d\theta - (8\pi + o(1)) \frac{\tilde{A}}{\lambda^2}.
$$

(134)

Finally, we estimate the denominator in $(Q)$. 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 $|u| \leq \frac{C}{\lambda \rho_0}$ (by the expression of $\varepsilon_0$ and the asymptotics of $G_\rho$), 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

$$
\int_{M \setminus \{\rho \leq 2\rho_0\}} |u|^4 \theta \wedge d\theta \leq C \frac{1}{\lambda^4} \int_{\rho_0}^{\infty} \rho^3 \mu^2 \mu^2 = O \left( \frac{1}{\lambda^4 \rho_0^5} \right) \ll \frac{1}{\lambda^2}.
$$

Moreover, from (112) and the expression of $\omega_\lambda$ we obtain

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

In conclusion, using (134) and the last three formulas, the Tanaka-Webster quotient $(Q)$ for the test function (109) becomes

$$
\frac{\int_M |\nabla_k u|^2 \theta \wedge d\theta}{\left( \int_M |u|^4 \theta \wedge d\theta \right)^2} = \frac{\int_{\{\rho \leq \rho_0\}} \omega^4 \theta \wedge d\theta - (C_1 + o(1)) \frac{\tilde{A}}{\lambda^2 \rho_0^2}}{\left( \int_{\{\rho \leq \rho_0\}} \omega^4 \theta \wedge d\theta \right)^2 + O \left( \frac{1}{\lambda^4} \log(\rho_0) \right)}.
$$
Since \( O \left( \frac{1}{N^2 \rho_0} \right) + O \left( \frac{1}{N^2 \log (\lambda \rho_0)} \right) \ll \frac{1}{N^2} \), from the last formula and (108) we find

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

which is the desired inequality.

The proof of Theorem 1.2 then follows from [29] in the case when \( M \) is CR equivalent to the 3-sphere, and from the variational argument in [28] in the complementary case.

**Remark 5.4** Since the minimization procedure for the Tanaka-Webster quotient is related to the positivity of the mass, in view of Proposition 4.4 there might be examples of pseudohermitian manifolds of positive Tanaka-Webster class for which there is no minimizer. In this case, the use of variational or topological methods (as in [23], [24]) seems to be a necessary tool in order to find conformal structures of constant Tanaka-Webster curvature.

### 6 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 [30].

#### 6.1 Variations of interesting quantities

Here we consider variations of some geometric quantities either under the conformal change of contact form (pp. 421-422 in [32]), or under the change of the pseudohermitian structure (pp. 231-232 in [19]).

**6.1.1 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

\[
\hat{\theta}^1 = e^f (\theta^1 + 2if^1 \theta);
\]

and that

\[
\hat{h}_{1\bar{T}} = h_{1\bar{T}} = 1,
\]

and that

\[
\hat{Z}_1 = e^{-f} Z_1; \quad \hat{T} = e^{-2f} \left( T + 2if^1 Z_1 - 2iZ_1 f^1 \right).
\]

Moreover we also have

\[
\hat{\omega}_1 = \omega_1 + 3 \left( f_1 \theta^1 - f^1 \theta^1 + i (f_{1\bar{1}} + f_{1\bar{T}} + 8f_1 f_{\bar{T}}) \theta. \right.
\]

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

\[
\hat{A}_{1\bar{1}} = e^{-2f} (A_{1\bar{1}} + 2if_{1\bar{1}} - 4if_1 f_{\bar{1}}); \quad \hat{R} = e^{-2f} (R - 4 \Delta_b f - 8f_1 f_{\bar{T}}).
\]

**6.1.2 Deformation of \( J \)**

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

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

This implies

\[
\dot{Z}_1 = -iE_{1\bar{T}}^1 Z_{1\bar{T}}; \quad \dot{\theta}^1 = -iE_{1\bar{T}}^1 \theta^1.
\]

45
and

\[ \omega_1 = i (A_{11} E_{11} + A_{11} E_{11}) \theta = i E_{11}^1 \theta - i E_{11} \theta^1; \quad A_{11}^1 = -i E_{11}^1. \]

We also have

\[ \hat{R} = i (E_{11} E_{11} - E_{11} E_{11}) - (A_{11} E_{11} + A_{11} E_{11}). \]

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

\[ \Delta_b = (Z_T Z_1 - \omega_1 (Z_T Z_1) + \text{conj.}. \]

From this formula, differentiating with respect to \( s \) one finds

\[ \Delta_b = -i E_{11} Z_1 Z_1 + i E_{11} Z_1 Z_1 + i E_{11} Z_1 Z_1 + \text{conj.} \]

\[ - \Delta_b = 2i E_{11} Z_1 Z_1 + E_{11} Z_1 Z_1 + \text{conj.}. \]

To derive these formulas we have used the above transformation laws for \( J, Z_1 \) and \( \omega_1 \).

If we differentiate once more we find that

\[ (E_{11,1}^1) = i E_{11} E_{11,1} + 2i E_{11} E_{11} + (E_{11})_T, \]

and hence

\[ - \Delta_b = 2i (E_{11} Z_1 Z_1 + E_{11} Z_1 Z_1 + \text{conj.}) \]

\[ (11) = 0; \quad (21) = 0; \quad (11)_T = 0; \quad (21)_T = 0. \]

Using similar formulas we can also deduce the expression of \( \hat{R} \).

### 6.2 CR normal coordinates

We recall the following result in [30] on page 313, Proposition 2.5.

**Proposition 6.1** Let \( \tilde{Z}_1 \) be a special frame dual to \( \tilde{\theta}^1 \) (such that \( \tilde{h}_{1T} = 2 \)). Let \( \theta^1 = \sqrt{2} \tilde{\theta}^1 \) be a unitary coframe (i.e., \( h_{11} = 1 \)). Then in pseudohermitian normal coordinates \((z, t)\) with respect to \( \tilde{Z}_1 \), \( \tilde{\theta}^1 \), we have

- (a) \( \theta_{(2)} = \theta_0 \); \quad \( \theta_{(3)} = 0 \); \quad \( \theta_{(m)} = \frac{1}{m} \sqrt{2} \left( i z \theta^1 - i \bar{\theta}^1 \right) \right)_{(m)} \), \quad \( m \geq 4 \);
- (b) \( \theta_{(1)} = \sqrt{2} dz \); \quad \( \theta_{(2)} = 0 \); \quad \( \theta_{(m)} = \frac{1}{m} \left( \sqrt{2} z \theta^1 + 2t A_{T1} \theta^1 - \sqrt{2} \bar{\theta} A_{TT} \theta \right) \right)_{(m)} \), \quad \( m \geq 3 \)
- (c) \( \omega^1_{(1)} = 0 \); \quad \( \omega^1_{(m)} = \frac{1}{m} \left( \sqrt{2} R (z \theta^1 - \bar{\theta}^1) + A_{11} (\sqrt{2} z \theta - 2 \theta^1) - A_{11,1} (\sqrt{2} \bar{\theta} - 2 \bar{\theta}^1) \right) \right)_{(m)} \), \quad \( m \geq 2 \).

**Definition 6.2** Given a three dimensional pseudohermitian manifold \((M, \theta)\) we define a real symmetric tensor \( Q \) as

\[ Q = Q_{jk} \theta^j \otimes \theta^k, \quad j, k \in \{0, 1, T\} \]

whose components with respect to any admissible coframe are given by

\[ Q_{11} = Q_{11} = 3i A_{11}; \quad Q_{1T} = Q_{11} = h_{11} R; \]

\[ Q_{01} = Q_{01} = Q_{01} = 4 A_{11} + i R_{11}; \quad Q_{00} = 16 \text{Im} A_{11,11} - 2 \Delta_b R. \]
We have then the following result, see page 315 in [30], Theorem 3.1.

**Proposition 6.3** 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 \( \theta \) such that all symmetrized covariant derivatives of \( Q \) with total order less or equal than \( N \) vanish at \( q \), that is

\[
Q_{(jk,L)} = 0 \quad \text{if} \quad O(jkL) \leq N.
\]

**Remark 6.4** (a) For a multi index \( L = (l_1, \ldots, l_s) \) we count its order as

\[
O(J) = O(j_1) + \cdots + O(j_s),
\]

where \( O(1) = O(\bar{1}) = 1 \) and where \( O(0) = 2 \).

(b) The symmetrized covariant derivatives are defined by

\[
Q_{(L)} = \frac{1}{s!} \sum_{\sigma \in S_s} Q_{\sigma L}; \quad \sigma L = (l_{\sigma(1)}, \ldots, l_{\sigma(s)}).
\]

Let us apply Proposition 6.3 for \( N = 4 \) and derive some consequences. At order 2, at \( q \) we have

\[
0 = Q_{11} = 3iA_{11}; \quad 0 = Q_{1\bar{1}} = R.
\]

At order 3 we have

\[
0 = Q_{01} = 4A_{11, 1} + iR, \quad 0 = Q_{10} = Q_{11, 1} + 3iA_{11, \bar{1}} + R, \quad 0 = 3iA_{11, \bar{1}} + 2R.
\]

These two equations imply that

\[
A_{11, \bar{1}} = R, \quad 0 = 3iA_{11, \bar{1}} + 2R.
\]

We also have

\[
0 = Q_{(11, 1)} = 4A_{11, 1} = 3iA_{11, 1}.
\]

At order 4 we find

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

and

\[
0 = Q_{10, 0} + Q_{01, T} + Q_{0T, 1} = R_0 + (4A_{11, 1} + iR)T + \left(4A_{\bar{T}, T} - iR\right)_{\bar{T}}.
\]

This quantity is equal to

\[
0 = R_0 + 4A_{11, \bar{T}} + 4A_{\bar{T}, 1} + iR_1 + \left(4A_{\bar{T}, T} - iR\right)_{\bar{T}}.
\]

We also have that

\[
0 = Q_{11, 0} + Q_{10, 1} + Q_{01, 1} = 3iA_{11, 0} + 2(4A_{11, 1} + iR_1)_1 = 3iA_{11, 0} + 8A_{11, 1} + 2iR_{11};
\]

\[
0 = Q_{(11, \bar{T})} = 4Q_{11, \bar{T}} + 4Q_{1\bar{T}, T} + 4Q_{\bar{T}, 11} + 4Q_{\bar{T}, T} + 4Q_{
\bar{T}, 1\bar{T}}.
\]

This quantity is equal to

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

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

\[ 24Q_{(11,11)} = 6(Q_{11,11} + Q_{11,11} + Q_{11,11} + Q_{11,11}) = 6(3i(A_{11,11} + A_{11,11} + 2R_{,11}), \]

and

\[ (145) \quad 0 = 3i(A_{11,11} + iA_{11,0} + 2RA_{11} + A_{11,11}) + 2R_{,11} = -3A_{11,0} + 6iA_{11,11} + 2R_{,11}. \]

From (144), (145) and the definition of Cartan tensor \( \Omega \) (see page 227 in [19]) we have that, at \( q \)

\[
\begin{aligned}
\begin{cases}
3iA_{11,0} + 8A_{11,11} + 2iR_{,11} = 0; \\
-3A_{11,0} + 6iA_{11,11} + 2R_{,11} = 0; \\
-6A_{11,0} - 4iA_{11,11} + R_{,11} = 6\Omega_{11},
\end{cases}
\end{aligned}
\]

where

\[ \Omega_{11} = \frac{4}{6} R_{,11} + i \frac{2}{6} R A_{11} - A_{11,0} - \frac{2}{3} i A_{11,11}. \]

Therefore we deduce that, at \( q \)

\[ A_{11,0} = -\frac{4}{5} \Omega_{11}; \quad A_{11,11} = \frac{12}{35} i \Omega_{11}; \quad R_{,11} = -\frac{6}{35} \Omega_{11}. \]

For \( N = 4 \), suppose we have chosen a contact form \( \hat{\theta} \) such that (143) holds true. Then one can check that

\[ \hat{\omega}^{1}_{(2)} = \hat{\omega}^{1}_{(3)} = 0; \quad \hat{\theta}^{1}_{(3)} = \hat{\theta}^{1}_{(4)} = 0; \quad \hat{\theta}^{1}_{(4)} = 0. \]

For example we have

\[ \hat{\omega}^{1}_{(2)} = \frac{1}{2} \left( \sqrt{2i} R(z\hat{\theta}^{1} - \zeta^{1}) + A_{11,11}(\sqrt{2}z\hat{\theta} - 2t\hat{\theta}^{1}) - A_{11,11}(\sqrt{2}\zeta\hat{\theta} - 2t\hat{\theta}^{1}) \right)_{(2)} \]

\[ = \frac{1}{2} \left( \sqrt{2}z(R\hat{\theta}^{1})(1) - \sqrt{2z}(R\hat{\theta}^{1})(1) + \sqrt{2z}(A_{11,11}\hat{\theta})(1) - 2t(A_{11,11}\hat{\theta})(0) \right) - \sqrt{2}(A_{11,11}\hat{\theta})(1) + 2t(A_{11,11}\hat{\theta})(0) \right) = 0, \]

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

\[ \hat{\omega}^{1}_{(4)} = \frac{1}{4} \left( \sqrt{2i} R(z\hat{\theta}^{1} - \zeta^{1}) + A_{11,11}(\sqrt{2}z\hat{\theta} - 2t\hat{\theta}^{1}) - A_{11,11}(\sqrt{2}\zeta\hat{\theta} - 2t\hat{\theta}^{1}) \right)_{(4)} \]

\[ = \frac{1}{4} \left( \sqrt{2}z(R\hat{\theta}^{1})(3) - \sqrt{2z}(R\hat{\theta}^{1})(3) + \sqrt{2z}(A_{11,11}\hat{\theta})(3) - 2t(A_{11,11}\hat{\theta})(2) \right) - \sqrt{2}(A_{11,11}\hat{\theta})(3) + 2t(A_{11,11}\hat{\theta})(2) \right) \]

\[ = \frac{1}{4} \left( 2R_{(2)} z d\tau - 2R_{(2)} \zeta d\tau + \sqrt{2}(A_{11,11}\hat{\tau})(1) z\theta_{0} - 2(A_{11,11}\hat{\tau})(1) t \sqrt{2} d\tau \right) - \sqrt{2}(A_{11,11}\hat{\tau})(1) z\theta_{0} + 2(A_{11,11}\hat{\tau})(1) t \sqrt{2} d\tau \]

\[ = \frac{1}{4} \left( \sqrt{2}R_{(2)} z - 2(A_{11,11}\hat{\tau})(1) t \right) \sqrt{2} d\tau + \frac{1}{4} \left( \sqrt{2}R_{(2)} z + 2(A_{11,11}\hat{\tau})(1) t \right) \sqrt{2} d\tau \]

\[ + \frac{1}{4} \left( (A_{11,11}\hat{\tau})(1) z - (A_{11,11}\hat{\tau})(1) z \right) \theta_{0}, \]

so we deduce

\[ \hat{\omega}^{1}_{(4)} = (-R_{,11}(q) z^{2} - R_{,11}(q) \zeta^{2} - A_{11,11}(q) z t) d\tau + (R_{,11}(q) z^{3} + R_{,11}(q) \zeta^{2} z + A_{11,11}(q) \zeta^{2} z) d\tau \]

\[ + \frac{1}{2} (A_{11,11}(q) z^{2} - A_{11,11}(q) \zeta^{2} \theta_{0}. \]
Hence we conclude
\[ \omega_1^1 = O(\rho^3)dz + O(\rho^3)d\bar{\tau} + O(\rho^3)\theta_0. \]
We also have
\[
\hat{\theta}_1^{(5)} = \frac{1}{5} \left( \sqrt{2}z\omega_1^1 + 2tA_{11}^T\hat{\theta}^1 - \sqrt{2}zA_{11}^T\theta \right)_{(5)} = \frac{1}{5} \left( \sqrt{2}z(\omega_1^1)_{(4)} + 2t(A_{11}^T\hat{\theta}^1)_{(3)} - \sqrt{2}z(A_{11}^T\theta)_{(4)} \right)
\]
and therefore we get
\[
\hat{\theta}_1^{(5)} = \frac{1}{20} \left( -4R_{11}(q)z^3\bar{\tau} - 4R_{11}(q)\bar{\tau}^3z - 4A_{11,T}(q)z^2t \right) \sqrt{2}dz
+ \left[ \frac{1}{5} \left( R_{11}(q)z^4 + R_{11}(q)z^2\bar{\tau}^2 + A_{11,T}(q)z\bar{\tau} t \right) + \frac{2}{5} A_{11,T}(q)z^2 t^2 + \frac{4}{5} (2A_{11,T}(q) - iA_{11,0}(q))z\bar{\tau} t \right] \sqrt{2}d\bar{\tau}
+ \left[ \frac{\sqrt{2}}{10} (A_{11,T}(q)z^3 - A_{11,T}(q)z\bar{\tau}^2) - \frac{\sqrt{2}}{5} A_{11,T}(q)z\bar{\tau} t - \frac{2\sqrt{2}}{5} (2A_{11,T}(q) - iA_{11,0}(q)) z\bar{\tau}^2 \right] \theta_0,
\]
which implies
\[ \hat{\theta}^1 = (1 + O(\rho^1)) \sqrt{2}dz + O(\rho^3)d\bar{\tau} + O(\rho^3)\theta_0. \]
We also have
\[ \hat{\theta}_1 = \frac{1}{6} \left( \sqrt{2}z\hat{\theta}^1 - \sqrt{2}z\bar{\theta}^1 \right)_{(6)} = \frac{\sqrt{2}}{6} \left( iz\hat{\theta}^1_{(5)} - iz\bar{\theta}^1_{(5)} \right), \]
and hence
\[ \hat{\theta} = (1 + O(\rho^4))\theta_0 + O(\rho^5)dz + O(\rho^5)d\bar{\tau}. \]
Let us now try to understand the behavior of the dual vectors. Let
\[ \hat{W}_1 = (1 + a)\hat{Z}_1 + b\hat{\tau}_1 + c\frac{\partial}{\partial t}, \]
where
\[ \hat{Z}_1 = \frac{1}{\sqrt{2}} \left( \frac{\partial}{\partial z} + iz\frac{\partial}{\partial \bar{\tau}} \right). \]
From these formulas, if we set
\[ \hat{\theta} = \theta_0 + \sum_{m \geq 6} \hat{\theta}_1^{(m)}; \quad \hat{\theta}^1 = \sqrt{2}dz + \sum_{m \geq 5} \hat{\theta}^1_{(m)}; \quad \hat{\theta}^T = \sqrt{2}d\bar{\tau} + \sum_{m \geq 5} \hat{\theta}_{(m)}^T, \]
we have that
\[
0 = \hat{\theta}(\hat{W}_1) = \left( \theta_0 + \sum_{m \geq 6} \hat{\theta}_1^{(m)} \right) \left( (1 + a)\hat{Z}_1 + b\hat{\tau}_1 + c\frac{\partial}{\partial t} \right)
= (1 + a)\theta_0(\hat{Z}_1) + b\theta_0(\hat{\tau}_1) + c\theta_0(\frac{\partial}{\partial t}) + (1 + a) \sum_{m \geq 6} \hat{\theta}_1^{(m)}(\hat{Z}_1) + b \sum_{m \geq 6} \hat{\theta}_1^{(m)}(\hat{\tau}_1) + c \sum_{m \geq 6} \hat{\theta}_{(m)}(\frac{\partial}{\partial t})
= c + O(\rho^5) + aO(\rho^5) + bO(\rho^5) + c(\rho^4)
\]
and hence we find that \( c = O(\rho^5) \).
Similarly
\[ 1 = \hat{\theta}^1(\hat{W}_1) \Rightarrow a = O(\rho^4); \quad 0 = \hat{\theta}^T(\hat{W}_1) \Rightarrow b = O(\rho^4). \]
Also, if we set
\[ \hat{T} = (1 + a)\frac{\partial}{\partial t} + b\hat{Z}_1 + c\hat{\tau}_1, \]
then from
\[ 1 = \hat{\theta}(\hat{T}); \quad 0 = \hat{\theta}^1(\hat{T}); \quad 0 = \hat{\theta}^T(\hat{T}) \]
49
we deduce that \( a = O(\rho^4), b = O(\rho^3), c = O(\rho^3) \), and hence we obtain

\[
\hat{T} = (1 + O(\rho^4)) \frac{\partial}{\partial t} + O(\rho^3)Z_1 + O(\rho^3)Z_T.
\]

In conclusion, we arrive to the following result.

**Proposition 6.5** In CR normal coordinates, for \( N = 4 \) we can choose a contact form \( \hat{\theta} \) such that in pseudohermitian normal coordinates \((z, t)\) we have that

\[
\hat{\theta} = (1 + O(\rho^4)) \theta_0 + O(\rho^5)dz + O(\rho^5)d\overline{z} + O(\rho^3)\theta_0;
\]

\[
\hat{\omega}_1 = O(\rho^5)dz + O(\rho^5)d\overline{z} + O(\rho^3)\theta_0;
\]

\[
\hat{W}_1 = (1 + O(\rho^4)) Z_1 + O(\rho^5)Z_T + O(\rho^5)\frac{\partial}{\partial t};
\]

\[
\hat{T} = (1 + O(\rho^4)) \frac{\partial}{\partial t} + O(\rho^3)Z_1 + O(\rho^3)Z_T;
\]

where

\[
\theta_0 = dt + izd\overline{z} - i\overline{z}dz;
\]

\[
Z_1 = \frac{1}{\sqrt{2}} \left( \frac{\partial}{\partial z} + i\frac{\partial}{\partial t} \right);
\]

\[
\rho^4 = t^2 + |z|^4.
\]

The above computation concluding the proof of Proposition 6.5 was first done by H.-L. Chiu in the summer of 2007 when he visited J.-H. Cheng.

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