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AMBIENT METRIC CONSTRUCTION OF Q-CURVATURE IN CONFORMAL AND CR GEOMETRIES

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1. Introduction

This article presents a geometric derivation of the Q-curvature in terms of the ambient metric associated with conformal and CR structures. The Q-curvature in conformal geometry is a scalar Riemannian invariant Q that is conformally invariant up to an error given by a conformally invariant power of the Laplacian. In dimension 2, the Q-curvature is the half of the scalar curvature, $Q_1 = R/2$, which satisfies

$$e^{2\Upsilon}\widehat{Q}_1 = Q_1 + \Delta\Upsilon \quad \text{whenever } \widehat{g} = e^{2\Upsilon}g.$$

In general even dimension n, the Laplacian Δ is replaced by a conformally invariant $(n/2)^{\text{th}}$ power of the Laplacian $P_{n/2}$ and the Q-curvature, $Q_{n/2}$, is $\frac{1}{2(n-1)}\Delta^{n/2}R$ modulo nonlinear terms in curvature. We here give a simple formula for $Q_{n/2}$ which directly follows from the ambient metric construction of $P_{n/2}$ given in [15]; this formula can be generalized to any invariant differential operators P on functions (densities of weight 0) that arise in the ambient metric construction. We also apply the construction of the Q-curvature to CR geometry; it then turns out that the Q-curvature gives the coefficient of the logarithmic singularity of the Szegö kernel of 3-dimensional CR manifolds.

The Q-curvature in general even dimensions was first defined by Branson [3] in a study of the functional determinant of the conformal Laplacian. He used an argument of analytic continuation in the dimension, in which the Q-curvature in dimension n is defined from $P_{n/2}$ in dimension $m > n$. For example, $Q_1 = R/2$ in dimension 2 is obtained from the zeroth order term of conformal Laplacian $P_1 = \Delta + \frac{(n-2)}{4(n-1)}R$ in dimension $n > 2$. It was thus natural to ask: what is $Q_{n/2}$ in n dimensional conformal geometry? An answer to this question was given by Graham-Zworski [17] in their study of the scattering for the Laplacian Δ_+ in the Poincaré metric associated with conformal structure $(M, [g])$ on the boundary at infinity. They gave a formula for the Q-curvature in terms of the scattering matrix, where the argument of analytic continuation in dimension is replaced by the analytic continuation in a spectral parameter. Their formulation of the Q-curvature was significantly simplified in Fefferman-Graham [10]; the Q-curvature

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is given as the logarithmic term in the formal solution to a Dirichlet problem for Δ_+. This construction has an intimate relation to the volume expansion for the a Poincaré metric [17]; in particular, it is shown that the integral of Q gives the coefficient of the log term of the expansion.

Our approach is directly related to the original derivation of the operator $P_{n/2}$ of [15] in terms of the ambient metric space, a formally constructed $(n+2)$-dimensional pseudo-Riemannian space $\widetilde{\mathcal{G}}$ that contains the metric bundle $\mathcal{G} = \{t^2 g \in S^2T^*M : t \in C^\infty(M)\}$ as a hypersurface. The invariant differential operator $P_{n/2}$ arises in two ways:

(a) as an operator on the homogeneous functions on $\mathcal{G}$ induced from the powers of the Laplacian $\widetilde{\Delta}^{n/2}$ on the ambient space;
(b) as an obstruction to the existence of a smooth homogeneous solution to $\widetilde{\Delta}F = 0$ with an initial condition on $\mathcal{G}$.

Corresponding to these derivations, we give two formulas for the Q-curvature in §2. In either case, our key observation is the following transformation law of $\log t$, where t is a conformal scale (a fiber coordinate of the bundle $\mathcal{G}$ determined by a section $g \in [g]$):

$$-\log \widehat{t} = -\log t + \Upsilon \quad \text{whenever} \quad \widehat{g} = e^{2\Upsilon} g.$$

In view of (a), we extend t off $\mathcal{G}$ and apply $\widetilde{\Delta}^{n/2}$ to $-\log t$. Then we see that its restriction to $\mathcal{G}$ gives the Q-curvature; the required transformation law is clear from that of $-\log t$. This formulation is naturally related to Branson's one. In the argument of analytic continuation in dimension m the function $\log t$ appears as the differential in m of the density $t^{(n-m)/2}$ at $m = n$. Corresponding to (b), we also express the Q-curvature as an obstruction to the existence of a smooth solution to $\widetilde{\Delta}F = 0$ with an initial condition $F|_{\mathcal{G}} = \log t$. Since the Laplace equation in the ambient metric can be reformulated as the one in the Poincaré metric, we see that this derivation is equivalent to that of Fefferman-Graham, mentioned above.

Note that there is another derivation of the invariant operators in terms of a bundle calculus associated with the conformal Cartan connection, which is called tractor calculus [4]. Corresponding to this derivation, Gover and Peterson [12] gave a tractor expression of the Q-curvature. Gover informed us that their formula can be translated into an ambient metric expression that is equivalent to our construction corresponding to (a). See also the remark at the end of §2.

In §3, we turn to CR geometry. For strictly pseudoconvex CR structures, the ambient metric is given as a Lorentz Kähler metric. The powers of the ambient Laplacian induce invariant powers of the sublaplacian $P_{n/2}$ and the ambient construction of Q-curvature is also valid. (For a comprehensive treatment of CR invariant operators see [11].) A new feature in this setting is that $P_{n/2}$ has a large null space, including the space of CR pluriharmonic functions $\mathcal{P}$. Thus the Q-curvature on $(2N-1)$-dimensional CR manifolds, Q_θ^{CR}, which is a local invariant of the pseudohermitian structure θ, satisfies

$$e^{2N\Upsilon} Q_{\hat{\theta}}^{\mathrm{CR}} = Q_{\theta}^{\mathrm{CR}} \quad \text{whenever } \hat{\theta} = e^{2\Upsilon}\theta \text{ with } \Upsilon \in \mathcal{P}. \tag{1.1}$$

If $N = 2$, it has been shown in [18] that this transformation law uniquely characterizes Q_θ^{CR} up to a constant multiple. As a consequence, we see that the leading term of the logarithmic singularity of the Szegö kernel, ψ, is a constant multiple of Q^{CR}, since the Szegö kernel enjoys the same transformation law. While such a simple characterization does not hold for higher dimensions, the transformation law still indicates an intimate link between the Q-curvature and the Szegö kernel.

2. Q-curvature in conformal geometry

2.1. Conformally invariant operators. We first recall basic materials on the ambient metric construction of the invariant operators from [9] and [15].

Let $(M, [g])$ be a conformal manifold of signature (p, q), $p + q = n \geq 3$. Then M admits the metric bundle $\mathcal{G} \subset S^2T^*M$, a ray bundle consisting of the metrics in the conformal class $[g]$. There are dilations $\delta_s : \mathcal{G} \to \mathcal{G}$ given by $\delta_s(g) = s^2 g$ for $s > 0$, and the homogeneous functions, with respect to δ_s, on $\mathcal{G}$ are called conformal densities; the space of densities of weight w is denoted by $\mathcal{E}(w)$, i.e.,

$$\mathcal{E}(w) = \{f \in C^\infty(\mathcal{G}) : \delta_s^* f = s^w f \text{ for any } s > 0\}.$$

Conformally invariant operators are then defined as operators acting on the conformal densities:

$$P : \mathcal{E}(w) \to \mathcal{E}(w').$$

A choice of representative $g \in [g]$ determines a trivialization

$$\mathcal{E}(w) \ni f \mapsto f_g := f \circ g \in C^\infty(M), \tag{2.1}$$

such that $f_{\widehat{g}} = e^{w\Upsilon} f_g$ when $\widehat{g} = e^{2\Upsilon} g$. Thus an invariant operator P defines, for each representative $g \in [g]$, an operator P_g on $C^\infty(M)$ such that

$$P_{\widehat{g}} = e^{w'\Upsilon} P_g e^{-w\Upsilon} \quad \text{whenever } \widehat{g} = e^{2\Upsilon} g.$$

In particular, if $w = 0$, then $\mathcal{E}(0) = C^\infty(M)$ and P acts on the functions on M. We say that P is an invariant diferential operator if each P_g is given by a differential operator on $C^\infty(M)$.

The ambient metric $\widetilde{g}$ is formally defined on $\widetilde{\mathcal{G}} = \mathcal{G} \times (-1, 1)$ along $\mathcal{G}$ which is now embedded as a hypersurface $\iota : \mathcal{G} \to \mathcal{G} \times \{0\} \subset \widetilde{\mathcal{G}}$. It is characterized by the following three conditions:

(1) $\widetilde{g}$ is an extension of the tautological two-tensor g_0 on $\mathcal{G}$, i.e., $\iota^*\widetilde{g} = g_0$;
(2) $\delta_s^*\widetilde{g} = s^2\widetilde{g}$ for any $s > 0$;
(3) $\widetilde{g}$ is an asymptotic solution to $\mathrm{Ric}(\widetilde{g}) = 0$ along $\mathcal{G}$.

When n is odd, these conditions uniquely determine a formal power series of $\widetilde{g}$ up to homogeneous diffeomorphisms that fix $\mathcal{G}$; but when n is even, $\widetilde{g}$ exists in general only to order $n/2$.

Many invariant differential operators can be constructed out of the ambient metric. The basic procedure is to construct a differential operator on the ambient space $\widetilde{\mathcal{G}}$ which preserves the homogeneity $\widetilde{P} : \widetilde{\mathcal{E}}(w) \to \widetilde{\mathcal{E}}(w')$ and then prove that $\widetilde{P}$ induces an operators $P : \mathcal{E}(w) \to \mathcal{E}(w')$, namely, prove that $(\widetilde{P}\widetilde{f})|_{\mathcal{G}}$ depends only on $\widetilde{f}|_{\mathcal{G}}$. We then call $\widetilde{P}$ an ambient extension of P. For example, the powers of the Laplacian $\widetilde{\Delta} = -\widetilde{\nabla}_I \widetilde{\nabla}^I$ in the ambient metric

$$\widetilde{P}_k = \widetilde{\Delta}^k : \widetilde{\mathcal{E}}(k - n/2) \to \widetilde{\mathcal{E}}(-k - n/2),$$

for $k > 0$ (and $k \le n/2$ if n is even) induce

$$P_k : \mathcal{E}(k - n/2) \to \mathcal{E}(-k - n/2).$$

The leading part of P_k for each representative g is the powers of the Laplacian Δ^k in g and hence P_k is called an invariant power of the Laplacian – see Proposition 2.1 of [15].

More operators have been constructed by Alexakis [1] by using the harmonic extension of densities. Denoting by T the infinitesimal generator of the dilations $T = \frac{d}{ds}\delta_s|_{s=1}$, we set $\widetilde{\rho} = \|T\|^2$; then $\widetilde{\rho} \in \mathcal{E}(2)$ and $\widetilde{\rho} = 0$ defines $\mathcal{G}$. Then the harmonic extension of densities are explicitly given by the following lemma, which is a part of Proposition 2.2 of [15].

Lemma 2.1. *Let $f \in \mathcal{E}(w)$ and set $k = n/2 + w$. If $k \notin \{1, 2, \dots\}$, then f admits an extension to $\widetilde{f}_m \in \widetilde{\mathcal{E}}(w)$ such that $\widetilde{\Delta}\widetilde{f}_m = O(\widetilde{\rho}^m)$ for any $m \ge 0$. Such an $\widetilde{f}_m$ is unique modulo $O(\widetilde{\rho}^{m+1})$ and is given by*

$$\widetilde{f}_m = E_m E_{m-1} \cdots E_1 \widetilde{f}, \quad \text{where} \quad E_l = 1 + \frac{1}{4l(k-l)}\widetilde{\rho}\,\widetilde{\Delta}$$

and $\widetilde{f} \in \widetilde{\mathcal{E}}(w)$ is an arbitrary extension of f. If $k \in \{1, 2, \dots\}$, then the same result is true with the restriction $m < k$.

Using this harmonic extension and $\widetilde{\nabla}^p \widetilde{R}$, the iterated covariant derivative of the curvature tensor of the ambient metric $\widetilde{g}$, we form a complete contraction

$$\widetilde{P}\widetilde{f} = \operatorname{contr}\Big(\widetilde{\nabla}^{p_1}\widetilde{R} \otimes \cdots \otimes \widetilde{\nabla}^{p_l}\widetilde{R} \otimes \widetilde{\nabla}^q \widetilde{f}_m\Big).$$

It defines a map $\widetilde{P} : \widetilde{\mathcal{E}}(w) \to \widetilde{\mathcal{E}}(w')$, where $w' = w - p_1 - \cdots - p_l - 2l - q$. If q is sufficiently small (e.g., $q \le m$) then the lemma above ensures that $\widetilde{P}$ induces an invariant operator $P : \mathcal{E}(w) \to \mathcal{E}(w')$.

Remark. In [1] it is shown that all conformally invariant differential operators $P : \mathcal{E}(w) \to \mathcal{E}(w')$ arise as above provided the dimension n is odd and $n/2 + w \notin \{1, 2, \dots\}$. The result of [1] applies also to nonlinear operators.

2.2. Q-curvatures in terms of the ambient metric. We now define Q-curvatures for the invariant operators constructed as above.

Theorem 2.2. *Let $P : \mathcal{E}(0) \to \mathcal{E}(w)$ be an invariant differential operator with an ambient extension $\widetilde{P} : \widetilde{\mathcal{E}}(0) \to \widetilde{\mathcal{E}}(w)$. For $g \in [g]$, choose $t \in \widetilde{\mathcal{E}}(1)$ such that $t(u^2 g) = u$ on $\mathcal{G}$. Then*

$$Q_g = -\big(\widetilde{P} \log t\big) \circ g$$

is independent of the extension of t off $\mathcal{G}$ and defines a function determined by g. Moreover, if $P1 = 0$, then Q_g satisfies the transformation law

$$e^{-w\Upsilon} Q_{\hat{g}} = Q_g + P_g \Upsilon \quad \text{whenever} \quad \widehat{g} = e^{2\Upsilon} g. \tag{2.2}$$

Proof. If t' is another function $\widetilde{\mathcal{E}}(1)$ which agrees with t on $\mathcal{G}$, then we have $t' = e^f t$ for an $f \in \widetilde{\mathcal{E}}(0)$ such that $f = O(\widetilde{\rho})$. So

$$\widetilde{P} \log t' - \widetilde{P} \log t = \widetilde{P} f = O(\widetilde{\rho}),$$

and hence $(\widetilde{P} \log t') \circ g = (\widetilde{P} \log t) \circ g$. To prove the transformation law, we extend Υ to $\Upsilon \in \widetilde{\mathcal{E}}(0)$ and set $\widehat{t} = e^{-\Upsilon} t$. Since $\widetilde{P}$ has no zeroth order term, we have $\widetilde{P} \log t \in \widetilde{\mathcal{E}}(w)$ so that

$$e^{-w\Upsilon} Q_{\hat{g}} = -e^{-w\Upsilon} \big(\widetilde{P} \log \widehat{t}\big) \circ \widehat{g} = -\big(\widetilde{P} \log \widehat{t}\big) \circ g.$$

Substituting $\widetilde{P} \log \widehat{t} = \widetilde{P} \log t - \widetilde{P} \Upsilon$ into the right-hand side, we get (2.2). □

In particular, if P is the invariant power of the Laplacian $P_{n/2}$ then $w = -n$ and $Q_g = -\big(\widetilde{\Delta}^{n/2} \log t\big) \circ g$. We now show that this Q_g agrees with the Q-curvature defined by Branson [3], which we recall briefly. For $m \geq n/2$, we denote by $P_{n/2,m}$ the invariant powers of Laplacian of order n in dimension m. Let $\widetilde{Q}_{n/2,m}$ be the zeroth order term of $P_{n/2,m}$ in the metric g. Then, noting $P_{n/2,n} 1 = 0$, we may write $\widetilde{Q}_{n/2,m} = (m - n)/2\, Q_{n/2,m}$ for a scalar Riemannian invariant of g. Moreover, from the construction of $P_{n/2,m}$, we see that $Q_{n/2,m}$ is expressed as a linear combination complete contractions of the tensor products of $\nabla^l R$, the coefficients of which are rational in m and regular at $m = n$. Thus we may substitute $m = n/2$ and define Q-curvature by $Q_{n/2,n}$.

In the identification (2.1) with respect to g, the constant function $1 \in C^\infty(M)$ corresponds to $t^w \in \mathcal{E}(w)$. Thus, extending t^w to $\widetilde{\mathcal{E}}(w)$, we have

$$\widetilde{Q}_{n/2,m} = P_{n/2,m} 1 = \big(\widetilde{\Delta}^{n/2} t^{(n-m)/2}\big) \circ g.$$

Substituting $t^{(n-m)/2} = 1 + (n - m)/2 \, \log t + O\big((n - m)^2\big)$ into the right-hand side gives

$$\widetilde{Q}_{n/2,m} = \frac{(n - m)}{2} \big(\widetilde{\Delta}^{n/2} \log t\big) \circ g + O\big((n - m)^2\big),$$

which implies $Q_{n/2,n} = -\big(\widetilde{\Delta}^{n/2} \log t\big) \circ g$ as claimed.

2.3. Q-curvature in terms of Poincaré metrics. There is another derivation of $P_{n/2}$, which was also given in [15]. For $f \in \mathcal{E}(0)$, take an extension $\widetilde{f} \in \widetilde{\mathcal{E}}(0)$ such that $\widetilde{\Delta}\widetilde{f} = O(\widetilde{\rho}^{n/2})$ – see Lemma 2.1. Then $\widetilde{\rho}^{1-n/2}\widetilde{\Delta}\widetilde{f}|_{\mathcal{G}}$ is shown to agree with $c_n P_{n/2} f$, where $c_n = 2^{2-n}((n/2-1)!)^{-2}$. This derivation of $P_{n/2}$ can be reformulated as follows:

Lemma 2.3. *Let n be even. For a representative $g \in [g]$, take t as in Theorem 2.2 and set $\rho = \widetilde{\rho}/(2t^2)$. Then, for each $f \in \mathcal{E}(0)$, there exists a formal solution to $\widetilde{\Delta}\widetilde{f} = 0$ of the form $\widetilde{f} = \widetilde{f}_0 + \eta\,\widetilde{\rho}^{n/2}\log\rho$ with $\widetilde{f}_0 \in \widetilde{\mathcal{E}}(0)$ such that $\widetilde{f}_0|_{\mathcal{G}} = f$ and $\eta \in \widetilde{\mathcal{E}}(-n)$. Here $\widetilde{f}_0 \mod O(\rho^{n/2})$ and $\eta \mod O(\rho^\infty)$ are determined by f, and moreover, $\eta|_{\mathcal{G}}$ is a non-zero constant multiple of $P_{n/2}f$.*

Proof. By taking the smooth part and the log term, we decompose $\widetilde{\Delta}\widetilde{f} = 0$ into a system of equations

$$\widetilde{\Delta}\widetilde{f}_0 + [\widetilde{\Delta}, \log\rho]\,\eta\widetilde{\rho}^{n/2} = 0, \quad \widetilde{\Delta}\,\eta = 0.$$

We solve this system by using Lemma 2.1. Noting that

$$[\widetilde{\Delta}, \log\rho]\,\eta\widetilde{\rho}^{n/2} = 2n\,\eta\widetilde{\rho}^{n/2-1} + O(\rho^{n/2}),$$

we first solve $\widetilde{\Delta}\widetilde{f}_0 = O(\rho^{n/2-1})$ and $\widetilde{\Delta}\eta = 0$ under the initial conditions $\widetilde{f}_0|_{\mathcal{G}} = f$ and $\eta|_{\mathcal{G}} = -c_n/(2n)\,P_{n/2}f$. Then we have $\widetilde{\Delta}\widetilde{f}_0 + [\widetilde{\Delta}, \log\rho]\,\eta\widetilde{\rho}^{n/2} = O(\rho^{n/2})$, and thus we may modify $\widetilde{f}_0$ so that $\widetilde{\Delta}\widetilde{f}_0 + [\widetilde{\Delta}, \log\rho]\,\eta\widetilde{\rho}^{n/2} = 0$. The uniqueness of η is clear from this construction. □

Corresponding to this derivation of $P_{n/2}$, we have the following characterization of the Q-curvature.

Theorem 2.4. *Let n be even. For a representative $g \in [g]$, take t as in Theorem 2.2 and set $\rho = \widetilde{\rho}/(2t^2)$. Then there is a formal solution to $\widetilde{\Delta}F = 0$ of the form*

$$F = \log t + \varphi + \eta\,\widetilde{\rho}^{n/2}\log\rho$$

with $\varphi \in \widetilde{\mathcal{E}}(0)$ such that $\varphi = O(\rho)$ and $\eta \in \widetilde{\mathcal{E}}(-n)$. Here $\varphi \mod O(\rho^{n/2})$ and $\eta \mod O(\rho^\infty)$ are determined by g and, moreover, $\eta \circ g$ is a constant multiple of the Q-curvature of $P_{n/2}$.

The proof of this theorem is just a straightforward modification of that of Lemma 2.3; the last statement follows form the fact that η is a multiple of $\widetilde{\Delta}^{n/2}\log t$ on $\mathcal{G}$. We will omit the details and, instead, we show that this theorem is equivalent to Theorem 3.1 of [10], which we state as Theorem 2.5 below.

Let $X = M \times (0,1)$ and identify M with a portion of the boundary $M \times \{0\}$. The Poincaré metric g_+ is a metric on X satisfying the following conditions: g_+ satisfies the Einstein equation $\mathrm{Ric}(g_+) + ng_+ = 0$ asymptotically along M, and if r is a defining function of M in X, then $h = r^{-2}g_+$ is smooth on $\overline{X} = M \times [0,1]$ and $h|_{TM} \in [g]$. Note that $r \mod O(r^2)$ corresponds to a representative $g \in [g]$. The higher jets of r can be uniquely determined by the normalization $\|d\log r\|_{g_+} = 1$.

Theorem 2.5. ([10]) *Let n be even. For a representative $g \in [g]$, take a defining function r such that $\|d\log r\|_{g_+} = 1$ and $(r^2 g_+)|_{TM} = g$. Then, there is an asymptotic solution to the equation*

$$\Delta_+ U = n,$$

of the form

$$U = \log r + A + B\, r^n \log r,$$

with $A, B \in C^\infty(\overline{X})$ which are even in r and $A|_M = 0$. Here $A \mod O(r^n)$ and $B \mod O(r^\infty)$ are formally determined by g, and moreover, $B|_M$ is a constant multiple of the Q-curvature.

To translate this theorem into Theorem 2.4, we recall the relation between the ambient metric and Poincaré metric from [9] and [17]. With respect to a suitable a decomposition of $\widetilde{\mathcal{G}} = \mathbb{R}_+ \times M \times (-1, 1)$, we have

$$\widetilde{g} = 2tdtd\rho + 2\rho dt^2 + t^2 \overline{g}_\rho, \tag{2.3}$$

where $t \in \mathbb{R}_+$ is homogeneous of degree 1, $\rho \in (-1, 1)$ and $\overline{g}_\rho$ is a one-parameter family of metrics on M such that $\overline{g}_0 = g$. Then $T = t\partial_t$ and $\widetilde{\rho} = 2t^2\rho$ hold. We embed $\overline{X} = M \times [0, 1] \ni (x, r)$ into $\widetilde{\mathcal{G}}$ by the map $\iota(x, r) = (1/r, x, -r^2/2)$ so that $\iota(\overline{X}) = \{2\widetilde{\rho} = -1, \rho \le 0\}$. Then $g_+ = \iota^*\widetilde{g}$ gives the Poincaré metric. Now set $s = t\sqrt{-2\rho} = t\, r$ and define new coordinates (s, x, r) of $\widetilde{\mathcal{G}}$ in which $\iota(X) = \{s = 1\}$. Then we have $\widetilde{g} = s^2 g_+ - ds^2$ and hence

$$\widetilde{\Delta} = s^{-2}(\Delta_+ + (s\partial_s)^2 + ns\partial_s),$$

where Δ_+ is considered as an operator in the variables (x, r). Thus

$$\begin{aligned} s^2\widetilde{\Delta}F &= s^2\widetilde{\Delta}(\log s - \log r + \varphi + \eta\, \widetilde{\rho}^{n/2} \log \rho) \\ &= n - \Delta_+(\log r - \varphi - \eta\, \widetilde{\rho}^{n/2} \log \rho) \end{aligned}$$

because $-\log r + \varphi + \eta\, \widetilde{\rho}^{n/2} \log \rho$ is homogeneous of degree 0. Now, restricting the both sides to $s = 1$, we get

$$(\widetilde{\Delta}F)\big|_{s=1} = n - \Delta_+ U,$$

where $U = -F\big|_{s=1}$ and it is of the form

$$U = \log r + A + B\, r^n \log r.$$

Therefore $\widetilde{\Delta}F = 0$ is equivalent to $\Delta_+ U = n$. Comparing the log term coefficients, we have $B(x, r) = -2(-1)^{n/2}\eta|_{(t,x,\rho)=(1,x,-r^2/2)}$.

2.4. Examples. We give two examples of the pairs (P, Q), an invariant operator P and the associated Q-curvature. It is a routine computation and we only outline the computation by quoting basic formulas from [9] and [15].

Fixing a representative $g \in [g]$, we take local coordinates (t, x_i, ρ) of $\widetilde{\mathcal{G}} = \mathbb{R}_+ \times M \times (-1, 1)$ such that (2.3) holds; we here rename the coordinates as $(x_I) = (x_0, x_i, x_\infty)$ and use capital indices $I, J, K, \ldots$ (resp. small indices $i, j, k, \ldots$) to ran through $0, 1, \ldots, n, \infty$ (resp. $1, \ldots, n$). With these coordinates, it is easy to compute the covariant derivatives of $\log t$. We have $\widetilde\nabla_I\widetilde\nabla_J \log t = 0$ except for the following two cases:

$$\widetilde\nabla_0\widetilde\nabla_0 \log t = -t^{-2}, \quad \widetilde\nabla_i\widetilde\nabla_j \log t = t^{-2}P_{ij} + O(\rho). \tag{2.4}$$

Here P_{ij} is the Rho tensor, the trace modification of the Ricci tensor of g, determined by

$$P_{ij} = \frac{1}{n-2}(R_{kij}{}^k - J\,g_{ij}), \quad J = P_i{}^i = \frac{1}{2(n-1)}R_{ij}{}^{ji}.$$

In particular, we see that $\widetilde\Delta \log t|_{\mathcal G} = -J$ is a constant multiple of the scalar curvature.

We next express the components of $\widetilde R_{IJKL}$ on $\mathcal G$ in terms of the curvature of g:

$$\widetilde R_{IJK0} = 0,\ \widetilde R_{ijkl} = t^2 W_{ijkl},\ \widetilde R_{ijk\infty} = t^2 C_{kij},\ \widetilde R_{\infty ij\infty} = \frac{t^2 B_{ij}}{n-4}. \tag{2.5}$$

(If $n=4$, $\widetilde R_{\infty ij\infty}$ is undetermined.) Here W, C and B, called the Weyl, Cotton and Bach tensor, respectively, are defined as follows: W_{ijkl} is the totally trace-free part of the curvature tensor R_{ijkl}; $C_{ijk} = \nabla_k P_{ij} - \nabla_j P_{ik}$, and $B_{ij} = \nabla^k C_{ijk} + P^{kl}W_{kijl}$. These relations and the usual symmetries of the curvature tensor determine all the components of $\widetilde R$.

Our first example of P is the operator $P^1 : \mathcal E(0) \to \mathcal E(-6)$ with the ambient expression

$$\widetilde P^1(\widetilde f) = \widetilde R_{IJK}{}^L \widetilde R^{IJKM}\widetilde\nabla_L\widetilde\nabla_M \widetilde f_1.$$

Recalling $\widetilde f_1 = \widetilde f + \frac{1}{2(n-2)}\widetilde\rho\widetilde\Delta\widetilde f$ and using

$$\widetilde R_{IJK}{}^L T_L = 0, \quad \widetilde\nabla_I T_J = g_{IJ} \text{ with } \quad 2\,T_I = \widetilde\nabla_I\,\widetilde\rho \tag{2.6}$$

(see (1.3)–(1.6) of [15]), we see that

$$\widetilde P^1(\widetilde f) = \widetilde R_{IJK}{}^L \widetilde R^{IJKM}\widetilde\nabla_L\widetilde\nabla_M \widetilde f + \frac{1}{n-2}\|\widetilde R\|^2\widetilde\Delta\widetilde f + O(\rho).$$

In terms of the representative metric g, it can be expressed as

$$P^1(f) = W_{ijk}{}^l W^{ijkm}\nabla_l\nabla_m f - 2C_{kij}W^{ijkl}\nabla_l f + \frac{1}{n-2}\|W\|^2\Delta f.$$

On the other hand, using (2.4) and (2.5), we can express the Q-curvature $Q^1 = -\widetilde P^1(\log t)\circ g$ as

$$Q^1 = -W_{ijk}{}^l W^{ijkm}P_{lm} + \|C\|^2 + \frac{1}{n-2}\|W\|^2 J.$$

Our next example is $P^2 : \mathcal E(0) \to \mathcal E(-6)$ induced by

$$\widetilde P^2(\widetilde f) = \widetilde R_{IJKL}(\widetilde\nabla^M \widetilde R^{IJKL})\widetilde\nabla_M \widetilde f_1.$$

Noting that $2\widetilde P^2(\widetilde f) = \widetilde\nabla^I(\|\widetilde R\|^2\widetilde\nabla_I\widetilde f_1)$, we have

$$2\widetilde P^2(\widetilde f) = \widetilde\nabla^I\big(\|\widetilde R\|^2\widetilde\nabla_I\widetilde f\big) + \frac{n-6}{n-2}\|\widetilde R\|^2\widetilde\Delta\widetilde f + O(\rho),$$

and from this one can easily deduce

$$2P^2(f) = \nabla^i\big(\|W\|^2\nabla_i f\big) + \frac{n-6}{n-2}\|W\|^2\Delta f.$$

The Q-curvature $Q^2 = -\widetilde{P}^2(\log t)\circ g$ is

$$Q^2 = 2\Big(W_{ijkl}\nabla^i C^{jkl} + W_{ijk}{}^l W^{ijkm}P_{lm} + 2\|C\|^2 - \frac{1}{n-2}\|W\|^2 J\Big).$$

Remark. The Q-curvature associated with $P^2 : \mathcal{E}(0) \to \mathcal{E}(-6)$ in dimension 6 has been obtained in Gover-Peterson [12]; their Q-curvature is $\frac{1}{8}\Delta\|W\|^2$. Our Q^2 is consistent with their formula because $Q^2 = \frac{1}{8}(\Delta\|W\|^2 - \widetilde{\Delta}\|\widetilde{R}\|^2\circ g)$ when $n = 6$ and $\widetilde{\Delta}\|\widetilde{R}\|^2\circ g$ is a conformal invariant – see [9].

3. Q-curvature in CR geometry

3.1. Ambient metric and invariant contact forms. We now turn to CR geometry. We first recall the ambient metric of [7] and [8]. Let M be a strictly pseudoconvex real hypersurface in $\mathbb{C}^N$ and let J be the complex Monge-Ampère operator

$$J[\rho] = (-1)^N \det\begin{pmatrix} \rho & \rho_j \\ \rho_{\overline{k}} & \rho_{j\overline{k}} \end{pmatrix}, \quad \rho_j = \frac{\partial\rho}{\partial z_j}, \text{ etc.} \tag{3.1}$$

Then there is a smooth defining function of M that is positive on the pseudoconvex side and satisfies $J[u] = 1 + O(u^{N+1})$; such a u is unique modulo $O(u^{N+2})$. The ambient metric lives on $\mathbb{C}^*\times\widetilde{M}$ for a small collar neighborhood $\widetilde{M}$ of M. It is the Lorentz-Kähler metric

$$\widetilde{g}[u] = -\sum_{j,k=0}^{N}\frac{\partial^2\big(|z_0|^2u(z)\big)}{\partial z_j\partial\overline{z}_k}\,dz_j d\overline{z}_k, \tag{3.2}$$

with $(z_0, z)\in\mathbb{C}^*\times\widetilde{M}$. Note that $J[u] = 1 + O(u^{N+1})$ implies $\mathrm{Ric}(\widetilde{g}) = O(u^N)$.

The defining function u also specifies a contact form $\theta[u] = \mathrm{Im}\,\partial u|_{TM}$ of M and $\widetilde{g}[u]$ induces a real Lorentz metric $g[u]$ on the circle bundle $S^1\times M$. Since $g[u]$ is shown to depend only on $\theta[u]$, we may write the metric as $g[\theta]$. This correspondence $\theta\mapsto g[\theta]$ can be extended to a general contact form θ of M in such a way that $g[e^{2\Upsilon}\theta] = e^{2\Upsilon}g[\theta]$ holds, and we have a conformal class of Lorentz metric $[g]$ on $S^1\times M$ – see [19]. For the conformal manifold $(S^1\times M, [g])$, the metric bundle and the ambient space are given by $\mathcal{G} = \mathbb{C}^*\times M$ and $\widetilde{\mathcal{G}} = \mathbb{C}^*\times\widetilde{M}$ respectively, and the metric $\widetilde{g}[u]$ satisfies the conditions (1), (2) and (3) of §2.1. Thus the definition of the ambient metric in conformal and CR cases are compatible, where $(2N-1)$-dimensional CR manifolds correspond to $2N$-dimensional Lorentzian conformal manifolds – see [9].

The contact form $\theta[u]$ defined above has special importance, and we call $\theta[u]$ an invariant contact form. This notion can be generalized to CR manifolds M: θ is an invariant contact form on M if it is locally given as an invariant contact form for some local embedding of M into $\mathbb{C}^N$. An intrinsic formulation of invariant contact form is also given ([6], [20]): θ is an invariant contact form if it is locally volume-normalized with respect to a closed $(N,0)$-form on M. From this characterization, it is straightforward to see that any two invariant contact forms θ and θ' satisfy $\theta' = e^{2\Upsilon}\theta$ with a CR pluriharmonic function Υ (that is, Υ is locally the real part of a CR function). Note that, when $N \geq 3$, Lee [20] showed that θ is an invariant contact form if and only if θ is pseudo-Einstein, that is, the Tanaka-Webster Ricci tensor of θ is a scalar multiple of the Levi form (this condition is vacuous when $N = 2$).

We next consider the CR analog of the operators P_k. CR densities of weight (w, w) are functions $f(z_0, z)$ on $\mathcal{G}$ such that $f(\lambda z_0, z) = |\lambda|^{2w} f(z_0, z)$ for any $\lambda \in \mathbb{C}^*$. The totality of such functions is denoted by $\mathcal{E}(w, w)$. For each θ, the metric $g[\theta]$ determines a S^1-subbundle of $\pi : \mathcal{G} \to M$. Restricting each $f \in \mathcal{E}(w, w)$ to the circle bundle, we obtain a function $\pi_* f$ on M; this correspondence gives an identification $\mathcal{E}(w, w) \cong C^\infty(M)$. Note also that $\mathcal{E}(w, w)$ can be regarded as a subspace of conformal densities $\mathcal{E}(2w)$ for the conformal manifold $(S^1 \times M, [g])$. As in the conformal case, we extend $\mathcal{E}(w, w)$ to the ambient space and define $\widetilde{\mathcal{E}}(w, w)$ to be the smooth functions on $\widetilde{\mathcal{G}}$ which are homogeneous of degree (w, w) in z_0 variable. Then the powers of the ambient Laplacian $\widetilde{\Delta}^k$ maps $\widetilde{\mathcal{E}}(w, w)$ into $\widetilde{\mathcal{E}}(w - k, w - k)$ and, for $w = k - N \leq 0$, it induces an operator $P_k : \mathcal{E}(w, w) \to \mathcal{E}(w - k, w - k)$. From this construction, it is clear that the CR invariant operator P_k is the restriction of the conformally invariant operator $P_k : \mathcal{E}(2w) \to \mathcal{E}(2w - 2k)$.

3.2. CR Q-curvature. The CR version of the Q-curvature is defined by

$$Q_\theta^{\mathrm{CR}} := \pi_* Q_g,$$

where Q_g is the Q-curvature, of the conformal P_N, in the metric $g = g[\theta]$, and where π is the projection $S^1 \times M \to M$. Since Q_g is S^1-invariant and pushes forward to a function on M. Then, as in the conformal case, we have

$$e^{2N\Upsilon} Q_{\hat\theta}^{\mathrm{CR}} = Q_\theta^{\mathrm{CR}} + P_N \Upsilon \quad \text{whenever } \widehat{\theta} = e^{2\Upsilon}\theta. \tag{3.3}$$

Here P_N is computed in θ.

Proposition 3.1. *If θ is an invariant contact form, then $Q_\theta^{\mathrm{CR}} = 0$.*

Proof. For the metric $g[\theta]$, we may take $|z_0|^2$ as a fiber coordinate of $\mathbb{C}^* \times M \to S^1 \times M$. Then $Q_\theta^{\mathrm{CR}} = -(\widetilde{\Delta}^N \log |z_0|^2) \circ g[\theta] = 0$ because $\widetilde{\Delta}$ kills pluriharmonic functions. □

In view of this proposition, we have another expression of Q^{CR}. Take an invariant contact form θ_0 as a reference and set

$$Q_\theta^{\mathrm{CR}} = e^{-2N\Upsilon} P_N \Upsilon, \tag{3.4}$$

where $\theta = e^{2\Upsilon}\theta_0$ and P_N is computed in θ_0. This is well-defined because Υ modulo additions of CR pluriharmonic functions is independent of the choice of θ_0 and CR pluriharmonic functions are killed by P_N.

If M is a real hypersurface in $\mathbb{C}^N$, then M admits a global invariant contact form θ so that $Q^{\mathrm{CR}}_\theta = 0$ on M. However, for abstract CR manifolds M, there is a topological obstruction for the global existence of an invariant contact form θ: the existence of θ implies the vanishing of the first Chern class of the holomorphic tangent bundle $c_1(T^{1,0}M)$ in $H^2(M,\mathbb{R})$. This obstruction, for $N \geq 3$, was first found by Lee [20] in the study of pseudo-Einstein contact form and his argument implicitly contains the proof for the $N = 2$ case. At present, we do not know if we can always choose θ so that Q^{CR}_θ vanishes globally.

Remark. The operators P_N were first introduced in Graham [13] as a compatibility operator for the Dirichlet problem for the Bergman Laplacian for the ball in $\mathbb{C}^N$. This construction of P_N was generalized, in [16], to the boundaries of strictly pseudoconvex domains in $\mathbb{C}^N$; the CR invariance of P_2 was realized later in [18]. Graham [13] proved that the kernel of P_N for the sphere agrees with the space of CR pluriharmonic functions (this can be partially generalized to the curved case [16]). As a result, on the sphere, we see from the expression (3.4) that $Q^{\mathrm{CR}}_\theta = 0$ if and only if θ is an invariant contact form.

3.3. Logarithmic singularity of the Szegö kernel. Now let M be the boundary of a strictly pseudoconvex domain Ω in $\mathbb{C}^N$. For a choice of contact form θ on M, we define $H^2_\theta(M)$ to be the kernel of $\overline{\partial}_b$ in $L^2(M)$ with respect to the volume element $\theta \wedge (d\theta)^{N-1}$. Then the Szegö kernel $K(x, y)$ is defined as the reproducing kernel of the Hilbert space $H^2_\theta(M)$. $K(x, y)$ can be extended to a holomorphic function $K(z, \overline{w})$ on $\Omega \times \overline{\Omega}$; its restriction to the diagonal $K(z, \overline{z})$ admits an expansion

$$K(z, z) = \varphi(z)u(z)^{-N} + \psi(z) \log u(z),$$

where φ, ψ are functions smooth up to the boundary and u is a defining function of Ω – see [8], [2]. This asymptotic expansion is locally determined by the CR structure of $\partial\Omega$ and θ. Moreover, $\psi_\theta = \psi|_M$ is shown to be a local pseudohermitian invariant of θ, that is, ψ_θ can be written as a linear combination of complete contractions, with respect to the Levi form, of the tensor products of Tanaka-Webster curvature and torsion and their covariant derivatives.

In general, there is no simple transformation law of the Szegö kernel under the scaling of contact form $\widehat{\theta} = e^{2\Upsilon}\theta$. But if Υ is CR pluriharmonic, we have $\widehat{K} = e^{-2N\Upsilon}K$, where Υ is extended to a pluriharmonic function in Ω. In particular, we obtain

$$e^{2N\Upsilon}\psi_{\hat{\theta}} = \psi_\theta.$$

In case $N = 2$, this transformation law is strong enough to characterize ψ_θ up to a constant multiple. In fact, we have

Theorem. ([18]) *Let $N = 2$. Suppose that S_θ is a scalar pseudohermitian invariant satisfying the transformation law*

$$e^{2N\Upsilon}S_{\hat{\theta}} = S_\theta \quad \textit{whenever } \widehat{\theta} = e^{2\Upsilon}\theta \textit{ and } \Upsilon \textit{ is CR pluriharmonic.} \tag{3.5}$$

Then S_θ is a constant multiple of

$$\Delta_b R - 2\,\mathrm{Im}\nabla^\alpha\nabla^\beta A_{\alpha\beta}, \tag{3.6}$$

where R is the Tanaka-Webster scalar curvature, A is the torsion, Δ_b is the sublaplacian computed in θ.

Since Q_θ^{CR} also satisfy the transformation law (3.5), the theorem above implies $\psi_\theta = c\,Q_\theta^{\mathrm{CR}}$ for a universal constant c, which can be identified by an explicit computation for an example (c.f. [18], [11]). Thus we have

Proposition 3.2. *If $N = 2$, then*

$$32\pi^2\psi_\theta = Q_\theta^{\mathrm{CR}} = \frac{4}{3}\big(\Delta_b R - 2\,\mathrm{Im}\nabla^\alpha\nabla^\beta A_{\alpha\beta}\big).$$

For $N \geq 3$, there are examples of pseudohermitian invariants that satisfy (3.5) for any $\Upsilon \in C^\infty(M)$ – see [8]. Such invariants are called CR invariants of weight N. Thus it is a natural conjecture that S is a constant multiple of Q^{CR} up to an addition of CR invariant of weight N. (In case $N = 2$, there is no CR invariant of weight 2 – see [14], and this conjecture is reduced to the theorem above.)

We finally note that the integral of the Q-curvature $L_M = \int_M Q_\theta^{\mathrm{CR}}\theta\wedge(d\theta)^{N-1}$ is independent of the choice of a contact form θ and gives a CR invariant; this follows from the analogous fact in the conformal case. In case $N = 2$, it turns out that $L_M = 0$ because (3.6) is the divergence of the one form $\nabla_\alpha R - i\nabla^\beta A_{\alpha\beta}$. We also see from the argument of §3.2 above that L_M vanishes if M admits a global invariant (or pseudo-Einstein) contact form. It should be interesting to find a link between L_M and the Chern class $c_1(T^{1,0}M)$, which obstructs the existence of an invariant contact form θ.

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