CR INVARIANT POWERS OF THE SUB-LAPLACIAN

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Abstract. CR invariant differential operators on densities with leading part a power of the sub-Laplacian are derived. One family of such operators is constructed from the “conformally invariant powers of the Laplacian” via the Fefferman metric; the powers which arise for these operators are bounded in terms of the dimension. A second family is derived from a CR tractor calculus which is developed here; this family includes operators for every positive power of the sub-Laplacian. This result together with work of Čap, Slovák and Souček imply in three dimensions the existence of a curved analogue of each such operator in flat space.

1. Introduction

Invariant differential operators have a long history of importance and this is particularly the case for operators of Laplace type. The conformally invariant Laplacian is the basic example in conformal geometry. A family of higher order generalizations of the conformal Laplacian with principal part a power of the Laplacian was constructed in [22] and has been the subject of recent interest. In CR geometry, the CR invariant sub-Laplacian of Jerison-Lee ([27]) plays a role analogous to that of the conformal Laplacian. In this paper we construct and study generalizations of the Jerison-Lee sub-Laplacian which are CR analogues of the “conformally invariant powers of the Laplacian”.

One can deduce the existence of some such operators in the CR case from the conformal operators via the Fefferman metric. Fefferman [12] showed that to a CR manifold $M$ of dimension $2n + 1$ one can associate a conformal structure on a circle bundle $\mathcal{C}$ of dimension $N = 2n + 2$. On conformal manifolds of dimension $N$, the construction in [22] produces for each $w$, such that $N/2 + w = k \in \mathbb{N}$ and $k \leq N/2$ if $N$ is even, a conformally invariant natural differential operator $P_k : \mathcal{E}(w) \to \mathcal{E}(w - 2k)$, with principal part $\Delta^k$, where $\mathcal{E}(w)$ denotes

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the space of conformal densities of weight $w$. As we explain in the
next section, on a CR manifold one can consider CR densities $E(w, w')$
parametrized by (bi-)weights $(w, w') \in \mathbb{C} \times \mathbb{C}$. It is necessary that
$w - w' \in \mathbb{Z}$ in order that $E(w, w')$ be well-defined and this is always
implicitly assumed. The space $E(w, w')$ of CR densities on $M$ can
be naturally regarded as a subspace of the space of conformal densities
$E(w + w')$ on $\mathcal{C}$. The operators $P_k$ for the Fefferman metric can be shown
to preserve the subspaces of CR densities and it is straightforward to
calculate the principal part of the induced operators. One thereby
obtains:

**Theorem 1.1.** Let $n + 1 + w + w' = k \in \mathbb{N}$ with $k \leq n + 1$. There is
a CR invariant natural differential operator

$$P_{w,w'} : E(w, w') \to E(w - k, w' - k)$$

whose principal part agrees with that of $\Delta^k_b$.

In the case that $M$ is a flat CR manifold, the hypothesis $k \leq n + 1$
is unnecessary in this construction and in the flat case the operators
$P_{w,w'}$ exist for all $(w, w')$ such that $n + 1 + w + w' \in \mathbb{N}$.

In the conformal case, it is conjectured that if $N$ is even and $k > N/2$,
there is no natural operator with principal part $\Delta^k$ mapping $E(-N/2 +
k) \to E(-N/2 - k)$. This has been established for $N = 4$, $k = 3$ ([21])
and $N = 6$, $k = 4$ ([35]). Our main result is the existence in the CR
case of the following family of operators, which includes operators of
higher orders. Set $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$.

**Theorem 1.2.** For each $(w, w')$ such that $n + 1 + w + w' = k \in \mathbb{N}$ and
$(w, w') \notin \mathbb{N}_0 \times \mathbb{N}_0$, there is a CR invariant natural differential operator

$$\mathcal{P}_{w,w'} : E(w, w') \to E(w - k, w' - k)$$

whose principal part agrees with that of $\Delta^k_b$.

In order to construct the operators $\mathcal{P}_{w,w'}$, we derive a tractor calculus
for CR geometry which we anticipate will be of independent interest.
The main ingredients are to define a tractor bundle, a complex vector
bundle of rank $n + 2$ over $M$, together with a CR invariant connection,
and an extension of this connection to a so-called tractor $D$ operator
between weighted tractor bundles. We give a direct derivation of these
in terms of the pseudohermitian Tanaka-Webster connection induced
by a choice of contact form on $M$, parallel to the derivation in [1] in
the projective and conformal cases. The tractor bundle and connection
can also be derived from the CR Cartan connection of Cartan, Tanaka,
Chern-Moser, but we found it preferable to proceed directly, especially
for the tractor $D$ calculus needed for the construction of the invariant operators. See [1], [9], [17], [4] for further discussion and background about tractors. Given this machinery, the construction of the operators $P_{w,w'}$ follows a similar construction of Eastwood and Gover in the conformal case described in [17], involving iterating tractor $D$'s. The operators so constructed are strongly invariant in the sense of [9], i.e. they act invariantly not just on scalar densities but also on density-valued tractors. Note that the tractor construction does not yield an operator in the case $w = w' = 0$ even though the construction via the Fefferman metric does; this is the only weight for which this occurs. However, when $n = 1$, a refinement of the tractor construction does produce a CR invariant (but not necessarily strongly invariant) operator $P_{0,0} : \mathcal{E}(0,0) \to \mathcal{E}(-2,-2)$, which by direct calculation can be seen to agree with $P_{0,0}$. Based on the situation in the conformal case ([18]), we do not anticipate that the operators $P_{w,w'}$ and $P_{w,w'}$ agree in general when both are defined. In fact, one must make choices of orderings and conjugations in defining $P_{w,w'}$, and one expects that different choices will in general lead to different operators. In the flat case, the tractor construction (suitably interpreted) also produces operators for all $(w,w')$ for which $n + 1 + w + w' \in \mathbb{N}$; these do agree with the corresponding operators constructed via the Fefferman metric.

A construction of invariant natural operators is given in [6] for general parabolic geometries, of which CR geometry is a special case. This construction produces curved analogues of many invariant operators on the flat homogeneous model, in the case when the flat operators are standard and act between irreducible bundles corresponding to integral non-singular highest weight vectors. For CR geometry with $n \geq 2$, any flat operator $P_{w,w'}$ satisfying these criteria has $\min\{w,w'\} \leq -n - 1$. So in these dimensions Theorem 1.2 substantially extends the results of [6]. However, the three dimensional case is special: the relevant parabolic is a Borel subalgebra, so all flat operators are standard. There do exist bundles $\mathcal{E}(w,w')$ with $w + w' + 2 \in \mathbb{N}$ corresponding to non-integral or singular highest weight vectors, for which [6] does not apply. However, one can check that if $(w,w') \in \mathbb{N}_0 \times \mathbb{N}_0$, then the highest weight vector for the bundle $\mathcal{E}(w,w')$ is integral and non-singular. We are not aware that it has been established in general that a given specific operator constructed in [6] has the desired principal part, or even is nonzero. However, it is possible to show that this is the case for all the operators which arise in three dimensional CR geometry. Therefore, in three dimensions Theorem 1.2 and [6] together yield the existence of a curved version of each of the flat operators:
Theorem 1.3. For each \((w, w')\) satisfying \(w + w' + 2 = k \in \mathbb{N}\), there is a natural differential operator on three dimensional CR manifolds mapping \(\mathcal{E}(w, w') \to \mathcal{E}(w - k, w' - k)\), whose principal part agrees with that of \(\Delta^k_b\).

Kengo Hirachi has informed us that he has established the existence of such an operator in three dimensions mapping \(\mathcal{E}(1, 1) \to \mathcal{E}(-3, -3)\) via the CR ambient metric with ambiguity derived in [26]. We are grateful to Andi Čap for pointing out to us the special applicability of [6] in the three dimensional case.

In Section 2 we review the basic facts about CR structures and pseudohermitian geometry. We derive the tractor bundle, its connection, curvature, and the tractor \(D\) operators in Section 3. These in turn are used in Section 4 to construct the operators \(P_{w,w'}\). The main point in proving Theorem 1.2 is that there are natural candidate operators which can be written down in terms of iterated tractor \(D\) operators whose principal part is a multiple of \(\Delta^k_b\) and it must be determined when the multiple is nonzero. This leads to some numerology in calculating the multiple for flat space. Finally in Section 5 we review Lee’s formulation of the Fefferman metric and the GJMS construction of the conformal operators and present the details of the proof of Theorem 1.1. We show how this derivation via the Fefferman metric can be reformulated in terms of Fefferman’s ambient metric and also in terms of the Kähler-Einstein metric of Cheng-Yau when \(M\) is a hypersurface in \(\mathbb{C}^{n+1}\), and close with a brief discussion of \(Q\)-curvature in the CR case. Our presentation in this section in terms of the Fefferman metric is influenced by the point of view explicated in [14]. In Sections 4 and 5 we also prove that the operators \(P_{w,w'}\) and \(P_{w,w'}\) are self-adjoint (for \(P_{w,w'}\) the orderings of the \(D\) operators in the iteration must be chosen appropriately).

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2. Pseudohermitian Geometry

A CR-structure on a \((2n + 1)\)-dimensional smooth manifold \(M\) is an \(n\)-dimensional complex subbundle \(T^{1,0} \subset CTM\) such that \(T^{1,0} \cap \overline{T^{1,0}} = \{0\}\) and satisfying the integrability condition \([T^{1,0}, T^{1,0}] \subseteq T^{1,0}\), where we have used the same notation \(T^{1,0}\) for the bundle and the space of its smooth sections. Set \(T^{0,1} = \overline{T^{1,0}}\) and define \(\Lambda^{1,0} \subset CT^*M\) by \(\Lambda^{1,0} = (T^{0,1})^*\). The canonical bundle \(\mathcal{K} := \Lambda^{n+1}(\Lambda^{1,0})\) is a complex line bundle on \(M\). We will assume that \(\mathcal{K}\) admits an \((n + 2)\text{nd}\) root and we fix a bundle denoted \(\mathcal{E}(1, 0)\) which is a \(-1/(n + 2)\) power of
K. The bundle $E(w, w') := (E(1, 0))^w \otimes (\overline{E(1, 0)})^{w'}$ of $(w, w')$-densities is defined for $w, w' \in \mathbb{C}$ satisfying $w - w' \in \mathbb{Z}$. (If $E(1, 0) \setminus \{0\}$ is viewed as a $\mathbb{C}^*$-principal bundle, then $E(w, w')$ is the bundle induced by the representation $\lambda \to \lambda^w \overline{\lambda}^{w'}$ of $\mathbb{C}^*$.) Without further comment, we will assume implicitly whenever we write $E(w, w')$ that $w, w' \in \mathbb{C}$ and $w - w' \in \mathbb{Z}$. We will also usually write $E(w, w')$ for the space of sections of this bundle; the interpretation should be clear from context.

The bundle $H = \text{Re}(T^{1,0})$ is a real $2n$-dimensional subbundle of $TM$. $H$ carries a natural almost complex structure map given by $J(Z + \overline{Z}) = i(Z - \overline{Z})$ for $Z \in T^{1,0}$, which induces an orientation on $H$. We will assume that $M$ is orientable, which implies that the bundle $H^\perp \subset T^*M$ admits a nonvanishing global section. A pseudohermitian structure on $M$ is the choice of such a contact 1-form $\theta$. We fix an orientation on the bundle $H^\perp$ and restrict consideration to $\theta$’s which are positive relative to this orientation. The Levi-form of $\theta$ is the Hermitian form $h$ on $T^{1,0}$ defined by

$$h(Z, \overline{W}) = -2i\theta(Z, \overline{W}).$$

We assume that the CR structure is nondegenerate, i.e. $h$ is a nondegenerate form, whose signature we denote by $(p, q)$, $p + q = n$. Given a pseudohermitian form $\theta$, define $T$ to be the unique vector field on $M$ satisfying

$$\theta(T) = 1 \text{ and } T \lrcorner d\theta = 0.$$  \hspace{1cm} (2.1)

An admissible coframe is a set of $(1, 0)$ forms $\{\theta^\alpha\}$, $\alpha = 1, \ldots, n$, which satisfy $\theta^\alpha(T) = 0$ and whose restrictions to $T^{1,0}$ form a basis for $(T^{1,0})^*$. We will use lower case Greek indices to refer to frames for $T^{1,0}$ or its dual. We may also interpret these indices abstractly, so will denote by $\mathcal{E}^\alpha$ the bundle $T^{1,0}$ (or its space of sections) and by $\mathcal{E}_\alpha$ its dual, and similarly for the conjugate bundles or for tensor products thereof. By integrability and (2.1), we have

$$d\theta = ih_{\alpha \beta} \theta^\alpha \wedge \overline{\theta^\beta}$$

for a smoothly varying Hermitian matrix $h_{\alpha \beta}$, which we may interpret as the matrix of the Levi form in the frame $\theta^\alpha$, or as the Levi form itself in abstract index notation.

It is shown in Lemma 3.2 of [30] (see also (4.3) of [31]) that if $\zeta$ is a (locally defined) nonvanishing section of $\mathcal{K}$, then there is a unique pseudohermitian form $\theta$ with respect to which $\zeta$ is volume normalized.
in the sense that
\[ \theta \wedge (d\theta)^n = i^{n^2} n! (-1)^q \theta \wedge (T \zeta) \wedge (T \overline{\zeta}). \]

This is equivalent to the requirement that \( \zeta \) have unit length with respect to the natural norm induced by \( \theta \) and \( h \). Upon replacing \( \zeta \) by \( \lambda \zeta \), where \( \lambda \) is a smooth \( C^\infty \)-valued function, \( \theta \) is replaced by \( |\lambda|^{2/n+2} \theta \). Now \( |\zeta|^{-2/n+2} := |\zeta|^{-1/(n+2)} \otimes \overline{\zeta}^{-1/(n+2)} \) is a section of \( K^{-1/n+2} \otimes \overline{K}^{-1/n+2} = E(1,1) \), so \( \theta := \theta \otimes |\zeta|^{-2/n+2} \) defines a section of \( T^*M \otimes E(1,1) \) which depends only on the CR structure. The Levi form of \( \theta \) scales the same way, so defines a canonical section \( h_{\alpha \beta} \) of \( E_{\alpha \beta}(1,1) \), where in general we denote the tensor product with a density bundle by omitting the second \( E \):

\[ E_{\alpha}(w,w') := E_{\alpha} \otimes E(w,w'). \]

We will use exclusively \( h_{\alpha \beta} \) and its inverse \( h^{\alpha \beta} \in E^{\alpha \beta}(1,-1) \) to raise and lower indices, so that raising and lowering indices changes weight. The choice of pseudohermitian form \( \theta \) on \( M \) is equivalent to the choice of a \( CR \)-scale \( 0 < t \in E(1,1) \) related by \( \theta = t \theta \), and we also have \( h_{\alpha \beta} = th_{\alpha \beta} \). If \( \Upsilon \in C^\infty(M) \), the change of pseudohermitian structure \( \hat{\theta} = e^{\Upsilon} \theta \) results in \( \hat{h}_{\alpha \beta} = e^{\Upsilon} h_{\alpha \beta} \) and \( \hat{t} = e^{-\Upsilon} t \). A pseudohermitian structure is said to be flat if it is locally equivalent to the Heisenberg group with its standard pseudohermitian structure. It is said to be \( CR \) flat if there is a rescaling of \( \theta \) which is pseudohermitian flat.

A choice of pseudohermitian structure determines a connection on \( TM \), the Tanaka-Webster, or pseudohermitian, connection ([33], [34]). It is given in terms of an admissible coframe by
\begin{equation}
\nabla \theta^\alpha = -\omega^\alpha_\beta \otimes \theta^\beta, \quad \nabla \theta = 0,
\end{equation}

where Webster’s connection 1-forms \( \omega^\alpha_\beta \) satisfy
\[ d\theta^\alpha = \theta^\beta \wedge \omega^\alpha_\beta + A^\alpha_\beta \theta \wedge \overline{\theta}, \]

and the pseudohermitian torsion tensor \( A_{\alpha \beta} = A_{\alpha \beta} \in E_{(\alpha \beta)} \) is symmetric. (According to our conventions for raising indices, \( A^\alpha_\beta \) is a section of \( E^\alpha_\beta(-1,-1) \).) In particular, this connection preserves \( T^{1,0} \), so induces connections on \( E^\alpha \) and \( E_\alpha \). One has \( \nabla h = 0 \). There is an induced connection on the canonical bundle, and therefore also on all the density bundles \( E(w,w') \).

**Proposition 2.1.** \( \nabla \theta = 0 \)

**Proof.** The definition is \( \theta = \theta \otimes |\zeta|^{-2/n+2} \), where \( \zeta \) is volume normalized with respect to \( \theta \). Since \( \nabla \theta = 0 \), it suffices to show that \( \nabla |\zeta|^2 = 0 \) for such \( \zeta \). Choose an admissible coframe \( \{ \theta^\alpha \} \) such that \( \zeta = \theta \wedge \theta^1 \wedge \cdots \wedge \theta^n \).
The condition that $\zeta$ is volume normalized is equivalent to $\det(h_{a\overline{\alpha}}) = (-1)^q$. By (2.2) we have

$$\nabla\zeta = -\omega^\alpha \otimes \zeta.$$  

(2.3)

It follows that $\nabla |\zeta|^2 = -(\omega^\alpha + \overline{\omega}^\alpha) \otimes |\zeta|^2$. However, from $\nabla h = 0$ one obtains $\omega^\alpha + \overline{\omega}^\alpha = h_{\alpha\overline{\alpha}}h_{\alpha\overline{\alpha}} = 0$ as desired. $\square$

From Proposition 2.1 we conclude that $\nabla t = 0$, where $t$ is the scale associated to $\theta$, and that $\nabla h = 0$.

The pseudohermitian connection preserves the splitting $\mathbb{CTM} = T^{1,0} \oplus T^{0,1} \oplus \text{span} T$. Therefore, if we decompose a tensor field relative to this splitting (and/or its dual), we may calculate the covariant derivative componentwise. Each of the components may be regarded as a section of a tensor product of $\mathcal{E}^\alpha$ or its dual or conjugates thereof. Therefore we will often restrict consideration to the action of the connection on $\mathcal{E}^\alpha$ or $\mathcal{E}_\alpha$. We will use indices $\alpha, \overline{\alpha}, 0$ for components with respect to the frame $\{\theta^\alpha, \theta^\overline{\alpha}, \theta\}$ and its dual, so that the 0-components incorporate weights. If $f$ is a (possibly density-valued) tensor field, we will denote components of the (tensorial) iterated covariant derivatives of $f$ in such a frame by preceding $\nabla$’s, e.g. $\nabla_\alpha \nabla_0 \cdots \nabla_\beta f$. As usual, such indices may alternately be interpreted abstractly. So, for example, if $f_\beta \in \mathcal{E}_\beta(w, w')$, we will consider $\nabla f$ as the triple $\nabla_\alpha f_\beta \in \mathcal{E}_{\alpha\beta}(w, w')$, $\nabla_\overline{\alpha} f_\beta \in \mathcal{E}_{\overline{\alpha}\beta}(w, w')$, $\nabla_0 f_\beta \in \mathcal{E}_\beta(w - 1, w' - 1)$.

The torsion and curvature of $\nabla$ can be described by structure equations for the forms $\omega^\alpha_\beta$ (see (2.2) above and (1.3) of [29]), or by commuting second derivatives on functions and 1-forms (see Lemma 2.3 of [31]. We generally follow the same conventions as [31], [29], except that we substitute $\theta, h$ for $\theta, h$ so that all quantities are naturally weighted.) These can be expressed in terms of the pseudohermitian curvature tensor $R_{\alpha\beta\gamma\delta} \in \mathcal{E}_{\alpha\beta\gamma\delta}(1,1)$, $A_{\alpha\beta}$, $\nabla_\gamma A_{\alpha\beta}$, and conjugates of the latter two. Flat pseudohermitian structures are characterized by the vanishing of $R_{\alpha\beta\gamma\delta}$ and $A_{\alpha\beta}$. The Webster-Ricci tensor is defined by

$$R_{\alpha\beta} = -R_{\beta\gamma} R^{\gamma}_{\alpha\beta} \in \mathcal{E}_{\alpha\beta}$$

and the Webster scalar curvature by

$$R = R_{\alpha\alpha} \in \mathcal{E}(-1, -1).$$

From these we define

$$P_{\alpha\beta} := \frac{1}{n+2} \left( R_{\alpha\beta} - \frac{1}{2(n+1)} R h_{\alpha\beta} \right).$$

We will also need to know how to commute derivatives of densities.
Proposition 2.2. If \( f \in \mathcal{E}(w, w') \), then
\[
\nabla_\alpha \nabla_\beta f - \nabla_\beta \nabla_\alpha f = 0
\]
(2.4)
\[
\nabla_\alpha \nabla_\beta f - \nabla_\beta \nabla_\alpha f = \frac{w - w'}{n + 2} R_{\alpha \beta} f - i h_{\alpha \beta} \nabla_0 f
\]
\[
\nabla_\alpha \nabla_0 f - \nabla_0 \nabla_\alpha f = \frac{w - w'}{n + 2} (\nabla_\gamma A_{\gamma \alpha}) f + A_{\alpha \gamma} \nabla_\gamma f.
\]

Proof. We first note that (2.4) holds when \( w = w' = 0 \), since in that case it agrees with Lemma 2.3 of [31]. Now it is a straightforward consequence of the definitions that if \( V \) is a vector bundle with connection over a manifold \( M \), which itself has a linear connection, if \( v^A \) is a section of \( V \), then
\[
[\nabla_i, \nabla_j]v^A = \Omega_{ij}^B v^B - T^k_{ij} \nabla_k v^A,
\]
(2.5)
where here \( i, j, k \) label \( TM \), \( \Omega \) denotes the curvature of the connection on \( V \), \( T^k_{ij} \) denotes the torsion of the connection on \( TM \), and the second covariant derivative is with respect to the coupled connection on \( T^* M \otimes V \). We first apply (2.5) taking \( V \) to be the trivial bundle with the flat connection over our pseudohermitian manifold with its connection: the case \( w = w' = 0 \). The curvature term vanishes, and we conclude that the torsion term in (2.5) is exactly the right hand side of (2.4) for \( w = w' = 0 \). Next let \( w = -(n+2), w' = 0 \), and take \( V = \mathcal{E}(w, w') = \mathcal{K} \) with its induced connection. The form of the torsion term in (2.5) is independent of the choice of \( V \), so takes exactly the same form as in the previous case. To identify the curvature term, observe that since \( \mathcal{K} \) is a line bundle, its curvature is a scalar 2-form on \( M \). Choose an admissible coframe and set \( \zeta = \theta \wedge \theta_1 \wedge \cdots \wedge \theta^n \). Then we have (2.3), so the connection form for \( \mathcal{K} \) relative to the frame \( \{ \zeta \} \) is \( -\omega_\alpha^\alpha \). The curvature of \( \mathcal{K} \) is therefore \( -2d\omega_\alpha^\alpha \). However, (2.3), (2.4) of [31] state that
\[
d\omega_\alpha^\alpha = R_{\alpha \beta} \theta_\beta \wedge \theta + \nabla_\beta A_{\beta \alpha} \theta_\alpha \wedge \theta - \nabla_\beta A_{\beta \alpha} \theta_\alpha \wedge \theta.
\]
Thus (2.5) reduces to (2.4) for \( w = -(n+2), w' = 0 \). The general case now follows upon conjugating, taking powers, and adding. \( \Box \)

Proposition 2.2 together with the formulae in Lemma 2.3 of [31] enable one to calculate the effect of commuting covariant derivatives on any weighted tensor field.

If \( \hat{\theta} = e^\gamma \theta \) is another pseudohermitian form, we can express the connection, curvature, and torsion for \( \hat{\theta} \) in terms of that for \( \theta \). We consider first the relation between the induced connections on tensor products of \( \mathcal{E}^\alpha \) or its dual or conjugates thereof. For efficiency in expressing the
transformation laws, we will denote covariant derivatives of $\Upsilon$ with indices: $\nabla_\alpha \nabla_\beta \Upsilon = \Upsilon_{\alpha \beta}$. One observes first that if $\{\theta^\alpha\}$ is an admissible coframe for $\theta$, then $\hat{\theta}^\alpha = \theta^\alpha + i\Upsilon^\alpha \theta$ defines an admissible coframe for $\hat{\theta}$. Since the restrictions of $\hat{\theta}^\alpha$ and $\theta^\alpha$ to $T^{1,0}$ agree, the components of a section $f$ of $\mathcal{E}^\alpha$ or its dual (or conjugates or tensor products) are the same in the two frames. We will denote by $\tilde{\nabla}_\alpha f$, $\tilde{\nabla}_\pi f$, and $\tilde{\nabla}_0 f$ the components of $\tilde{\nabla} f$ relative to $\{\hat{\theta}^\alpha, \hat{\theta}^\pi, \theta\}$. For example, if $f$ is an unweighted function, one obtains upon changing frames that

$$
(2.6) \quad \tilde{\nabla}_\alpha f = \nabla_\alpha f, \quad \tilde{\nabla}_\pi f = \nabla_\pi f, \quad \tilde{\nabla}_0 f = \nabla_0 f + i\Upsilon^\pi \nabla_\pi f - i\Upsilon^\gamma \nabla_\gamma f.
$$

The connection forms $\hat{\omega}_\alpha^\beta$ for $\tilde{\nabla}$ can be expressed in terms of $\omega_\alpha^\beta$ and $\Upsilon$; this is Lemma 3.4 of [29]. It is straightforward to use this to calculate the analogue of (2.6) for a section $\tau_\beta$ of $\mathcal{E}_\beta$. One obtains:

\[
\begin{align*}
\tilde{\nabla}_\alpha \tau_\beta &= \nabla_\alpha \tau_\beta - \Upsilon_\beta \tau_\alpha - \Upsilon_\alpha \tau_\beta \\
\tilde{\nabla}_\pi \tau_\beta &= \nabla_\pi \tau_\beta + h_{\beta \alpha} \Upsilon^\gamma \tau_\gamma \\
\tilde{\nabla}_0 \tau_\beta &= \nabla_0 \tau_\beta + m \Upsilon^\pi \nabla_\pi \tau_\beta - i(\Upsilon^\gamma \Upsilon_\gamma \tau_\beta - i(\Upsilon^\gamma \Upsilon_\gamma \tau_\beta - i(\Upsilon^\gamma \Upsilon_\gamma \tau_\beta).
\end{align*}
\]

(2.7)

We also need to know how the connection transforms on densities.

**Proposition 2.3.** If $f \in \mathcal{E}(w, w')$, then

\[
\begin{align*}
\tilde{\nabla}_\alpha f &= \nabla_\alpha f + w_\alpha f \\
\tilde{\nabla}_\pi f &= \nabla_\pi f + w' \Upsilon \nabla_\pi f \\
\tilde{\nabla}_0 f &= \nabla_0 f + i\Upsilon^\pi \nabla_\pi f - i\Upsilon^\gamma \nabla_\gamma f \\
&\quad + \frac{1}{n+2} \left[(w + w') \Upsilon_0 + iw\Upsilon_\gamma - iw' \Upsilon_\gamma + i(w' - w) \Upsilon_\gamma \Upsilon_\gamma\right] f
\end{align*}
\]

**Proof.** As in the proof of Proposition 2.2, if we establish the result for $w = -(n + 2)$, $w' = 0$, the general case follows by conjugating, taking powers, and adding. Let $\zeta = \theta \wedge \theta^1 \wedge \cdots \wedge \theta^n$ be a section of $\mathcal{K} = \mathcal{E}(-(n + 2), 0)$. Then $\nabla \zeta$ is given by (2.3). However, also $\zeta = e^{-\gamma} \hat{\theta} \wedge \hat{\theta}^1 \wedge \cdots \wedge \hat{\theta}^n$, so applying (2.3) again gives $\tilde{\nabla} \zeta = -(\hat{\omega}_\alpha^\alpha + d\Upsilon) \otimes \zeta$. Therefore

$$
\tilde{\nabla} \zeta - \nabla \zeta = -(\hat{\omega}_\alpha^\alpha - \omega_\alpha^\alpha + d\Upsilon) \otimes \zeta.
$$

Now Lemma 3.4 of [29] gives $\hat{\omega}_\alpha^\beta - \omega_\alpha^\beta$ in terms of $\Upsilon$. Contracting, adding $d\Upsilon$, and reformulating the result in terms of components yields the desired formulae.

The curvature and torsion also transform under the pseudohermitian change. From Lemma 2.4 of [31] one obtains

$$
(2.8) \quad \tilde{\mathcal{P}}_{\alpha \beta} = \mathcal{P}_{\alpha \beta} - \frac{1}{2} \left(\Upsilon_{\alpha \beta} + \Upsilon_{\beta \alpha}\right) - \frac{1}{2} \Upsilon_\gamma \Upsilon^\gamma h_{\alpha \beta}.
$$
\[
\hat{A}_{\alpha\beta} = A_{\alpha\beta} + i\Upsilon_{\alpha\beta} - i\Upsilon_{\alpha}\Upsilon_{\beta}.
\]

We also will need the transformation laws for two other objects. Set 
\[ P = P_\alpha^\alpha = \frac{1}{2(n+1)}R \]
and define
\[
T_\alpha = \frac{1}{n+2}(\nabla_\alpha P - i\nabla^\beta A_{\alpha\beta}) \in \mathcal{E}_\alpha(-1,-1),
\]
\[ S = -\frac{1}{n}(\nabla^\alpha T_\alpha + \nabla^{\alpha\beta}T_{\alpha\beta} + P_{\alpha\beta}P^{\alpha\beta} - A_{\alpha\beta}A^{\alpha\beta}) \in \mathcal{E}(-2,-2). \]

Straightforward calculation using the formulae discussed above and the Bianchi identities of Lemma 2.2 of [31] gives:
\[
\hat{T}_\alpha = T_\alpha + \frac{i}{2}\Upsilon_{\alpha\beta}Y^{\beta} - iA_{\alpha\beta}Y^{\beta} + \frac{1}{2}Y_{\alpha\beta}Y^{\beta} - \frac{1}{2}Y^{\alpha\beta}Y_{\beta} - \frac{1}{2}Y_{\beta}Y^{\beta}Y_{\alpha},
\]
\[
\hat{S} = S + \frac{i}{2}\Upsilon_{\alpha\beta}Y^{\beta} - \frac{1}{4}(Y_{\alpha\beta}Y^{\beta} - A_{\alpha\beta}Y^{\beta} - A_{\sigma\tau}Y^{\sigma}Y^{\tau})
\]
\[
- 3P_{\alpha\beta}Y^{\alpha}Y^{\beta} - \frac{1}{2}(Y_{\alpha\beta}Y^{\alpha}Y^{\beta} + Y_{\beta}Y^{\alpha}Y^{\beta})
\]
\[
+ \frac{1}{2}(Y_{\alpha\beta}Y^{\alpha}Y^{\beta} + Y_{\beta}Y^{\alpha}Y^{\beta}) + \frac{3}{4}(Y_{\alpha}Y^{\alpha})^2.
\]

We derived the expressions for \( T_\alpha \) and \( S \) from the condition that they satisfy transformation laws of this form, which we needed to construct the tractor connection in the next section. Only later did we observe that they occur already in [30] as components of the connection forms and Ricci tensor of the Fefferman metric. Also, \( T_\alpha \) and a variant of \( S \) arise in [29], where they were combined with \( P_{\alpha\beta} \) and \( A_{\alpha\beta} \) to form a 2-tensor on \( M \) which was used to construct a version of pseudohermitian normal coordinates. In that work, only the part of the transformation laws involving highest derivatives (counted non-isotropically) of \( \Upsilon \) was relevant. The version of \( S \) in [29] therefore does not include the \( P_{\alpha\beta}P^{\alpha\beta} - A_{\alpha\beta}A^{\alpha\beta} \) term, which however is important for us.

3. TRACTORS

The pseudohermitian connection depends on the choice of \( \theta \). In this section we construct a vector bundle of rank \( n + 2 \) over \( M \), the tractor bundle, together with a CR invariant tractor connection. We also show how to extend this connection to a CR invariant tractor \( D \) operator on weighted tractors which can be iterated.

For a given choice of \( \theta \), the (co-)tractor bundle \( \mathcal{E}_A \) is realized as a direct sum
\[
\mathcal{E}_A = \mathcal{E}(1,0) \oplus \mathcal{E}_\alpha(1,0) \oplus \mathcal{E}(0,-1).
\]
The realization corresponding to \( \hat{\theta} = e^{\bar{T}\theta} \) is identified with that for \( \theta \) via
\[
\begin{pmatrix}
\hat{\sigma} \\
\hat{\tau}_\alpha \\
\hat{\rho}
\end{pmatrix} =
\begin{pmatrix}
\sigma \\
\tau_\alpha + \bar{\Upsilon}_\alpha \sigma \\
\rho - \gamma^{\beta} \tau_\beta - \frac{1}{2} (\gamma^{\beta} \gamma_\beta + i \gamma_0) \sigma
\end{pmatrix} = M_\Gamma \begin{pmatrix}
\sigma \\
\tau_\beta \\
\rho
\end{pmatrix},
\]
where \( \sigma \in \mathcal{E}(1,0) \), \( \tau_\beta \in \mathcal{E}_\beta(1,0) \), \( \rho \in \mathcal{E}(0, -1) \), and
\[
M_\Gamma = \begin{pmatrix}
1 & 0 & 0 \\
\gamma_\alpha & 0 & 0 \\
-\frac{1}{2} \left( \gamma^{\gamma} \gamma_\gamma + i \gamma_0 \right) & -\gamma^{\beta} & 1
\end{pmatrix}.
\]
Recalling (2.6), it is easily checked that these identifications are consistent upon changing to yet a third \( \theta \). We may therefore mod them out to obtain a bundle \( \mathcal{E}_A \) determined solely by the CR structure. (More formally, the total space of the bundle \( \mathcal{E}_A \) can be defined to be the disjoint union of one copy of the total space of \( \mathcal{E}(1,0) \oplus \mathcal{E}_\alpha(1,0) \oplus \mathcal{E}(0, -1) \) for each global section \( \theta \), modulo the equivalence relation (3.2). The smooth structure on this total space and the linear structure on the fibers are inherited from that of any of the realizations.) The subspaces \( \{ \sigma = 0 \} \) and \( \{ \sigma = \tau_\alpha = 0 \} \) are preserved by the identifications, so determine canonical subbundles of \( \mathcal{E}_A \). This composition series structure is what remains of the direct sum decomposition (3.1) after making the identifications. The vector given by \( \sigma = \tau_\alpha = 0, \rho = 1 \) is preserved by \( M_\Gamma \), so defines an invariant section of \( \mathcal{E}_A(0,1) = \mathcal{E}_A \otimes \mathcal{E}(0,1) \) which we denote by \( Z_A \). The matrix \( M_\Gamma \) is in \( SU(h_{AB\bar{\gamma}}) \), where
\[
h_{AB\bar{\gamma}} = \begin{pmatrix}
0 & 0 & 1 \\
0 & h_{AB\bar{\gamma}} & 0 \\
1 & 0 & 0
\end{pmatrix}.
\]
It follows that \( h_{AB\bar{\gamma}} \) defines an invariant Hermitian metric on \( \mathcal{E}_A \), and that \( \mathcal{E}_A \) has an invariant volume form. We denote by \( \mathcal{E}_A^\Gamma \) the conjugate bundle, by \( \mathcal{E}^A \) the dual bundle (the tractor bundle), and we use \( h_{AB\bar{\gamma}} \) and its inverse to raise and lower tractor indices.

We define a connection on \( \mathcal{E}_A \) as follows. If
\[
v_A = \begin{pmatrix}
\sigma \\
\tau_\alpha \\
\rho
\end{pmatrix}
\]
is a section of \( \mathcal{E}_A \) in the realization determined by \( \theta \), set
\[
\nabla_\beta v_A = \begin{pmatrix}
\nabla_\beta \sigma - \tau_\beta \\
\nabla_\beta \tau_\alpha + i A_{\alpha\beta} \sigma \\
\nabla_\beta \rho - P_{\beta} \omega \tau_\alpha + T_\beta \sigma
\end{pmatrix},
\]
\[
(3.3) \quad \nabla_\beta v_A = \left( \begin{array}{c}
\nabla_\beta \tau_\alpha + h_{\alpha \beta \rho} + P_{\alpha \beta \sigma} \\
h_{\alpha \beta \rho} + iA_{\beta \rho} - T_{\beta \sigma}
\end{array} \right),
\]
\[
\nabla_0 v_A = \left( \begin{array}{c}
\nabla_0 \tau_\alpha - iP_{\alpha \beta \tau_\beta} + \frac{i}{n+2}P_{\alpha \tau_\alpha} + 2iT_{\alpha \sigma} \\
\nabla_0 \rho + \frac{i}{n+2}P_{\rho} + 2iT_{\alpha \tau_\alpha} + iS_{\sigma}
\end{array} \right),
\]
where \(T_\alpha\) and \(S\) were defined in §2, and where the \(\nabla\)'s on the right hand side refer to the pseudohermitian connection on the appropriate weighted bundles. This operation satisfies a Leibnitz formula so defines a connection on \(E_A\). It is a direct calculation using the transformation formulae in the previous section to show that the definition is independent of the choice of \(\theta\), and therefore CR invariant. For example, consider the second component of \(\nabla_\beta v_A\). Using (2.7), Proposition 2.3, and (2.9), we obtain
\[
\hat{\nabla}_\beta \hat{\tau}_\alpha + i\hat{A}_{\alpha \beta} = \hat{\nabla}_\beta (\tau_\alpha + \Upsilon_\alpha) + i\hat{A}_{\alpha \beta} =
\]
\[
= (\nabla_\beta \tau_\alpha + iA_{\alpha \beta} + \Upsilon_\alpha (\nabla_\beta \sigma - \tau_\beta))
\]
as desired. (Here we verified the full transformation law, but it suffices to check invariance to first order in \(\Upsilon\).) This connection induces connections on the dual and conjugate and tensor product bundles, and a calculation shows that \(\nabla h_{AB} = 0\) (reflecting a Hermitian symmetry inherent in (3.3)). Therefore differentiation commutes with raising and lower tractor indices.

One can calculate the curvature of the tractor connection from (2.5), using the commutation formulae and Bianchi identities of [31]. The result is the following:
\[
\Omega_{\rho \sigma A}^B = 0, \quad \Omega_{\rho \sigma A}^B = 0, \quad \Omega_{\rho A}^B = \left( \begin{array}{ccc}
0 & 0 & 0 \\
iV_{\rho \sigma} & S_{\rho \sigma A} & 0 \\
U_{\rho \sigma} & -iV_{\rho \sigma} & 0
\end{array} \right),
\]
\[
\Omega_{\rho A}^B = \left( \begin{array}{ccc}
0 & 0 & 0 \\
Q_{\rho \sigma} & V_{\rho \sigma} & 0 \\
Y_{\rho} & -iU_{\rho \sigma} & 0
\end{array} \right), \quad \Omega_{\rho A}^B = \left( \begin{array}{ccc}
0 & 0 & 0 \\
-iU_{\rho \sigma} & -V_{\rho \sigma} & 0 \\
-Y_{\rho} & -Q_{\rho \sigma} & 0
\end{array} \right),
\]
where the component tensors are given by
\[
S_{\alpha \beta \sigma} = R_{\alpha \beta \rho \sigma} - P_{\alpha \beta \rho} - P_{\rho \sigma}h_{\alpha \beta} - P_{\alpha \sigma}h_{\rho \beta} - P_{\rho \beta}h_{\alpha \sigma} - P_{\rho \sigma}h_{\alpha \beta} - P_{\rho \beta}h_{\alpha \sigma} - P_{\rho \sigma}h_{\alpha \beta} - P_{\rho \beta}h_{\alpha \sigma},
\]
\[
V_{\alpha \beta \rho} = \nabla_\beta A_{\alpha \rho} + i\nabla_\rho P_{\alpha \beta} - iT_{\rho \alpha \beta} - 2iT_{\alpha \tau_\alpha} - iS_{\sigma} - 2iT_{\alpha \tau_\alpha} - iS_{\sigma}.
\]
$U_{\alpha\beta} = \nabla_\alpha T_\beta + \nabla_\beta T_\alpha + P_{\alpha}^\gamma P_{\gamma\beta} - A_{\alpha\gamma} A^{\gamma\beta} + Sh_{\alpha\beta}$

$Q_{\alpha\beta} = i \nabla_\alpha A_{\alpha\beta} - 2i \nabla_\beta T_\alpha + 2P_{\alpha}^\gamma A_{\gamma\beta}$

$Y_{\alpha} = \nabla_0 T_\alpha - i \nabla_\alpha S + 2i P_{\alpha}^\gamma T_\gamma - 3A_{\alpha} T_{\alpha}$

$V_{\beta\alpha\sigma} = \overline{V}_{\beta\sigma\alpha}, \quad Q_{\alpha\beta} = \overline{Q}_{\beta\alpha}, \quad Y_{\beta} = \overline{Y}_{\beta}$

and have the properties:

$S_{\alpha\beta\gamma\rho} = S_{\rho\beta\alpha\gamma}, \quad S^\alpha_{\beta\rho\sigma} = 0$

$V_{\alpha\beta\gamma} = V_{\gamma\beta\alpha}, \quad V^\alpha_{\beta\gamma} = 0$

$U_{\alpha\beta} = \overline{U}_{\beta\alpha}, \quad U^\alpha_{\beta} = 0$

$Q_{\alpha\beta} = Q_{\beta\alpha}$

This should be compared with the curvature of Chern’s Cartan connection (see [7], [34]). We observe for future reference that the vanishing trace conditions above imply

(3.4) $\Omega_{\rho}^{\rho A B} = 0$.

Next we use the tractor connection to construct a CR invariant second order differential operator $D$ between tractor bundles. Let us write $\mathcal{E}^*(w, w')$ to indicate any weighted tractor bundle (with arbitrary lists of conjugated and/or unconjugated upper and/or lower indices). The tractor $D$ operator

$D_A : \mathcal{E}^*(w, w') \to \mathcal{E}_A \otimes \mathcal{E}^*(w - 1, w')$

is defined by

$D_A f = \left( \begin{array}{c} w(n + w + w') f \\ (n + w + w') \nabla_\alpha f \\ -(\nabla^\beta \nabla_\beta f + iw \nabla_0 f + w(1 + \frac{w' - w}{n+2}) Pf) \end{array} \right)$

in the realization determined by a choice of $\theta$. Here $\nabla_\alpha f$ refers to the tractor connection defined above coupled with the pseudohermitian connection on the relevant density bundle. The $\nabla^\beta$ in the bottom component additionally couples the pseudohermitian connection on $\mathcal{E}_\beta$.

That this definition is CR invariant is again a direct calculation of its transformation under change of $\theta$. The tractor indices on $f$ play no role whatsoever in this calculation since the tractor connection is invariant. The first component does not depend on $\theta$, as required. For the second component, by Proposition 2.3 we have $\overline{\nabla}_\alpha f = \nabla_\alpha f + w \Upsilon_\alpha f$, which is precisely what is required by the identification. The third follows upon transforming the connection using (2.7) and Proposition 2.3 and substituting the contraction of (2.8). Conjugation produces the operator

$D_\Pi : \mathcal{E}^*(w, w') \to \mathcal{E}_\Pi \otimes \mathcal{E}^*(w, w' - 1)$. 
Both $D_A$ and $\Pi_A$ clearly commute with raising and lowering tractor indices. A straightforward calculation from the definition shows that one has

\begin{equation}
D_A Z^A f = (n + w + w' + 2)(n + w + 1)f
\end{equation}

for $f \in \mathcal{E}^*(w, w')$, where here and in what follows we view $Z^A$ as a multiplication operator and we omit the parentheses when composing operators.

One motivation for the $D_A$ operator is its interpretation in flat space. The flat model can be taken to be a real hyperquadric in $\mathbb{C}P^{n+1}$; A section of $\mathcal{E}(w, w')$ can be interpreted as a function on the associated affine null cone $N$ which is homogeneous of degree $(w, w')$. If $n + w + w' \neq 0$, such a function $f$ has a homogeneous extension $\tilde{f}$ off $N$ which is harmonic to first order with respect to the corresponding Laplacian, and one has

\[ D_A f = (n + w + w') \partial_A \tilde{f} |_N. \]

A similar interpretation can be made in the curved case when $M$ is a hypersurface in $\mathbb{C}^{n+1}$; in this situation the extension is required to be harmonic to first order with respect to Fefferman’s ambient metric. Details of this and further connections between tractors and the ambient construction will be given in [5].

It is often useful to decompose $D_A$ into two pieces. Given a choice of $\theta$, let us write $\Box : \mathcal{E}^*(w, w') \to \mathcal{E}^*(w - 1, w' - 1)$ for the operator appearing in the bottom slot of the above formula for the tractor $D$ operator; that is

\begin{equation}
\Box f := \nabla^\alpha \nabla_\alpha f + i w \nabla_0 f + w(1 + \frac{(w' - w)}{n + 2}) P f,
\end{equation}

and by $\overline{\Box} : \mathcal{E}^*(w, w') \to \mathcal{E}^*(w - 1, w' - 1)$ the corresponding conjugate operator given by

\[ \overline{\Box} f := \nabla_\alpha \nabla^\alpha f - i w' \nabla_0 f + w'(1 - \frac{(w' - w)}{n + 2}) P f. \]

We also define $\tilde{D}_A : \mathcal{E}^*(w, w') \to \mathcal{E}_A \otimes \mathcal{E}^*(w - 1, w')$ by

\[ \tilde{D}_A f := \begin{pmatrix} w f \\ \nabla_\alpha f \\ 0 \end{pmatrix}, \]

with conjugate $\tilde{D}_A : \mathcal{E}^*(w, w') \to \mathcal{E}_A^* \otimes \mathcal{E}^*(w, w' - 1)$. Then clearly we have

\begin{equation}
D_A f = (n + w + w') \tilde{D}_A f - Z_A \Box f.
\end{equation}
A direct calculation shows that as operators on any weighted tractor bundle,

\[(\Box, Z_A) = \tilde{D}_A\, .\]

Another calculation (using (3.4)) gives

\[(\Box - \Box) = (n + w + w')(i\nabla_0 + \frac{(w' - w)}{n + 2}P)\]

on \(\mathcal{E}^*(w, w')\). The operators \(\Box\) and \(\tilde{D}_A\) depend on the choice of \(\theta\) and are not CR invariant.

4. Inv\ant Operators Via Tractors

A first attempt to use tractors to construct an invariant operator from densities to densities would be to form \(D_A D^A f\). However, direct calculation shows that this vanishes identically for \(f\) a tractor field of any weight. Note, though, that if \(f\) has weight \((w, w')\) satisfying \(n + w + w' = 0\), then from (3.7)

\[D_A f = -Z_A \Box f.\]

Therefore, \(\Box\) is a CR invariant differential operator

\[\Box : \mathcal{E}^*(w, w') \to \mathcal{E}^*(w - 1, w' - 1), \quad n + w + w' = 0.\]

This is a generalization of the sub-Laplacian of Jerison-Lee ([27]), which is \(\Box\) on \(\mathcal{E}(-\frac{n}{2}, -\frac{n}{2})\). The operator \(\Box\) is also CR invariant when \(n + w + w' = 0\), but from (3.9) we conclude that \(\Box = \Box\) for such \((w, w')\).

It follows immediately from these observations and the invariance of \(D_A\) that for \(k \geq 1\), the operator

\[D^B \cdots D^A \Box D_A \cdots D_B : \mathcal{E}^*(w, w') \to \mathcal{E}^*(w - k, w' - k)\]

is CR invariant if \(n + w + w' = k - 1\). Variants of this operator can also be formed which are invariant between the same spaces by replacing some of the indices by barred indices and by reordering the \(D\) factors independently on either side of the \(\Box\). It is not hard to see that in any choice of CR scale, the principal part of any such operator agrees with a multiple of that of \(\Delta_b^k\), where \(\Delta_b = -(\nabla^\alpha \nabla_\alpha + \nabla^\pi \nabla_\pi)\). However, the multiple can vanish. By calculating these operators explicitly in flat space, we will determine when the multiple is nonzero and thereby prove the following strengthening of Theorem 1.2.

**Theorem 4.1.** For each \((w, w')\) such that \(n + w + w' + 1 = k \in \mathbb{N}\) and \((w, w') \notin \mathbb{N}_0 \times \mathbb{N}_0\), there is a CR invariant natural differential operator

\[P_{w,w'} : \mathcal{E}^*(w, w') \to \mathcal{E}^*(w - k, w' - k)\]
whose principal part agrees with that of $\Delta^k_b$.

For fixed $(w, w')$ as in Theorem 4.1 we shall in general obtain several operators $\mathcal{P}_{w,w'}$ corresponding to different choices of barred and unbarred indices and different orderings of the $D$ factors. We shall see that these operators all agree for a flat CR structure.

It is straightforward but tedious to check directly from the definition that for a flat pseudohermitian structure,

\[ [D_B, D_C] = 0, \quad [D_B, D_C] = 0, \quad \text{and} \quad [\bar{D}_B, D_C] = 0 \]

as operators on any weighted tractor bundle. Since $D_A$ is CR invariant, this remains true if the structure is only CR flat. So in the flat case, it is clear that the order of the $D$ factors is irrelevant.

The following proposition calculates the operators in flat space. The proof of Theorem 4.1 only uses the cases $k_1 = 0$ or $k_2 = 0$, but we include the general case for completeness.

**Proposition 4.2.** Let $(w, w')$ satisfy $n + w + w' + 1 = k \in \mathbb{N}$. Let $k_1, k_2 \in \mathbb{N}_0$ be such that $k_1 + k_2 = k - 1$. For a flat pseudohermitian structure, we have as operators on $E^*(w, w')$:

\[ (4.3) \quad \Box^{D_B \cdots D_I \bar{D}_J \cdots \bar{D}_Q}_{k_1} = (-1)^{k-1} Z_B \cdots Z_I Z_J \cdots Z_Q \Box^k \]

\[ (4.4) \quad D^Q \cdots D^I D^I \cdots D^B \Box^{D_B \cdots D_I \bar{D}_J \cdots \bar{D}_Q}_{k_1} \]

\[ = (-1)^{k-1}(k - 1)! \prod_{i=0}^{k_1-1} (w - i) \prod_{j=0}^{k_2-1} (w' - j) \Box^k \]

\[ (4.5) \quad \Box^k = \Box^k. \]

We have written $\Box^k$ for the $k$-fold composition of $\Box$ with itself. Note that each factor is acting on a different density space, so each $\Box$ in the composition is really a different operator. In case $k_1$ or $k_2$ equals 0, the empty product in (4.4) is to be interpreted as 1.

**Proof of Theorem 4.1 using Proposition 4.2.** Conjugating if necessary, we may assume without loss of generality that $w \notin \mathbb{N}_0$. Set $k_1 = k - 1, k_2 = 0$. The numerical factor on the right hand side of (4.4) is then nonzero. Since the principal part of $-2\Box$ agrees with that of $\Delta_b$, we may define $\mathcal{P}_{w,w'}$ by multiplying the left hand side of (4.1) by the appropriate constant. It is clear that $\mathcal{P}_{w,w'}$ is a CR invariant operator,
and expanding (4.1) shows that it is natural in the sense that it is
given by a universal formula in terms of the pseudohermitian metric,
curvature, torsion, and connection. In flat space it has the correct
principal part, and it is easily seen that the correction terms in curved
space are of lower order.

We remark that the proof shows that in Theorem 4.1 a stronger sta-
tement can be made about the principal part of $P_{w,w'}$: its nonisotropic
principal part, in which derivatives with respect to $T$ are weighted by
a factor of 2, agrees with that of $(-2\Box)^k$.

The proof of Proposition 4.2 is preceded by three lemmas.

Lemma 4.3. Let $k_1, k_2 \in \mathbb{N}_0$ and let $(w, w')$ satisfy $n+w+w' = k_1+k_2$.
For a CR flat structure, we have as operators on $\mathcal{E}^*(w, w')$:

$$\Box_{k_1} D_B \cdots D_I D_J \cdots D_Q = (-1)^{k_1+k_2} Z_B \cdots Z_I Z_J \cdots Z_Q \Box_{k_1,k_2}$$

for a differential operator $\Box_{k_1,k_2}$.

Proof. It follows from (3.7) that if $f \in \mathcal{E}^*(w, w')$, then

$$Z_A \Box_{B} D_B \cdots D_I D_J \cdots D_Q f = -D_A D_B D_C \cdots D_I D_J \cdots D_Q f.$$

Skewing on $A$ and $B$ and recalling (4.2) gives

$$Z_{[A} \Box_{B]} D_C \cdots D_I D_J \cdots D_Q f = 0.$$

Again using (4.2), we can commute the $D$’s to conclude that the com-
mutator can be taken on any of the unbarred indices:

$$Z_{[A} \Box_{B]} \cdots D_I D_J \cdots D_Q f = 0$$

for $F = B, C, \cdots I$. Recalling (3.9), we obtain similarly

$$Z_{[A} \Box_{B]} \cdots D_I D_J \cdots D_M |D_{N]} D_P \cdots D_Q f = 0$$

for $N = J \cdots \bar{Q}$. Therefore

$$\Box_{k_1,k_2}$$

must be proportional to each of $Z_B, \cdots, Z_Q$, and the result follows.

Lemma 4.4. In Lemma 4.3, we have $\Box_{k_1,k_2} = \Box_{k_1',k_2'}$ if $k_1+k_2 = k_1'+k_2'$.

Proof. It suffices to show that for $k_2 \geq 1$ we have $\Box_{k_1,k_2} = \Box_{k_1+1,k_2-1}$
as operators on $\mathcal{E}^*(w, w')$ with $(w, w')$ as in Lemma 4.3. This is a
consequence of (3.7), (4.2) and (3.9) as follows:

\[-1 \cdot k_1 + k_2 Z_A Z_B \cdots Z_I Z_J \cdots Z_Q \Box_{k_1,k_2} = Z_A \Box D_B \cdots D_I D_J \cdots D_Q \]

\[-D_A D_B \cdots D_I D_J \cdots D_Q = D_J \Box D_A D_B \cdots D_I D_K \cdots D_Q \]

\[= (−1)^{k_1+k_2} Z_A Z_B \cdots Z_I Z_J \cdots Z_Q \Box_{k_1+1,k_2−1}. \]

**Lemma 4.5.** For flat pseudohermitian structures, we have

\[\Box, \tilde{D}_A = 0, \quad \Box^k, Z_A = k\Box^{k−1}\tilde{D}_A\]

on any weighted tractor bundle.

**Proof.** The first equation follows by direct calculation from the definitions. The second is a consequence of the first together with (3.8).

**Proof of Proposition 4.2.** According to Lemmas 4.3 and 4.4, in order to establish (4.3) it suffices to show that for \(k \geq 1\), we have for flat pseudohermitian structures \(\Box_{k−1,0} = \Box^k\) as operators on \(E^*(w,w')\) for \(n + w + w' + 1 = k\). We prove this by induction on \(k\). The case \(k = 1\) is clear. Suppose the statement is true for \(k\) and let \(f \in E^*(w,w')\) with \(n + w + w' = k\). Note that it follows from Lemma 4.3 that

\[Z_A \Box_{k−1,0} f = -\Box_{k−1,0} D_A f.\]

Combining this with the induction hypothesis and then using (3.7) and Lemma 4.5 gives

\[Z_A \Box_{k,0} f = -\Box^k D_A f = -\Box^k(k\tilde{D}_A - Z_A \Box)f = Z_A \Box^{k+1} f,\]

as desired.

Now (4.4) follows upon repeatedly applying (3.5) and its conjugate to (4.3), and (4.5) follows upon comparing (4.3) for \(k_2 = 0\) with the conjugate of (4.3) for \(k_1 = 0\), recalling from (3.9) that \(\Box = \Box^\ast\) on \(E^*(w,w')\) for \(n + w + w' = 0\).

For CR flat structures, Lemmas 4.3 and 4.4 show that the operator \(\Box_{k_1,k_2}\) is CR invariant and depends only on \(k_1 + k_2\), and its principal part is easily determined. It follows that for CR flat structures we can extend the definition of \(P_{w,w'}\) to the case \(n + w + w' + 1 = k \in \mathbb{N}\) without the restriction \(k \leq n + 1\) by setting \(P_{w,w'} = (−2)^k \Box_{k_1,k_2}\). Then
for CR flat structures $\mathcal{P}_{w,w'}$ is independent of the choice of barred and unbarred indices (and of their ordering, as already observed).

In the curved case, one expects by analogy with the conformal case (see the discussion in [17], [9]) that it is no longer generally true that $\Box D_B \cdots D_I D_J \cdots D_Q$ is proportional to $Z_B \cdots Z_I Z_J \cdots Z_Q$, necessitating the application of $D^Q \cdots D^J D^I \cdots D^B$ as in (4.4) and leading to the condition $(w, w') \notin \mathbb{N}_0 \times \mathbb{N}_0$ in Theorem 4.1. However, for $k = 2$ this is not necessary even in the curved case: if $f \in \mathcal{E}(w, w')$ with $n + w + w' = 1$, one can see by direct calculation from the definitions that the first two slots of $\Box D_A f$ vanish, so we have $4 \Box D_A f = -Z_AL_{w,w'}f$ for a fourth order operator $L_{w,w'}$ whose principal part agrees with that of $\Delta^2$. Applying $D^A \Phi$ shows that $L_{w,w'} = \mathcal{P}_{w,w'}$ if $w \neq 0$, so in this case nothing new is obtained. However, if $n = 1$ we conclude the existence of an invariant operator $L_{0,0} : \mathcal{E}(0, 0) \to \mathcal{E}(-2, -2)$ not covered by Theorem 4.1. For $n = 1$, we may therefore extend the definition of the family $\mathcal{P}_{w,w'}$ by setting $\mathcal{P}_{0,0} = L_{0,0}$. We shall recover $\mathcal{P}_{0,0}$ and show the existence of higher dimensional analogues mapping $\mathcal{E}(0, 0) \to \mathcal{E}(-n - 1, -n - 1)$ in the next section using the ambient metric.

Next we show that as long as the $D$’s are ordered consistently, the operators $\mathcal{P}_{w,w'}$ constructed in Theorem 4.1 are self-adjoint. Observe first that under the change of scale $\hat{\theta} = e^{\Theta} \theta$, the volume form $\theta \wedge (d\theta)^n$ multiplies by $e^{(n+1)\Theta}$, so the bundle of volume densities can be canonically identified with $\mathcal{E}(-n - 1, -n - 1)$ and $\int_M f$ is invariantly defined for $f \in \mathcal{E}(-n - 1, -n - 1)$. (Throughout this discussion we assume that all sections are compactly supported.) In general, if $L : E \to F$ is a differential operator between complex vector bundles $E$ and $F$, then the formal adjoint $L^* : F^* \otimes \mathcal{E}(-n - 1, -n - 1) \to E^* \otimes \mathcal{E}(-n - 1, -n - 1)$ is defined by

$$\int_M \langle Lu, v \rangle = \int_M \langle u, L^*v \rangle$$

for $u \in \Gamma(E)$, $v \in \Gamma(F^* \otimes \mathcal{E}(-n - 1, -n - 1))$, where $L^*$ denotes the conjugate of the dual bundle to $E$. We have $\mathcal{E}(w, w') = \mathcal{E}(-w', -w)$. If $n + w + w' + 1 = k \in \mathbb{N}$, then by our implicit assumption that $w - w' \in \mathbb{Z}$ it follows that $w, w' \in \mathbb{R}$, so the operators $\mathcal{P}_{w,w'} : \mathcal{E}(w, w') \to \mathcal{E}(w - k, w' - k)$ constructed in Theorem 4.1 have the property that also $\mathcal{P}_{w,w'}^* : \mathcal{E}(w, w') \to \mathcal{E}(w - k, w' - k)$. Recall that the operators $\mathcal{P}_{w,w'}$ depend on a choice of ordering of barred and/or unbarred indices before and after the middle $\Box$. We shall say that the indices are ordered...
Proposition 4.6. If \((w, w')\) is as in Theorem 4.1 and if the indices are ordered consistently, then \(\mathcal{P}_{w, w'} : \mathcal{E}(w, w') \to \mathcal{E}(w - k, w' - k)\) is self-adjoint.

Proof. The proposition clearly follows if we show that \(\Box\) is self-adjoint on \(\mathcal{E}^*(w, w')\) for \(n + w + w' = 0\) and that

\[
\int_M D_A f \cdot g^A = \int_M f \cdot D_A g^A
\]

for \(f \in \mathcal{E}^*(w, w')\), \(g^A \in \mathcal{E}^A \otimes \mathcal{E}^*(-n - w, -n - w' - 1)\), where the suppressed tractor indices on \(f\) and \(g^A\) are the same and we have denoted by \('\cdot'\) the full contraction of these tractor indices.

An easy calculation shows that the divergence operator \(f_\alpha \to \nabla^\alpha f_\alpha\) is CR invariant : \(\mathcal{E}_\alpha(-n, -n) \to \mathcal{E}(-n - 1, -n - 1)\) and integration by parts (see (2.18) of [31]) shows that

\[
\int_M \nabla^\alpha f_\alpha = 0
\]

for \(f_\alpha \in \mathcal{E}_\alpha(-n, -n)\). Also it is easily seen from (3.6), (2.4) and (3.4) that

\[
n\Box = n\nabla^\alpha \nabla_\alpha + w[\nabla^\alpha, \nabla_\alpha] + w(n + w - w') P
\]

on \(\mathcal{E}^*(w, w')\). Therefore for \(f \in \mathcal{E}^*(w, w'), g \in \mathcal{E}^*(-n - w, -n - w')\) we have

\[
n \int_M \Box f \cdot g = \int_M (n\nabla^\alpha \nabla_\alpha f + w[\nabla^\alpha, \nabla_\alpha] f + w(n + w - w') P f) \cdot g
\]

\[
= \int_M f \cdot (n\nabla_\alpha \nabla^\alpha g + w[\nabla_\alpha, \nabla^\alpha] g + w(n + w - w') P g)
\]

\[
= \int_M f \cdot (n\nabla^\alpha \nabla_\alpha g - (n + w)[\nabla^\alpha, \nabla_\alpha] g + w(n + w - w') P g)
\]

\[
= n \int_M f \cdot (\Box g + (n + w + w') P g).
\]

Self-adjointness of \(\Box\) when \(n + w + w' = 0\) follows immediately from this together with the fact that \(\Box = \overline{\Box}\) when \(n + w + w' = 0\). Finally,
if \( f \in \mathcal{E}^*(w, w') \) and
\[
g_A = \begin{pmatrix} \sigma \\ \tau \alpha \\ \rho \end{pmatrix} \in \mathcal{E}_A \otimes \mathcal{E}^*(\omega, \omega' - n - w' - 1),
\]
then the definition of \( D_A \) gives
\[
D_A f \cdot g_A = w(n + w + w') f \cdot \rho + (n + w + w') \nabla_\alpha f \cdot \tau^\alpha - \square f \cdot \sigma,
\]
while a computation shows that
\[
D_A g_A = w(n + w + w') \rho - (n + w + w') \nabla_\alpha \tau^\alpha - (\square + (n + w + w') \rho) \sigma.
\]
Therefore (4.6) follows from (4.7) and (4.8).

5. Invariant Operators Via Fefferman Metric

In this section we review Lee’s formulation ([30]) of the Fefferman conformal structure and the construction in [22] of the invariant powers of the Laplacian on a conformal manifold via the ambient metric. Combining these produces CR invariant powers of the sub-Laplacian. For a hypersurface in \( \mathbb{C}^{n+1} \), this construction can be expressed in terms of Fefferman’s original formulation, and reexpressed in terms of the associated Cheng-Yau metric.

In Lee’s formulation (see also [11], [3]), the Fefferman metric of a CR manifold \( M \) lives on the circle bundle \( K^*/\mathbb{R}_+ \), where \( K \) denotes the canonical bundle of \( M \), and \( K^* = K \setminus 0 \). A section \( \zeta \) of \( K^* \) determines a fiber variable \( \psi \) on \( K^*/\mathbb{R}_+ \) by the requirement that \( e^{i\psi} \zeta \) be in the given \( \mathbb{R}_+ \)-equivalence class. Suppose that \( \theta \) is a choice of pseudohermitian form, that \( \zeta \) is volume normalized with respect to \( \theta \), and choose an admissible coframe \( \theta^\alpha \) such that \( \zeta = \theta \wedge \theta^1 \wedge \cdots \wedge \theta^n \). The 1-form \( \sigma \) on \( K^*/\mathbb{R}_+ \) defined by
\[
(n + 2) \sigma = d\psi + i \omega^\alpha - \frac{1}{2(n + 1)} R \theta
\]
is independent of the choice of \( \zeta \) and \( \theta^\alpha \), so depends only on \( \theta \) and is globally defined. The Fefferman metric associated to \( \theta \) is the metric of signature \( (2p + 1, 2q + 1) \) given by
\[
g = h_{\alpha\beta} \theta^\alpha \cdot \theta^\beta + 2 \theta \cdot \sigma.
\]
In [30] it is shown that if \( \hat{\theta} = e^\tau \theta \), then \( \hat{g} = e^{\tau} g \), so that the conformal class of \( g \) is CR invariant. Lee also explicitly calculated the connection forms and Ricci curvature of \( g \). From his expression for the connection, it follows that all components of the curvature tensor of
and its iterated covariant derivatives are given by universal expressions in the pseudohermitian metric, curvature and torsion and their pseudohermitian covariant derivatives.

As in Section 2, we assume that $\mathcal{K}$ admits an $(n+2)^{\text{nd}}$ root, which we fix. For our purposes it will be useful to work on the circle bundle $\mathcal{C} = (\mathcal{K}^*)^{1/(n+2)}/\mathbb{R}_+$. The Fefferman metric pulls back via the $(n+2)^{\text{nd}}$ power map to a metric on $\mathcal{C}$ which we shall also denote by $g$. A fiber variable $\gamma$ on $\mathcal{C}$ satisfies $(n+2)^{\gamma} = \psi$.

The metric bundle of a manifold $\mathcal{C}$ of dimension $N$ with a conformal class of metrics $[g]$ of signature $(P,Q)$ is the ray subbundle $G \subset S^2T^*\mathcal{C}$ of multiples of the metric: if $g$ is a representative metric, then the fiber of $G$ over $p \in \mathcal{C}$ is $\{t^2g(p) : t > 0\}$. The bundle of conformal densities of weight $w \in \mathbb{C}$ is $E(w) = G - w/2$, where by abuse of notation we have denoted by $G$ also the line bundle associated to the ray bundle defined above. The main result of [22] is the existence, for $k \in \mathbb{N}$ satisfying $k \leq N/2$ if $N$ is even, of a conformally invariant natural differential operator $P_k : E(-N/2+k) \to E(-N/2-k)$ with principal part equal to that of $\Delta^k$. These operators are constructed in [22] using the ambient metric of [15]. Denote by $\pi : G \to \mathcal{C}$ the natural projection of the metric bundle, and by $g$ the tautological symmetric 2-tensor on $G$ defined for $(p,g) \in G$ and $X,Y \in T_p G$ by $g(X,Y) = g(\pi_\ast X, \pi_\ast Y)$. There are dilations $\delta_s : G \to G$ for $s > 0$ given by $\delta_s(p,g) = (p, s^2 g)$, and we have $\delta_s^* g = s^2 g$. Denote by $S$ the infinitesimal dilation vector field $S = \frac{d}{ds}\delta_s|_{s=1}$. Define the ambient space $\tilde{G} = G \times (-1,1)$. Identify $G$ with its image under the inclusion $i : G \to \tilde{G}$ given by $i(g) = (g, 0)$ for $g \in G$. The dilations $\delta_s$ and infinitesimal generator $S$ extend naturally to $\tilde{G}$. The ambient metric $\tilde{g}$ is a metric of signature $(P+1,Q+1)$ on $\tilde{G}$ which satisfies the initial condition $i^*\tilde{g} = g$, is homogeneous in the sense that $\delta_s^* \tilde{g} = s^2 \tilde{g}$, and is an asymptotic solution of $\text{Ric}(\tilde{g}) = 0$ along $G$. For $N$ odd, these conditions uniquely determine a formal power series expansion for $\tilde{g}$ up to diffeomorphism, but for $N$ even and $N > 2$, a formal power series solution exists in general only to order $N/2$.

An element of $E(w)$ can be regarded as a homogeneous function of degree $w$ on $G$. It is shown in [22] that the same operator $P_k$ arises in two ways:

1. By extending a density $f \in E(-N/2+k)$ to a function $\tilde{f}$ homogeneous of degree $-N/2+k$ on $\tilde{G}$, applying $\tilde{\Delta}^k$, where $\tilde{\Delta}$ denotes the Laplacian in the metric $\tilde{g}$, and restricting back to $G$: $P_k f = \tilde{\Delta}^k \tilde{f}|_G$. 
(2) As the normalized obstruction to extending \( \tilde{f} \in \mathcal{E}(-N/2 + k) \)
to a smooth function \( \tilde{F} \) homogeneous of degree \(-N/2 + k\) on \( \tilde{G} \), such that \( \tilde{F} \) satisfies \( \tilde{\Delta} \tilde{F} = 0 \) to infinite order along \( G \).

For \( N \) even, the condition \( k \leq N/2 \) is needed to ensure that the construction does not involve too many derivatives of the ambient metric. We remark that 2. above can be restated in terms of non-smooth solutions: there are infinite order formal solutions whose expansion includes a log term, and the invariant operator applied to \( f \) can be characterized as a multiple of the restriction to \( G \) of the coefficient of the log term of a formal solution which equals \( f \) on \( G \).

Let now \( M \) be a CR manifold of dimension \( 2n+1 \). We associate to \( M \) its Fefferman conformal manifold \((\mathcal{C}, [g])\), of dimension \( N = 2n+2 \). Volume normalization gives a canonical identification between \((\mathcal{K}^*)^{1/(n+2)}\) (with usual scalar multiplication) and the metric bundle of \((\mathcal{C}, [g])\) (with dilations \( \delta_s \)) as \( \mathbb{R}_+ \)-principal bundles over \( \mathcal{C} \). Now a CR density \( f \in \mathcal{E}(w, w') \) may be viewed as a smooth function on \((\mathcal{K}^*)^{1/(n+2)}\) homogeneous of degree \((w, w')\) in the sense that \( f(\lambda \xi) = \lambda^w \lambda^{w'} f(\xi) \) for \( \xi \in (\mathcal{K}^*)^{1/(n+2)} \). Therefore \( \mathcal{E}(w, w') \) may be regarded as the subspace of the space of conformal densities \( \mathcal{E}(w + w') \) which satisfy

\[
(e^{i\phi})^* f = e^{i(w-w')\phi} f, \quad \phi \in \mathbb{R},
\]

where on the left hand side, \((e^{i\phi})^*\) denotes pull back by the isometry of \((\mathcal{C}, g)\) given by multiplication by \( e^{i\phi} \).

**Proof of Theorem 1.1.** The conformally invariant operator \( P_k \) of [22] satisfies \( P_k : \mathcal{E}(w + w') \to \mathcal{E}(w + w' - 2k) \). Since multiplication by \( e^{i\phi} \) is an isometry of \((\mathcal{C}, g)\) and \( P_k \) is a natural operator, it follows that \( P_k f \) satisfies (5.1) if \( f \) does. Therefore \( P_k \) induces an operator from \( \mathcal{E}(w, w') \) to \( \mathcal{E}(w - k, w' - k) \). Define \( P_{w, w'} = 2^{-k} P_k \big|_{\mathcal{E}(w, w')} \). The CR invariance of \( P_{w, w'} \) follows from the conformal invariance of \( P_k \). Using the formulae in [30] for the connection of the Fefferman metric, one can see without difficulty that any component of an iterated covariant derivative of \( f \in \mathcal{E}(w, w') \) with respect to the Levi-Civita connection of \( g \) has a universal expression in terms of pseudohermitian covariant derivatives of \( f \) and the pseudohermitian metric, torsion and curvature. Since \( P_k \) is a natural differential operator associated to pseudo-Riemannian manifolds, it follows that \( P_{w, w'} \) is a natural differential operator associated to pseudohermitian manifolds in the sense that it also has such a universal expression. It is easily seen that the principal part of \( P_{w, w'} \) agrees with that of \( \Delta^k_b \). \qed
For \( k = 1 \) it is straightforward to carry out the calculation of \( P_{w,w'} \) from the conformal Laplacian \( P_1 \); one finds in that case that \( P_{w,w'} = P_{w,w'} = -2\Box \).

The conformal operators \( P_k \) have been shown in [24] and [16] to be self-adjoint; the argument in [16] is formal and valid in general signature. From this, the self-adjointness of \( P_{w,w'} \) is an easy consequence:

**Proposition 5.1.** If \( n + w + w' + 1 = k \leq n + 1 \), then the operator \( P_{w,w'} : \mathcal{E}(w, w') \to \mathcal{E}(w - k, w' - k) \) is self-adjoint.

**Proof.** If \( f_1, f_2 \in \mathcal{E}(w, w') \), then \( P_{w,w'}f_1 \overline{f_2} = 2^{-k}P_k f_1 \overline{f_2} \in \mathcal{E}(-n - 1, -n - 1) \subset \mathcal{E}(-N) \) is invariant under rotation in \( \mathcal{C} \). It follows that \( \int_M P_{w,w'}f_1 \overline{f_2} \) is a constant multiple of \( \int_C P_k f_1 \overline{f_2} \), so the self-adjointness of \( P_{w,w'} \) follows from that of \( P_k \). \( \square \)

A nondegenerate hypersurface \( M \subset \mathbb{C}^{n+1} \) inheirits a CR structure. This was the setting for Fefferman’s original construction of the ambient metric and conformal metric in [12], [13]. The ambient metric is defined above on \( \mathcal{G}_\mathbb{C} \times (-1, 1) = (K_M)^{1/(n+2)} \times (1, 1) \), which we may identify with \( (K_{\mathbb{C}^{n+1}})^{1/(n+2)} \) over a neighborhood \( U \subset \mathbb{C}^{n+1} \) of \( M \), since \( K_M \) is the restriction of \( K_{\mathbb{C}^{n+1}} \). Introduce a variable \( z^0 \in \mathbb{C} \), which is interpreted as a fiber coordinate on \( (K_{\mathbb{C}^{n+1}})^{1/(n+2)} \) relative to the trivialization defined by \( dz^1 \wedge \cdots \wedge dz^{n+1} \). So the ambient metric is defined on \( \mathbb{C}^* \times U \). Fefferman showed that \( M \) has a smooth defining function \( \phi \) which solves \( J(\phi) = 1 + O(\phi^{n+2}) \), where

\[
J(\phi) = (-1)^{p+1} \det \begin{pmatrix} \phi & \phi_B \\ \phi_a & \phi_{aB} \end{pmatrix}_{1 \leq a,b \leq n+1}
\]

Here the subscripts denote coordinate derivatives and the Levi form \( -\phi_{aB}T_{1,a}M \) has signature \((p, q), p+q = n \). The function \( Q := -|z^0|^2 \phi(z) \) satisfies \((-1)^{q+1} \det(\partial^2_{AB}Q) = |z^0|^{2(n+1)} J(\phi) \), where \( A, B = 0, \ldots, n+1 \). The Hermitian matrix \( (\partial^2_{AB}Q) \) is therefore nondegenerate and defines a Kähler metric \( \tilde{g} \) of signature \((p + 1, q + 1) \) which is approximately Ricci flat along \( M \). This metric is clearly homogeneous of degree 2 and it is shown in [30] that its restriction to \( S^1 \times M \) (Fefferman’s original definition of the Fefferman metric) agrees with the definition above for the Fefferman metric of the pseudohermitian form \( \theta = i(\partial - \overline{\partial}) \phi/2 \). Therefore the Kähler metric \( \tilde{g} \) is the ambient metric associated to \( M \).

We remark that in this formulation, the pseudohermitian form \( \theta = i(\partial - \overline{\partial}) \phi/2 \) is not general: the condition \( J(\phi) = 1 \) on \( M \) means that the closed form \( dz^1 \wedge \cdots \wedge dz^{n+1} \) is volume normalized with respect to \( \theta \). This forces conditions on \( \theta \): if \( n > 1 \) then \( \theta \) is pseudo-Einstein ([31]); the corresponding condition for \( n = 1 \) is given in [25]. Invariance under
rescaling $\theta$ is replaced by invariance under biholomorphic changes of coordinates.

For $M$ a hypersurface in $\mathbb{C}^{n+1}$, a section of $\mathcal{E}(w, w')$ can be regarded as a function on $\mathbb{C}^* \times M$ homogeneous of degree $(w, w')$ in $z^0$. The invariant operators $P_{w,w'}$ are therefore realized as the obstruction to extending such a function to be homogeneous and harmonic with respect to the Laplacian $\tilde{\Delta}$ in the Kähler metric $\tilde{g}$, or equivalently by applying $\tilde{\Delta}^k$ to an arbitrary homogeneous extension.

We next show how this realization of the operators $P_{w,w'}$ can be reformulated in terms of the Kähler metric

$$
\begin{align*}
g_{\alpha\beta} &= (\log \phi^{-1})_{\alpha\beta} \\
\end{align*}
$$
on $\{\phi > 0\} \subset \mathbb{C}^{n+1}$. If $\phi$ solves $J(\phi) = 1$ exactly, then $g$ is the Kähler-Einstein metric of Cheng-Yau [8]. We begin by considering the relationship between the Laplacians of $\tilde{g}$ and $g$ for a general metric of the form (5.2), not necessarily assuming that $\phi$ is an approximate solution of $J(\phi) = 1$. We continue to use capital indices $A, B$ which run between 0 and $n+1$, so for example

$$
\begin{align*}
\tilde{g}_{\alpha\beta} &= \left( \frac{\phi}{|z^0|} \phi^\alpha \phi^\beta \right).
\end{align*}
$$
Lower case indices $a, b$ will be raised and lowered using

$$
\begin{align*}
g_{a\bar{b}} &= -\phi^{-1} \phi_a \phi_{\bar{b}} + \phi^{-2} \phi_a \phi_{\bar{a}}
\end{align*}
$$
and its inverse.

As observed in [32], the choice of defining function $\phi$ determines near $M$ a $(1, 0)$ vector field $\xi^a$ and a scalar function $r$ (called the transverse curvature in [23]), as follows. Observe first that since $\phi_{\bar{a}}|_{T^{1,0}M}$ is non-degenerate, there is a unique direction in $T^{1,0} \mathbb{C}^{n+1}$ which is orthogonal to ker $\partial \phi$ with respect to $\phi_{\alpha\bar{b}}$. Therefore, near $M$ there is a unique $(1, 0)$ vector field $\xi^a$ satisfying

$$
\begin{align*}
\phi_{a\bar{b}} \xi^\bar{b} &= r \phi_a, \\
\xi^a \phi_a &= 1
\end{align*}
$$
for some uniquely determined smooth function $r$, and we have

$$
\begin{align*}
r &= \phi_{a\bar{b}} \xi^a \xi^{\bar{b}}.
\end{align*}
$$

Proposition 5.2. When acting on functions which are homogeneous of degree $(w, w')$ with respect to $z^0$, we have

$$
\begin{align*}
\phi |z^0|^2 \tilde{\Delta} &= \Delta_g + \frac{w' \phi}{1 - r\phi} \xi^a \partial_a + \frac{w^2 \phi}{1 - r\phi} \xi^\bar{a} \partial_{\bar{a}} - \frac{ww' \phi}{1 - r\phi}.
\end{align*}
$$

Here $\tilde{\Delta}$ denotes the Kähler Laplacian $-\tilde{g}^{AB} \partial_A \partial_B$ and similarly for $\Delta_g$. 

Proof. Our first observation is a matrix factorization of $\tilde{g}$ given by (5.3):

$$\tilde{g}_{AB} = \begin{pmatrix} \phi^{1/2} & 0 \\ z^0 \phi^{-1/2} \phi_a & z^0 \phi^{-1/2} \delta_a^c \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & g_{cc} \end{pmatrix} \begin{pmatrix} \phi^{1/2} & z^0 \phi^{-1/2} \phi_a \\ z^0 \phi^{-1/2} \delta_a^c & z^0 \phi^{1/2} \gamma_{cc} \end{pmatrix}.$$  

Taking inverses and multiplying out gives

$$\begin{pmatrix} |z^0|^2 \phi \end{pmatrix} \tilde{g}^{AB} = \begin{pmatrix} |z^0|^2 (\phi^{-2} \phi_a - a) & -z^0 \phi^{-1} \phi_a \\ -z^0 \phi^{-1} \phi_a & g^{ab} \end{pmatrix},$$

from which we obtain

$$\begin{pmatrix} |z^0|^2 \phi \end{pmatrix} \tilde{\Delta} = \Delta g + \phi^{-1} \phi_a \partial_a z^0 \partial_0 + \phi^{-1} \phi_a \partial_a z^0 \partial_0 - (\phi^{-2} \phi_a - 1) |z^0|^2 \partial_a^2,$$

We want to rewrite the coefficients of the last three terms. Define $l_{ab} = r \phi_a \phi_b - \phi_{ab}$ so that $l_{ab} \xi^b = 0$. Then $l_{ab}$ is nondegenerate on ker $\partial$ so we may consider its inverse there, extend to annihilate $\phi_a$, and thus obtain a tensor $k^{ab}$ defined by the relations $k^{ab} \phi_b = 0$ and $k^{ab} l_{bc} = \delta_a^c - \xi^a \phi_b$. Now (5.4) gives $g_{ab} = \phi^{-1} (l_{ab} + (1 - r \phi) \phi^{-1} \phi_a \phi_b)$, so $g^{ab} = (k^{ab} + \phi (1 - r \phi)^{-1} \xi^a \xi^b)$. From this we conclude that $\phi^{-1} g^{ab}$ extends smoothly across $\phi = 0$, and that

$$\phi^a = \frac{\phi^2}{1 - r \phi} \xi^a, \quad \phi^a \phi_a = \frac{\phi^2}{1 - r \phi}.$$ 

Substituting into (5.10) and using homogeneity gives (5.7). 

Remarks. The factorization (5.8) also gives a direct relation between the metrics $\tilde{g}$ and $g$: $\tilde{g} = (|z^0|^2 \phi) \left[ g - (\frac{d\phi}{\phi} + \frac{\partial \phi}{\phi}) (\frac{\xi^a}{\phi} + \frac{\phi_a}{\phi}) \right]$. Note that $Q = -|z^0|^2 \phi$ is the $\tilde{g}$-length squared of the $(1, 0)$ Euler field $z^0 \partial_0$.

Define differential operators in a neighborhood of $M$ in $\mathbb{C}^{n+1}$ by

$$\Delta_{w, w'} = \phi^{-1} \Delta g + \frac{w'}{1 - r \phi} \xi^a \partial_a + \frac{w}{1 - r \phi} \xi^b \partial_b - \frac{w w'}{1 - r \phi}.$$ 

By the observation in the proof of Proposition 5.2, $\Delta_{w, w'}$ has coefficients smooth near $M$. It follows from Proposition 5.2 that extending a section of $\mathcal{E}(w, w')$ to be harmonic with respect to $\tilde{\Delta}$ is the same as extending the corresponding function on $M$ to be annihilated by $\Delta_{w, w'}$. Therefore we conclude:

Proposition 5.3. If $w + w' + n + 1 = k \leq n + 1$, the invariant operator $P_{w, w'}$ is the (normalized) obstruction to extending a smooth function on $M$ to a smooth solution of $\Delta_{w, w'} = 0$, where $\phi$ is chosen to solve $J(\phi) = 1 + O(\phi^{n+2})$. 

In particular, $P_{0,0}$ is the obstruction to smoothly solving $\Delta_g u = 0$ with $u$ having prescribed boundary value.

In the setting of Proposition 5.3, the obstruction, or compatibility operators, were studied in [19], [20], [23]. In [20], the operators $P_{w,w'}$ were calculated explicitly for the sphere and the Heisenberg group with their usual defining functions, which solve $J(u) = 1$ exactly. Of course in this flat situation, the ambient metric is invariantly defined to all orders, so the invariant operators $P_{w,w'}$ exist without the restriction $k \leq n + 1$. The result is that each $P_{w,w'}$ is a product of various of the Folland-Stein operators $\Delta_b + i\alpha T$ on the Heisenberg group, or the analogous operators of Geller on the sphere. One can explicitly check that for the Heisenberg group, the operator $P_{w,w'}$ in [20] agrees with the operator $P_{w,w'} = (-2\Box)^k$ derived via tractors for flat pseudohermitian structures in Proposition 4.2.

In [23], a connection on a neighborhood of $M$ in $\mathbb{C}^{n+1}$ associated to an arbitrary defining function $\phi$ was derived along with an explicit formula for $\Delta_g$ in terms of this connection (Proposition 2.1 of [23]). This together with the expressions for the curvature of this connection given in [23] (for commuting derivatives) in principle enable explicit calculation of the obstruction operators in the curved case in terms of pseudohermitian curvature and torsion and their derivatives, and the transverse curvature $r$ and its derivatives. For general $\phi$, the obstruction operator was calculated in [23] for $n = 1$ and $w = w' = 0$ to be:

$$\Delta^2_b + T^2 + 4 \text{Im} \nabla_\beta (A^{\alpha\beta} \nabla_\alpha),$$

where all the quantities involved are those for the pseudohermitian structure induced by $\phi$ on $M$. The CR invariance of this operator was observed in [25], from which one concludes that for $n = 1$, $P_{0,0}$ is given by this formula for any choice of pseudohermitian structure. Direct calculation shows that the operator $P_{0,0} : \mathcal{E}(0,0) \to \mathcal{E}(-2,-2)$ discussed after the proof of Proposition 4.2 agrees with $P_{0,0}$.

When $w = w'$, the invariant operators can also be characterized as obstructions, or equivalently as log term coefficients, when solving $(\Delta_g + w(n+1+w))u = 0$. This is analogous to the corresponding characterization of the conformal operators $P_k$ given in [24]. The resolvent $(\Delta_g - s(n+1-s))^{-1}$ has been studied in [10].

**Proposition 5.4.** If $u$ is a function on $\mathbb{C}^{n+1}$, then

$$\tilde{\Delta}(|z|^2 \phi^w u) = (|z|^2 \phi)^w u.$$
Therefore, if \(n + 1 + 2w \in \mathbb{N} \) and \(w \leq 0\), then \(P_{w, w} f\) is the (normalized) obstruction to solving \((\Delta g + w(n + 1 + w))u = 0\) with \(\phi^w u\) smooth and \(\phi^w u = f\) on \(M\), where \(\phi\) is chosen to solve \(J(\phi) = 1 + O(\phi^{n+2})\).

\[\phi^w u = f\text{ on } M, \quad \phi \text{ is chosen to solve } J(\phi) = 1 + O(\phi^{n+2}).\]

Proof. The relation (5.13) is a direct calculation from (5.7). One expands the right hand side of (5.7) applied to \(\phi^w u\) using the Leibnitz rule and simplifies using (5.5), (5.6), (5.11), and the fact that \(g^{a b} \phi_{a b} = \phi(1 - r\phi)^{-1}((n + 1) r\phi - n)\).

This latter is a consequence of substituting (5.4) into \(g^{a b} \phi_{a b} = n + 1\). □

We remark that there is a similar relation in the case \(w \neq w'\) in terms of a family of modifications of \(\Delta g\) by both first and zeroth order terms, obtained by calculating \(\bar{\Delta}((z^0)^w (z^0)^{w'} \phi^{w + w'}/2 u)\).

We close with a brief discussion of CR \(Q\)-curvature, considered also in [14]. First recall Branson’s ([2]) formulation of \(Q\)-curvature in conformal geometry. For this discussion denote by \(P^N_k\) the operator \(P_k\) in dimension \(N\). Fix \(k \in \mathbb{N}\). The construction of [22] shows that the operator \(P^N_k\) is natural in the strong sense that \(P^N_k f\) may be written as a linear combination of complete contractions of products of covariant derivatives of the curvature tensor of a representative for the conformal structure with covariant derivatives of \(f\), with coefficients which are rational in the dimension \(N\). Also, the zeroth order term of \(P^N_k\) may be written as \(P^N_k 1 = (N/2 - k)Q^N_k\) for a scalar Riemannian invariant \(Q^N_k\) with coefficients which are rational in \(N\) and regular at \(N = 2k\). The \(Q\)-curvature in even dimension \(N\) is then defined as \(Q = Q^N_{N/2}\). An analytic continuation argument in the dimension then shows that under the conformal rescaling \(\hat{g} = e^{2\Upsilon} g\), we have \(e^{N\Upsilon} \hat{Q} = Q + P_{N/2} \Upsilon\).

If \(M\) is a pseudohermitian manifold, the \(Q\)-curvature of its Fefferman metric is invariant under rotations, so defines a function on \(M\) which we denote by \(Q_F\). It is then natural to define the CR \(Q\)-curvature of \((M, \theta)\) by \(Q_{\theta} = 2^{-n} Q_F\). Observations above imply that \(Q_{\theta}\) is given by a universal formula in the pseudohermitian metric, torsion, curvature and their covariant derivatives. The transformation law for conformal \(Q\)-curvature gives immediately that if \(\hat{\theta} = e^\Upsilon \theta\), then

\[(5.14) \quad e^{(n+1)\Upsilon} Q_{\hat{\theta}} = Q_{\theta} + P_{0,0} \Upsilon.\]

For \(N = 4\), the conformal \(Q\)-curvature is given by \(6Q = \Delta K + K^2 - 3|\text{Ric}|^2\), where \(K\) denotes the scalar curvature. Using Lee’s formulae for \(\Delta, K\), and \(\text{Ric}\), it is straightforward to calculate this for the Fefferman metric; one obtains that the \(Q\)-curvature for 3-dimensional CR
powers of the sub-Laplacian is given by:

\[(5.15) \quad 3Q_\theta = 2(\Delta_b R - 2 \Im \nabla^\alpha \nabla^\beta A_{\alpha\beta}).\]

This quantity was introduced by Hirachi [25], who showed that it gives the coefficient of the log term in the Szegö kernel. He also established the transformation law (5.14) in terms of the operator (5.12) by direct calculation.

The role of \(Q\)-curvature in CR geometry is not clear. In the conformal case, the total \(Q\)-curvature \(\int Q\) is an interesting invariant of a compact conformal manifold. However, since the expression in (5.15) is a divergence, it follows that we have \(\int_M Q_\theta = 0\) for the corresponding integral for 3-dimensional CR manifolds. Also, the \(Q\)-curvature vanishes identically for a hypersurface in \(\mathbb{C}^{n+1}\) with pseudohermitian structure induced by a solution of \(J(\phi) = 1 + O(\phi)\). A proof of this fact using a characterization of \(Q\)-curvature in terms of the ambient metric is given in [14]. It can also be seen directly from the definition by noting that the zeroth order term \(P_{k1}^N\) for the conformal operator for the Fefferman metric is a multiple of \((\bar{\Delta}^k|z^0|^{k-N/2})|z^0=1\). However, already \(\bar{\Delta}|z^0|^{k-N/2} = -g^{0\bar{0}} \partial_{\bar{0}}^2|z^0|^{k-N/2}\) vanishes to second order at \(k = N/2\).

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