Complex Geometry, Lect. Notes in Pure and Appl. Math. **143**, 67-76, Dekker, 1993

SCALAR PSEUDO-HERMITIAN INVARIANTS AND THE SZEGÖ KERNEL ON THREE-DIMENSIONAL CR MANIFOLDS

Kengo Hirachi

Department of Mathematics, Osaka University
Toyonaka, Osaka, 560, Japan

Introduction

Let M be a three-dimensional strictly pseudoconvex CR manifold which bounds a relatively compact domain in $\mathbb{C}^2$. We fix a Levi metric on M, which is called a pseudo-hermitian structure, and define the Szegö kernel with respect to the volume element associated with the metric. In this note, we give an invariant-theoretic characterization of ψ_0 the first invariant in the logarithmic term of Fefferman's asymptotic expansion of the Szegö kernel, and write down the invariant in terms of geometric local pseudo-hermitian invariants.

In computing the invariant, we also find that the transformation law of ψ_0, under the change of pseudo-hermitian structure, can be expressed by using a fourth-order linear differential operator $\mathcal{C}_\theta$ on M, which was introduced in [GL] as the compatibility operator for a degenerate Dirichlet problem (for example, in case M is the sphere $\mathcal{C}_\theta = \Box_b\overline{\Box}_b$, where $\Box_b$ is the Kohn Laplacian). See Corollary 1 below. This formula enables us to reduce the analysis of ψ_0 to that of the differential equation $\mathcal{C}_\theta f = g$. In particular, by studying the global solutions to $\mathcal{C}_\theta f = 0$, we can show that ψ_0 vanishes globally on M if and only if the Szegö kernel is defined with respect to an invariant volume element introduced in [F2], see also [H], under the assumption that M has a transversal symmetry. See Corollary 2 below.

For the Szegö kernel defined with respect to the invariant volume element, we have obtained, in [HKN], some detailed results on its asymptotic expansion. Thus, if we combine the results on the invariant Szegö kernel and the above characterization of the invariant volume element, we can prove that the Szegö kernel has no logarithmic singularity if and only if M is spherical, without assuming any condition on the choice of volume element. See Corollary 3. In this characterization of spherical surfaces, the assumption that the logarithmic term vanishes *globally* is essential, while in the case of the Bergman kernel, this type of result holds under a local vanishing condition of the logarithmic term on a piece of the boundary, see [G, Theorem 3.2] and [B]. We can not expect such a localized result for the Szegö kernel, without specifying the choice of volume element as in [HKN, Remark 2] or [Ha], see Remark 1.1 below. A counter example can be found in [Fu], see Remark 1.2 below.

This work was supported by Grant-in-Aid for Scientific Research, The Ministry of Education, Science and Culture.

The plan of this note is as follows: after a review of some geometric identities on pseudo-hermitian manifolds in §2, we first use in §3 Weyl's classical invariant theory for the unitary group $U(1)$ to see that the first invariant in the logarithmic term ψ_0 is written as a linear combination of the "Weyl invariants" constructed from the curvature and the torsion of the Tanaka-Webster connection. To determine the coefficients in the linear combination, we derive in §4 the transformation law of ψ_0 under a change of pseudo-hermitian structure, which is forced by the transformation law of the Szegö kernel, and show in §5 that the transformation law uniquely characterizes ψ_0 up to a constant multiple. The evaluation of the constant will be done in §6. Finally, in §7, we discuss the equation $\mathcal{C}_\theta f = 0$ and give the proofs of corollaries.

1. Results

Let $\Omega \subset \mathbb{C}^2$ be a strictly pseudoconvex domain with smooth boundary M. We fix a pseudo-hermitian structure on M by giving a contact form θ. Then it was shown in [F1] and [B-S] that the Szegö kernel defined with respect to the volume element $\theta \wedge d\theta$ has the asymptotic expansion

$$S(z,\overline{z}) = \varphi(z)\rho(z)^{-2} + \psi(z)\log\rho(z) \quad \text{with} \quad \varphi,\psi \in C^\infty(\overline{\Omega}),$$

where ρ is a defining function of Ω with $\rho > 0$ in Ω.

Main Theorem. *The boundary value of the log term coefficient $\psi_0 = \psi|_M$ is given by*

$$\psi_0 = \frac{1}{24\pi^2}(\Delta_b R - 2\,\mathrm{Im} A_{11,}{}^{11}),$$

where Δ_b is the sublaplacian, R is the Webster scalar curvature, and $A_{11,}{}^{11}$ is the contraction of the second covariant derivative of the Webster torsion.

In proving this formula, we also get the transformation law of ψ_0:

Corollary 1. *If $\widetilde{\theta} = e^{2f}\theta$ is another pseudo-hermitian structure, then ψ_0 transforms according to*

$$\widetilde{\psi}_0 = e^{-4f}(\psi_0 + \frac{1}{2\pi^2}\mathcal{C}_\theta f), \quad \text{where} \quad \mathcal{C}_\theta f = f_{\overline{1}}{}^{\overline{1}}{}_1{}^1 + i(A_{11}f^1)^{,1}.$$

Here the indices 1 and $\overline{1}$ indicate the covariant derivatives, see §2 for definition.

By evaluating the explicit formula of ψ_0, we can prove $\psi_0 = 0$ if $\theta \wedge d\theta$ is the invariant volume element up to multiplication by a CR-pluriharmonic function, see §7 below; this fact also follows from Graham's result [G], see [HKN]. Moreover, in case Ω has a transversal symmetry, we can also prove its converse.

Corollary 2. *Assume that Ω has a transversal symmetry (see [GL]). Then $\psi_0 = 0$ if and only if $\theta \wedge d\theta$ is the invariant volume element up to multiplication by a CR-pluriharmonic function.*

Combining this corollary and [HKN, Remark 2], we get

Corollary 3. *Assume that Ω has a transversal symmetry and that $\psi = O(\rho^3)$. Then the boundary M is spherical, i.e. locally CR-isomorphic to the sphere.*

Remark 1.1. In Hanges [Ha], he computed ψ_0 for the domains in $\mathbb{C}^2$ with transversal symmetries. The computation was done with respect to a specific choice of volume element. By using the formula, he proved a similar result to our corollary 3 in case the Szegö kernel is defined with respect to that specific volume element.

Remark 1.2. Fuks [Fu] derived the explicit formula for the Szegö kernel of the tube domain $\{(z,w) \in \mathbb{C}^2 : \operatorname{Im} z \operatorname{Im} w > 1,\ \operatorname{Im} z > 0\}$ with a suitable choice of volume element on the boundary, see the formula (4.126) in [Fu]. This Szegö kernel contains no logarithmic singularity. Since we can check that this Szegö kernel satisfies the holonomic system given by Kashiwara's theorem, see [HKN, §2], the singularity of the Szegö kernel can be localized, and thus we can make an example of a bounded domain for which the logarithmic term of the Szegö kernel vanishes on a non-spherical piece of its boundary.

2. Pseudo-hermitian geometry

Let M be a C^∞ real three-dimensional manifold. A *CR structure* on M is a complex one-dimensional subbundle $T^{1,0} \subset \mathbb{C}TM$ satisfying $T^{1,0} \cap \overline{T^{1,0}} = \{0\}$. We will always assume that the structure is *strictly pseudoconvex*: for some choice of a real one-form θ annihilating $T^{1,0}$, the *Levi form* $L_\theta(V, \overline{W}) = -id\theta(V \wedge \overline{W})$ gives a hermitian metric on $T^{1,0}$. A choice of a such one-form θ defines a *pseudo-hermitian structure* on M, and it induces a natural linear connection called the *Tanaka-Webster connection* [T], [W]. We shall quickly review the definition.

Let $\{T, Z_1, Z_{\bar 1}\}$ be a frame of $\mathbb{C}T$, where Z_1 is any local frame of $T^{1,0}$, $Z_{\bar 1} = \overline{Z}_1$ and T is the *characteristic vector field*, that is, the unique real vector field such that $\theta(T) = 1,\ T \rfloor d\theta = 0$. Then $\{\theta, \theta^1, \theta^{\bar 1}\}$, the coframe dual to $\{T, Z_1, Z_{\bar 1}\}$, satisfies

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

for some positive function $h_{1\bar 1}$. We call the one-form θ^1 an *admissible coframe*. In terms of this frame, the Tanaka-Webster connection ∇ is defined by the relations

$$\begin{aligned} &\nabla Z_1 = \omega_1{}^1 \otimes Z_1, \quad \nabla Z_{\bar 1} = \omega_{\bar 1}{}^{\bar 1} \otimes Z_{\bar 1}, \quad \nabla T = 0, \\ &d\theta^1 = \theta^1 \wedge \omega_1{}^1 + A_{\bar 1}{}^1 \theta \wedge \theta^{\bar 1}, \quad \omega_{1\bar 1} + \omega_{\bar 1 1} = dh_{1\bar 1} \end{aligned}$$

for a one-form $\omega_1{}^1$, with $\omega_{\bar 1}{}^{\bar 1} = \overline{\omega_1{}^1}$, and a function $A_{\bar 1}{}^1$, called the *Webster torsion*.

We denote the components of covariant derivatives of a tensor by indices proceeded by a comma; as in $\nabla(A_1{}^{\bar 1} Z_{\bar 1} \otimes \theta^1) = (A_1{}^{\bar 1}{}_{,1}\theta^1 + A_1{}^{\bar 1}{}_{,\bar 1}\theta^{\bar 1} + A_1{}^{\bar 1}{}_{,0}\theta) \otimes Z_{\bar 1} \otimes \theta^1$. For a scalar functions, we usually omit the comma. The structure equation for the Tanaka-Webster connection [L2] is then given by

$$d\omega_1{}^1 = R\, h_{1\bar 1}\theta^1 \wedge \theta^{\bar 1} + A_1{}^{\bar 1}{}_{,\bar 1}\theta^1 \wedge \theta - A_{\bar 1}{}^1{}_{,1}\theta^{\bar 1} \wedge \theta, \tag{2.1}$$

where R is a function called the *Webster curvature*, and the *Bianchi identity* is

$$R_{,0} = A_{11,}{}^{11} + A_{\bar 1 \bar 1,}{}^{\bar 1 \bar 1}. \tag{2.2}$$

Here we use $h_{1\bar{1}}$ and its inverse $h^{1\bar{1}}$ in the usual way to raise and lower indices.

Now we shall collect some fundamental formulas used below. First recall [L2, Lemma 2.3] that the covariant derivatives of a function u satisfy

$$u_1{}^1 - u^1{}_1 = iu_0, \quad u_{01} - u_{10} = A_{11}u^1, \quad u_{11}{}^1 - u_1{}^1{}_1 = iu_{10} + R\,u_1. \tag{2.3}$$

The transformation law of the connection under a change of pseudo-hermitian structure was computed in [L1, §5]. Let $\widetilde{\theta} = e^{2f}\theta$ be a new pseudo-hermitian structure. Then we can define an admissible coframe by $\widetilde{\theta}^1 = e^f(\theta^1 + 2if^1\theta)$. With this coframe, the connection form and the torsion tensor are given by

$$\widetilde{\omega}_1{}^1 = \omega_1{}^1 + 3(f_1\theta^1 - f_{\bar{1}}\theta^{\bar{1}}) + i(f_1{}^1 + f_{\bar{1}}{}^{\bar{1}} + 8f_1f^1)\theta, \tag{2.4}$$

$$\widetilde{A}_{11} = e^{-2f}(A_{11} + 2if_{11} - 4if_1f_1), \tag{2.5}$$

and thus the Webster curvature transforms as

$$\widetilde{R} = e^{-2f}(R - 4f_1{}^1 - 4f_{\bar{1}}{}^{\bar{1}} - 8f_1f^1). \tag{2.6}$$

Here covariant derivatives in the right sides are taken with respect to the pseudo-hermitian structure θ and an admissible coframe θ^1. Note also that the dual frame of $\{\widetilde{\theta}, \widetilde{\theta}^{\,1}, \widetilde{\theta}^{\,\bar{1}}\}$ is given by $\{\widetilde{T}, \widetilde{Z}_1, \widetilde{Z}_{\bar{1}}\}$, where

$$\widetilde{T} = e^{-2f}(T + 2if^{\bar{1}}Z_{\bar{1}} - 2if^1Z_1), \quad \widetilde{Z}_1 = e^{-f}Z_1.$$

Finally we shall recall [S, Lemma 1.8] the transformation law of the *sublaplacian* Δ_b on functions defined by $\Delta_b u = -(u_1{}^1 + u_{\bar{1}}{}^{\bar{1}})$. If we denote by $\widetilde{\Delta}_b$ the sublaplacian associated with $\widetilde{\theta}$, then we get

$$\widetilde{\Delta}_b u = e^{-2f}(\Delta_b u - 2f^1u_1 - 2f^{\bar{1}}u_{\bar{1}}). \tag{2.7}$$

3. Scalar pseudo-hermitian invariants

Our proof of Main Theorem begins with a study of scalar pseudo-hermitian invariants; as we see in the lemma below, our object ψ_0 is a scalar pseudo-hermitian invariant.

By a *scalar pseudo-hermitian invariant* we mean a polynomial Q in the components of the curvature and the torsion of the Tanaka-Webster connection and their covariant derivatives which is invariant under a change of frame of $T^{1,0}$. A scalar pseudo-hermitian invariant defines a C^∞ function $Q(\theta)$ on each pseudo-hermitian manifold (M, θ) by evaluating the polynomial at each point. We also call this assignment of functions a scalar pseudo-hermitian invariant and will identify two invariant polynomials if they define the same assignment.

The simplest scalar pseudo-hermitian invariant is of course the Webster curvature R. Other examples of scalar pseudo-hermitian invariants can be constructed out of

$R, A_{11}, A_{\bar{1}\,\bar{1}}$ and their covariant derivatives in Z_1 and $Z_{\bar{1}}$ by taking tensor products and contracting:

$$\mathrm{contraction}(R_{,\alpha_1\cdots\alpha_n} \otimes \cdots \otimes R_{,\alpha'_1\cdots\alpha'_m} \otimes A_{\beta_1\beta_2,\beta_3\cdots\beta_p} \otimes \cdots \otimes A_{\beta'_1\beta'_2,\beta'_3\cdots\beta'_q})$$

is a scalar pseudo-hermitian invariant, called a *Weyl invariant*, for any choice of indices such that the numbers of 1 and $\bar{1}$ are the same. The contraction is taken with respect to the Levi metric $h_{1\bar{1}}$ for some pairing of holomorphic and antiholomorphic indices.

Since a scalar pseudo-hermitian invariant is an invariant polynomial under the action of the unitary group $U(1)$, the classical invariant theory identifies all such invariant polynomials. This leads to the conclusion that every scalar pseudo-hermitian invariant is a linear combination of the Weyl invariants. Note that the Weyl invariants contain no terms containing covariant derivatives in T; such terms can be expressed as the polynomials in the components of the tensors which contain no T covariant derivatives, by using, e.g. (2.2) and (2.3).

Lemma 3.1. *The first invariant in the log term of the Szegö kernel ψ_0 is a scalar pseudo-hermitian invariant, and thus ψ_0 is written as a linear combination of the Weyl invariants.*

Proof. In [BGS, Theorem 7.30] the same type of result was proved in the case of the asymptotic expansion of the heat kernel for $\Box_b$. The argument used there can be also applied to our case, if we fix a defining function (or a phase function) and employ the algorithm of computing the Szegö kernel given in [B-S, §4] or [HKN]. This implies that ψ_0 is written as a polynomial in the components of the curvature, the torsion tensor, and their covariant derivatives. Since we know that ψ_0 is independent of a choice of defining function, ψ_0 must be an invariant polynomial. □

4. Transformation law of the Szegö kernel

This section derives the following transformation law.

Proposition 4.1. *Let S and $\widetilde{S}$ be the Szegö kernels defined with respect to pseudo-hermitian structures θ and $\widetilde{\theta}$ on M respectively. If we have $\widetilde{\theta} = e^{2f}\theta$ for a CR-pluriharmonic function in a neighborhood of p in M, then there exists a neighborhood U of p in $\mathbb{C}^2$ such that*

$$\widetilde{S}(z,\overline{z}) \equiv e^{-4f(z)}S(z,\overline{z}) \mod C^\infty(U\cap\overline{\Omega}), \tag{4.2}$$

where $f(z)$ is identified with its pluriharmonic extension to $U\cap\Omega$. In particular, the log term coefficients of S and $\widetilde{S}$ satisfy

$$\widetilde{\psi}(z) = e^{-4f(z)}\psi(z) \quad \text{on} \quad U\cap M. \tag{4.3}$$

Proof. It was shown in [B-S] that the Szegö projector on (M,θ) is micro-locally characterized as the unique Fourier integral operator $\mathbb{S}$, which we call the *local Szegö projector*, satisfying

$$\mathbb{S}\sim\mathbb{S}^*\sim\mathbb{S}^2,\quad \overline{\partial}_b\mathbb{S}\sim 0,\quad \mathrm{Id}\sim\mathbb{S}+\mathbb{L}\overline{\partial}_b \quad \text{for some regular operator } \mathbb{L}. \tag{4.4}$$

Here "$\sim$" means that the operators of each side differs by an operator of degree $-\infty$ (i.e. an operator with C^∞ kernel function). We shall construct operators $\mathbb{S}'$ and $\mathbb{L}'$ which satisfy (4.4), near p, with respect to the volume element $\widetilde{\theta} \wedge d\widetilde{\theta}$ from $\mathbb{S}$ and f.

Let F be a function on M which is CR-holomorphic in a neighborhood p and satisfies $\mathrm{Re}F = 2f$, and we regard e^{-F} as the operator, on functions and one-forms, defined by the multiplication $u \mapsto e^{-F}u$. Then $e^{-F} : L^2(M, \theta \wedge d\theta) \to L^2(M, \widetilde{\theta} \wedge d\widetilde{\theta})$ is unitary, and we have $\overline{\partial}_b(e^F u) = e^F\, \overline{\partial}_b u$ for any function u with support in a small neighborhood of p. Thus we see that $\mathbb{S}' = e^{-F}\ \mathbb{S}\ e^F$ and $\mathbb{L}' = e^{-F}\ \mathbb{L}\ e^F$ satisfy (4.4), near p, with respect to the volume element $\widetilde{\theta} \wedge d\widetilde{\theta}$. Therefore, we get $\widetilde{\mathbb{S}} \sim e^{-F}\ \mathbb{S}\ e^F$, near p, by the uniqueness of the local Szegö projector. If we rewrite this formula in terms of kernel functions, we get (4.2). □

5. Invariant-theoric characterization of ψ_0

In §§3 and 4 we have shown that ψ_0 is a scalar pseudo-hermitian invariant and satisfies the transformation law (4.3). In this section we show that the transformation law uniquely determines the scalar pseudo-hermitian invariant ψ_0 up to a constant multiple.

Theorem 5.1. *Let Q be a scalar pseudo-hermitian invariant on three-dimensional CR manifolds which satisfies the transformation law*

$$Q(e^{2f}\theta) = e^{-4f} Q(\theta) \quad \text{for any CR-pluriharmonic function } f. \tag{5.2}$$

Then there exists a constant c such that

$$Q = c\,(\Delta_b R - 2\,\mathrm{Im}A_{11,}{}^{11}). \tag{5.3}$$

We begin by showing that the right side of (5.3) satisfies the transformation law (5.2).

Lemma 5.4. *The divergence of the one-form $W_1\theta^1 = (R_{,1} - iA_{11,}{}^1)\theta^1$ is written as*

$$W_{1,}{}^1 = -\frac{1}{2}\Delta_b R + \mathrm{Im}A_{11,}{}^{11} \tag{5.5}$$

and, if $\widetilde{\theta} = e^{2f}\theta$, then W_1 and $W_{1,}{}^1$ transform as follows:

$$\widetilde{W}_1 = e^{-3f}(W_1 - 6P_1 f), \quad \text{where} \quad P_1 f = f_{\overline{1}}{}^{\overline{1}}{}_1 + iA_{11}f^1, \tag{5.6}$$

$$\widetilde{W}_{1,}{}^1 = e^{-4f}(W_{1,}{}^1 - 6C_\theta f), \quad \text{where} \quad C_\theta f = (P_1 f)_,{}^1. \tag{5.7}$$

In [L2, Proposition 3.4] it was shown that a C^∞ real function on an open set U satisfies $P_1 f = 0$ if and only if f is CR-pluriharmonic on U. Thus (5.7) implies that $W_{1,}{}^1$ satisfies the transformation law (5.2).

Proof of Lemma 5.4. In view of (2.2) and $R_{,1}{}^{1} - R_{,}{}^{1}{}_{1} = iR_{,0}$ which follows from (2.3), we have

$$W_{1,}{}^{1} = R_{,1}{}^{1} - iA_{11,}{}^{11} = \frac{1}{2}(R_{,1}{}^{1} + R_{,}{}^{1}{}_{1} - iA_{11,}{}^{11} + iA_{\bar{1}\bar{1},}{}^{\bar{1}\bar{1}})$$
$$= -\frac{1}{2}\Delta_b R + \mathrm{Im} A_{11,}{}^{11}.$$

This proves (5.5).

To simplify the computation of the transformation laws, we shall work with an admissible coframe θ^1 for which $\omega_1{}^1 = 0$ at a point $p \in M$, so that the first covariant derivatives at p are equal to ordinary derivatives, see [L2, Lemma 2.1]. At the point p, we compute

$$\begin{aligned}
\widetilde{R}_{,1} &= \widetilde{Z}_1 \widetilde{R} = e^{-f} Z_1 e^{-2f}(R - 4f_1{}^1 - 4f_{\bar{1}}{}^{\bar{1}} - 8f_1 f^1) \\
&= e^{-3f}(R_{,1} - 2Rf_1 - 4f_1{}^1{}_1 - 4f_{\bar{1}}{}^{\bar{1}}{}_1 - 8f_{11}f^1 + 8f_1{}^1 f_1 + 16 f_1 f_1 f^1), \\
i\widetilde{A}_{11,\bar{1}} &= i\left(\widetilde{Z}_{\bar{1}} - 2\widetilde{\omega}_1{}^1(\widetilde{Z}_{\bar{1}})\right)\widetilde{A}_{11} \\
&= ie^{-f}(Z_{\bar{1}} + 6f_{\bar{1}})e^{-2f}(A_{11} + 2if_{11} - 4if_1 f_1) \\
&= e^{-3f}(iA_{11,\bar{1}} + 4iA_{11}f_{\bar{1}} - 2f_{11\bar{1}} + 8f_{1\bar{1}}f_1 - 8f_{11}f_{\bar{1}} + 16f_1 f_1 f_{\bar{1}}).
\end{aligned}$$

Contracting the second equation with respect to the Levi metric $\widetilde{h}_{1\bar{1}} = h_{1\bar{1}}$, we get

$$\widetilde{R}_{,1} - i\widetilde{A}_{11,}^{1} = e^{-3f}(R_{,1} - iA_{11,}{}^{1} - 4f_1{}^1{}_1 - 4f_{\bar{1}}{}^{\bar{1}}{}_1 + 2f_{11}{}^1 - 2Rf_1 - 4iA_{11}f^1).$$

So using $-4f_1{}^1{}_1 + 2f_{11}{}^1 - 2Rf_1 = -2f_{\bar{1}}{}^{\bar{1}}{}_1 - 2iA_{11}f^1$, which follows from (2.3), we obtain (5.6). To prove (5.7), by using (2.4), we compute

$$\begin{aligned}
\widetilde{W}_{1,\bar{1}} &= \left(\widetilde{Z}_{\bar{1}} - \widetilde{\omega}_1{}^1(\widetilde{Z}_{\bar{1}})\right)\widetilde{W}_1 = e^{-f}(Z_{\bar{1}} + 3f_{\bar{1}})e^{-3f}(W_1 - 6P_1 f) \\
&= e^{-4f} Z_{\bar{1}}(W_1 - 6P_1 f) = e^{-4f}\left(W_{1,\bar{1}} - 6(P_1 f)_{,\bar{1}}\right).
\end{aligned}$$

If we contract this equation, we get (5.7). □

Proof of Theorem 5.1. Suppose we have a scalar pseudo-hermitian invariant Q satisfying (5.2). First we consider the effect of a *change of scale* in the Levi metric, that is, to consider the case f is a constant function. Then, as in [BGS, §8] and [S, §5], we see that the possible Weyl invariants in Q are

$$R_{,1}{}^{1}, \quad R_{,\bar{1}}{}^{\bar{1}}, \quad A_{11,}{}^{11}, \quad A_{\bar{1}\bar{1},}{}^{\bar{1}\bar{1}}, \quad |R|^2, \quad |A_{11}|^2.$$

Since we know $\mathrm{Re}A_{11,}{}^{11} = \mathrm{Im}R_{,1}{}^{1} = R_{,0}$ from (2.2) and (2.3), Q can be written in the form

$$Q = c_1\Delta_b R + c_2 \mathrm{Im} A_{11,}{}^{11} + c_3|R|^2 + c_4|A_{11}|^2 + c_5 R_{,0}.$$

Now we shall determine the coefficients. To simplify computation, we work on the Heisenberg group $\mathbb{H}^3 = \mathbb{C} \times \mathbb{R}$ with the CR structure given by $Z_1 = \partial/\partial z + i\bar{z}\partial/\partial t$. On

$\mathbb{H}^3$ with the standard pseudo-hermitian structure $\theta_0 = \frac{1}{2}(dt + izd\overline{z} - i\overline{z}dz)$, the curvature and the torsion vanish, and thus we can compute R and A_{11} for the pseudo-hermitian structure $\theta = e^{2f}\theta_0$ from (2.5) and (2.6):

$$R = -4e^{-2f}\left(Z_1 Z_{\overline{1}} f + Z_{\overline{1}} Z_1 f + 2(Z_1 f)(Z_{\overline{1}} f)\right),$$
$$A_{11} = 2i\, e^{-2f}\left(Z_1 Z_1 f - 2(Z_1 f)(Z_1 f)\right).$$

Note that Z_1 is normalized by the Levi metric associated with θ_0. For the determination of the coefficients, it is enough to compute Q for some simple examples of CR-pluriharmonic functions f.

First, we consider the case $f = a\,\mathrm{Re}(z + z^2)$, where a is a real constant. Then we get

$$|R|^2 = 4a^4 + O(1), \quad |A_{11}|^2 = (a^2 - 2a)^2 + O(1),$$

where $O(1)$ indicates some smooth function which vanishes at the origin $(0, 0) \in \mathbb{H}^3$. To verify $\Delta_b R$ we use (2.7):

$$\begin{aligned}\Delta_b R &= e^{-2f}\left(-Z_1 Z_{\overline{1}} - Z_{\overline{1}} Z_1 - 2(Z_1 f) Z_{\overline{1}} - 2(Z_{\overline{1}} f) Z_1\right) R \\ &= 2(Z_1 Z_{\overline{1}} + Z_{\overline{1}} Z_1 + a Z_{\overline{1}} + a Z_1) e^{-2f} |a + 2az|^2 + O(1) \\ &= -8a^2(a-2) + O(1).\end{aligned}$$

Since we have shown in Lemma 5.4 that $\Delta_b R - 2\,\mathrm{Im} A_{11,}{}^{11}$ satisfies (5.2), we also get

$$\mathrm{Im} A_{11,}{}^{11} = \frac{1}{2}\Delta_b R = -4a^2(a-2) + O(1).$$

For the evaluation of $R_{,0}$ we use $T = e^{-2f}\left(\partial/\partial t + 2i(Z_1 f) Z_{\overline{1}} - 2i(Z_{\overline{1}} f) Z_1\right)$ and get

$$R_{,0} = TR = -2\left(\frac{\partial}{\partial t} + iaZ_{\overline{1}} - iaZ_1\right) e^{-2f}|a + 2az|^2 + O(1) = O(1).$$

To sum up, we have shown that the value of $Q(\exp(a\mathrm{Re}(z + z^2))\theta_0)$ at the origin is

$$-4a^2(a-2)(2c_1 + c_2) + 4a^4 c_3 + (a^2 - 2a)^2 c_4,$$

which must vanishes for every $a \in \mathbb{R}$. Thus we get $2c_1 + c_2 = 0$ and $c_3 = c_4 = 0$. So Q is written as $c_1(\Delta_b R - 2\,\mathrm{Im} A_{11,}{}^{11}) + c_5 R_{,0}$. To determine c_5 we compute $R_{,0}$ for the CR-pluriharmonic function $f = t + |z|^2$ and get $R_{,0} = 32 + O(1)$. On the other hand, we know $\Delta_b R - 2\,\mathrm{Im} A_{11,}{}^{11} = 0$ for the pseudo-hermitian structure $\exp(2(t + |z|^2))\theta_0$. Thus c_5 must vanish. □

6. Determination of the universal constant

By Theorem 5.1, we have $\psi_0 = c\,(\Delta_b R - 2\mathrm{Im} A_{11,}{}^{11})$ for some constant c which depends on neither a choice of domain nor a choice of pseudo-hermitian structure. In order to determine the constant, we shall compute the Szegö kernel S on the Heisenberg group with the pseudo-hermitian structure $\theta = \exp(2|z|^4)(dt + izd\overline{z} - i\overline{z}dz)$. We embed $\mathbb{H}^3$ by $(z, t) \mapsto (z, (|z|^2 - it)/2) \in \mathbb{C}^2$, so that $\mathbb{H}^3$ is defined by $\rho = w + \overline{w} - z\overline{z} = 0$.

Lemma 6.1. *Set $\gamma_\varepsilon = (0, \varepsilon/2)$. Then, as $\varepsilon \to +0$, we have*

$$S(\gamma_\varepsilon, \overline{\gamma_\varepsilon}) = \frac{1}{4\pi^2}\varepsilon^{-2} + \left(\frac{2}{\pi^2} + O(\varepsilon)\right)\log\varepsilon. \tag{6.2}$$

Proof. We employ the method used in [HKN, §2]. Since the volume element $\theta\wedge d\theta$ corresponds to the δ-function $4\exp(4|z|^4)\delta(\rho)$, we get

$$4\exp(4|z|^4)\delta(\rho) = 4\sum_{n=0}^{\infty}\frac{4^n}{n!}z^{2n}(D_zD_w^{-1})^{2n}\delta(\rho).$$

Thus we have

$$\begin{aligned} S =& \Big(4\sum_{n=0}^{\infty}\frac{4^n}{n!}z^{2n}(D_zD_w^{-1})^{2n}\Big)^{*-1}\frac{1}{\pi^2}\rho^{-2} \\ =&\frac{1}{4\pi^2}(1-4D_z^2z^2D_w^{-2})\rho^{-2} + (\text{terms of weight} > 0). \end{aligned}$$

Since $(D_z^2z^2D_w^{-2}\rho^{-2})|_{\gamma_\varepsilon} = -2\log\varepsilon$, we get (6.2). $\square$

On the other hand, we see from (5.7) that the value of $\Delta_b R - 2\,\mathrm{Im}A_{11,}{}^{11}$ at the origin is $12(P_1 f)_,{}^1 = 12 f_{\bar 1}{}^{\bar 1}{}_1{}^1 = 12 Z_{\bar 1}Z_1Z_1Z_{\bar 1}|z|^4 = 48$. Therefore we find $c = 1/24\pi^2$. This concludes the proof of Main Theorem.

7. Proofs of corollaries

Corollary 1 has been proved in Lemma 5.4, so we begin with the proof of Corollary 2.

We first recall that the invariant volume element $\theta\wedge d\theta$ is defined by the normalization

$$\theta\wedge d\theta = i\theta\wedge(T\rfloor\zeta)\wedge(T\rfloor\bar\zeta) \tag{7.1}$$

with the closed $(2,0)$-form $\zeta = dz_1\wedge dz_2$. This definition is equivalent to the one given in [F2] and [HKN], see [H]. We denote the contact form satisfying this condition by θ_0. To evaluate ψ_0 for this volume element, we use the following lemma, which is an analogy of [L2, Theorem 4.2].

Lemma 7.2. *Let θ be a pseudo-hermitian structure on a three-dimensional CR manifold. Then $W_1 = R_{,1} + iA_{11,}{}^1 = 0$ in a neighborhood of a point $p\in M$ if and only if there exists a closed $(2,0)$-form ζ in a neighborhood of p satisfying* (7.1).

Proof. If we take the exterior differential of the one-form $\omega_1{}^1 + iR\,\theta$, and use (2.1), we obtain

$$d(\omega_1{}^1 + iR\,\theta) = i\,(W_1\theta^1 + W_{\bar 1}\theta^{\bar 1})\wedge\theta.$$

Thus we see that $W_1 = 0$ if and only if $\omega_1{}^1 + iR\,\theta$ is closed. This fact corresponds to [L2, Lemma 4.1], and thus the arguments in the proof of [L2, Theorem 4.2] also hold just as well in this case. $\square$

In particular, $\psi_0 = -\dfrac{1}{12\pi^2}W_{1,}{}^1 = 0$ for the invariant volume element. Thus, for the volume element $e^f\theta_0\wedge d\theta_0$ with CR-pluriharmonic function f, we also get $\psi_0 = 0$ by the transformation law (4.3).

In order to prove the only if part of Corollary 2, we use the following:

Proposition 7.3. *Let M be a compact three-dimensional CR manifold which has a transversal symmetry, and θ be any pseudo-hermitian structure on M. Then a C^∞ real function f satisfies $C_\theta f = 0$ on M if and only if f is CR-pluriharmonic.*

Proof. In [GL, Proposition 3.2], they proved this statement under the assumption that θ is normalized by the symmetry. In case θ is not normalized, we write $\theta = e^{2g}\widetilde{\theta}$ with a normalized pseudo-hermitian structure $\widetilde{\theta}$. Then the lemma below shows $C_{\widetilde{\theta}} f = e^{4g} C_\theta f = 0$, which implies that f is CR-pluriharmonic.

Conversely, if f is CR-pluriharmonic, then we have $C_\theta f = (P_1 f),{}^1 = 0$. □

Lemma 7.4. *Let θ and $\widetilde{\theta}$ be pseudo-hermitian structures on a three-dimensional CR manifold. If $\widetilde{\theta} = e^{2g}\theta$, then we have $C_{\widetilde{\theta}} = e^{-4g} C_\theta$.*

Proof. Take a real function f and define another contact form by $\widehat{\theta} = e^{2f}\widetilde{\theta} = e^{2(f+g)}\theta$. Then we have the transformation formulas of $W_{1,}{}^1$

$$\begin{aligned} \widehat{W}_{1,}{}^1 &= e^{-4f}(\widetilde{W}_{1,}{}^1 - 6C_{\widetilde{\theta}} f), \\ \widehat{W}_{1,}{}^1 &= e^{-4(f+g)}(W_{1,}{}^1 - 6C_\theta f - 6C_\theta g), \\ \widetilde{W}_{1,}{}^1 &= e^{-4g}(W_{1,}{}^1 - 6C_\theta g). \end{aligned}$$

These equations imply $C_{\widetilde{\theta}} f = e^{-4g} C_\theta f$. □

If ψ_0 vanishes for a volume element $\theta \wedge d\theta$, then, writing $\theta \wedge d\theta = e^{4f}\theta_0 \wedge d\theta_0$, we get $\psi_0 = \dfrac{1}{2\pi^2} e^{-4f} C_{\theta_0} f = 0$. Thus Proposition 7.3 implies that f is CR-pluriharmonic, which proves Corollary 2.

Finally we shall prove Corollary 3. By Corollary 2, we see that the volume element is a CR-pluriharmonic function multiple of the invariant volume element. Thus the transformation law (4.2) implies that the Szegö kernel defined with respect to the invariant volume element also has the logarithmic term which vanishes to the third order at the boundary. Thus [HKN, Remark 2] implies that the boundary is spherical.

References

[B] Boutet de Monvel, L., *Le noyau de Bergman en dimension* 2, Séminaire équations aux dérivées partielles 1987-88, Ecole Polytech. Palaiseau.

[B-S] Boutet de Monvel, L. and Sjöstrand, J., *Sur la singularité des noyau de Bergman et de Szegö*, Astérisque **34-35** (1976), 123–164.

[BGS] Beals, R., Greiner, P. C. and Stanton, N. K., *The heat equation on a CR manifold*, J. Differential Geom. **20** (1984), 343–387.

[F1] Fefferman, C., *The Bergman kernel and biholomorphic mappings of pseudoconvex domains*, Invent. Math. **26** (1974), 1–65.

[F2] Fefferman, C., *Parabolic invariant theory in complex analysis*, Adv. in Math. **31** (1979), 131–262.

[Fu] Fuks, B. A., *Introduction to the Theory of Analytic Functions of Several Complex Variables*, Transl. Math. Monographs Vol. 8, Amer. Math. Soc., 1963 (Russian original in 1962).

[G] Graham, C. R., *Scalar boundary invariants and the Bergman kernel*, in Complex analysis II, Lecture Notes in Math. 1276, Springer,1987, pp.108-135.

[GL] Graham, C. R. and Lee, J. M., *Smooth solutions of degenerate Laplacians on strictly pseudoconvex domains*, Duke Math. J. **57** (1988), 697–720.

[Ha] Hanges, N., *Explicit formulas for the Szegö kernel for some domains in C^2*, J. Functional Analysis **88** (1990), 153–165.

[H] Hirachi, K., *Transformation law for the Szegö projectors on CR manifolds*, Osaka J. Math. **27** (1990), 301–308.

[HKN] Hirachi, K., Komatsu, G. and Nakazawa, N., *Two methods of determining local invariants in the Szegö kernel*, in the present volume.

[L1] Lee, J. M., *The Fefferman metric and pseudohermitian invariants*, Trans. Amer. Math. Soc. **296** (1986), 411–429.

[L2] Lee, J. M., *Pseudo-Einstein structures on CR manifolds*, Amer. J. Math. **110** (1988), 157–178.

[S] Stanton, N. K., *Spectral invariants of CR manifolds*, Michigan Math. J. **36** (1989), 267–288.

[T] Tanaka, N., *A differential geometric study of strongly pseudo-convex manifolds*, Kinokuniya Company Ltd., Tokyo, 1975.

[W] Webster, S. M., *Pseudohermitian structures on a real hypersurface*, J. Differential Geom. **13** (1978), 25–41.