Clay Mathematics Proceedings
Volume 12, 2009

A Microlocal Approach to Fefferman's Program in Conformal and CR Geometry

Raphaël Ponge

Motivated by the analysis of the singularity of the Bergman kernel of a strictly pseudoconvex domain $D \subset \mathbb{C}^{n+1}$, Fefferman [**Fe2**] launched the program of determining *all* local invariants of a strictly pseudoconvex CR structure. This program was subsequently extended to deal with local invariants of other parabolic geometries, including conformal geometry (see [**FG1**]). Since Fefferman's seminal paper further progress has been made, especially recently (see, e.g., [**Al2**], [**BEG**], [**GH**], [**Hi1**], [**Hi2**]). In addition, there is a very recent upsurge of new conformally invariant Riemannian differential operators (see [**Al2**], [**Ju**]).

In this article we present the results of [**Po4**] on the logarithmic singularities of the Schwartz kernels and Green kernels of *general* invariant pseudodifferential operators in conformal and CR geometry. This connects nicely with results of Hirachi ([**Hi1**], [**Hi2**]) on the logarithmic singularities of the Bergman and Szegö kernels on boundaries of strictly pseudoconvex domains.

The main result in the conformal case (Theorem 3) asserts that in odd dimension, as well as in even dimension below the critical weight (i.e. half of the dimension), the logarithmic singularities of Schwartz kernels and Green kernels of conformally invariant Riemannian ΨDOs are linear combinations of Weyl conformal invariants, that is, of local conformal invariants arising from complete tensorial contractions of covariant derivatives of the ambient Lorentz metric of Fefferman-Graham ([**FG1**], [**FG2**]). Above the critical weight the description in even dimension involves the ambiguity-independent Weyl conformal invariants recently defined by Graham-Hirachi [**GH**], as well as the exceptional local conformal invariants of Bailey-Gover [**BG**]. In particular, by specializing this result to the GJMS operators of [**GJMS**], including the Yamabe and Paneitz operators, we obtain invariant expressions for the logarithmic singularities of the Green kernels of these operators (see Theorem 4).

In the CR setting the relevant class of pseudodifferential operators is the class of Ψ_HDOs introduced by Beals-Greiner [**BGr**] and Taylor [**Tay**]. In this context the main result (Theorem 6) asserts that the logarithmic singularities of Schwartz kernels and Green kernels of CR invariant Ψ_HDOs are local CR invariants, and below the critical weight are linear combinations of complete tensorial contractions

Research partially supported by NSERC Discovery Grant 341328-07 (Canada) and by a New Staff Matching Grant of the Connaught Fund of the University of Toronto (Canada).

of covariant derivatives of the curvature of the ambient Kähler-Lorentz metric of Fefferman [**Fe2**]. As a consequence this allows us to get invariant expressions for the logarithmic singularities of the Green kernels of the CR GJMS operators of [**GG**] (see Theorem 7).

The setup of the the first part of the paper, Sections 1–5, is conformal geometry. The main results on the logarithmic singularities of conformally invariant ΨDOs are presented in Section 5. In the previous sections, we review the main definitions and examples concerning local conformal invariants and conformally invariant differential operators (Section 1), conformally invariant ΨDOs (Section 2), the logarithmic singularity of the Schwartz kernel of a ΨDO (Section 3) and the program of Fefferman in conformal geometry (Section 4).

The setup of the second part, Sections 6–10, is pseudo-Hermitian and CR geometry. In Section 6, we review the motivating example of the Bergman kernel of a strictly pseudoconvex domain. Section 7 is an overview of the main facts about the Heisenberg calculus. In Section 8, we present important definitions and properties concerning pseudo-Hermitian geometry, local pseudo-Hermitian invariants and pseudo-Hermitian invariant Ψ_HDOs. In Section 9, we review the main facts about local CR invariants, CR invariant operators and the program of Fefferman in CR geometry. In Section 10, we present the main results concerning the logarithmic singularities of CR invariant operators.

This proceeding is a survey of the main results of [**Po4**].

1. Conformal Invariants

Up to Section 5, we denote by M a Riemannian manifold of dimension n and we denote by g_{ij} and R_{ijkl} its metric and curvature tensors. As usual we shall use the metric and its inverse g^{ij} to lower and raise indices. For instance, the Ricci tensor is $\rho_{jk} = R_{ijk}{}^{i} = g^{il}R_{ijkl}$ and the scalar curvature is $\kappa_g = \rho_j{}^{j} = g^{ji}\rho_{ij}$.

1.1. Local conformal invariants. In the sequel we denote by $M_n(\mathbb{R})_+$ the open subset of $M_n(\mathbb{R})$ consisting of positive definite matrices.

Definition 1. *A local Riemannian invariant of weight w is the datum on each Riemannian manifold (M^n, g) of a function $\mathcal{I}_g \in C^\infty(M)$ such that:*

(i) *There exist finitely many functions $a_{\alpha\beta}$ in $C^\infty(M_n(\mathbb{R})_+)$ such that, in any local coordinates,*

$$\mathcal{I}_g(x) = \sum a_{\alpha\beta}(g(x))(\partial^\alpha g(x))^\beta. \tag{1}$$

(ii) *For all $t > 0$,*

$$\mathcal{I}_{tg}(x) = t^{-w}\mathcal{I}_g(x). \tag{2}$$

Using Weyl's invariant theory for $O(n)$ (see, e.g, [**Gi**]) we obtain the following determination of local Riemannian invariants.

Theorem 1 (Weyl, Cartan). *Any local Riemannian invariant is a linear combination of Weyl Riemannian invariants, that is, of complete contractions of the curvature tensor and its covariant derivatives.*

For instance, the only Weyl Riemannian invariant of weight 1 is the scalar curvature κ_g. In weight 2 the Weyl Riemannian invariants are

$$|\kappa_g|^2, \qquad |\rho|^2 := \rho^{ij}\rho_{ij}, \qquad |R|^2 := R^{ijkl}R_{ijkl}, \qquad \Delta_g\kappa_g, \tag{3}$$

where Δ_g denotes the Laplace operator of (M, g). In weight 3 there are 17 Weyl invariants (see [**Gi**]).

DEFINITION 2. *A local conformal invariant of weight w is a local Riemannian invariant $\mathcal{I}_g$ such that*

$$\mathcal{I}_{e^f g}(x) = e^{-wf(x)}\mathcal{I}_g(x) \qquad \forall f \in C^\infty(M, \mathbb{R}). \tag{4}$$

The most fundamental conformally invariant tensor is the Weyl curvature tensor W_{ijkl}. Using complete contractions of k-fold tensor powers of W we get local conformal invariants of various weights. For instance, the following are local conformal invariants

$$|W|^2 := W^{ijkl}W_{ijkl}, \tag{5}$$

$$W_{ij}{}^{kl}W_{lk}{}^{pq}W_{pq}{}^{ij}, \qquad W_i{}^{jk}{}_l W^i{}_{pk}{}^q W_j{}^{pl}{}_q. \tag{6}$$

Here $|W|^2$ has weight 2, while the other two invariants have weight 3.

Other local conformal invariants can be obtained in terms of the ambient metric of Fefferman-Graham ([**FG1**], [**FG2**]; see Section 4 below).

1.2. Conformally invariant operators.

DEFINITION 3. *A Riemannian invariant differential operator of weight w is the datum on each Riemannian manifold (M^n, g) of a differential operator P_g on M such that:*

(i) *There exist finitely many functions $a_{\alpha\beta\gamma}$ in $C^\infty(M_n(\mathbb{R})_+)$ such that, in any local coordinates,*

$$P_g = \sum a_{\alpha\beta\gamma}(g(x))(\partial^\alpha g(x))^\beta D_x^\gamma. \tag{7}$$

(ii) *We have*

$$P_{tg} = t^{-w}P_g \qquad \forall t > 0. \tag{8}$$

DEFINITION 4. *A conformally invariant differential operator of biweight (w, w') is a Riemannian invariant differential operator P_g such that*

$$P_{e^f g} = e^{w'f}P_g e^{-wf} \qquad \forall f \in C^\infty(M, \mathbb{R}). \tag{9}$$

An important example of a conformally invariant differential operator is the Yamabe operator,

$$\Box_g := \Delta_g + \frac{n-2}{4(n-1)}\kappa_g, \tag{10}$$

where Δ_g denotes the Laplace operator. In particular,

$$\Box_{e^{2f}g} = e^{-(\frac{n}{2}+1)f}\Box_g e^{(\frac{n}{2}-1)f} \qquad \forall f \in C^\infty(M, \mathbb{R}). \tag{11}$$

A generalization of the Yamabe operator is provided by the GJMS operators of Graham-Jenne-Mason-Sparling [**GJMS**]. For $k = 1, \ldots, \frac{n}{2}$ when n is even, and for all non-negative integers k when n is odd, the GJMS operator of order k is a differential operator $\Box_g^{(k)}$ such that

$$\Box_g^{(k)} = \Delta_g^{(k)} + \text{ lower order terms}, \tag{12}$$

and which satisfies

$$\Box_{e^{2f}g}^{(k)} = e^{-(\frac{n}{2}+k)f}\Box_g^{(k)} e^{(\frac{n}{2}-k)f} \qquad \forall f \in C^\infty(M, \mathbb{R}). \tag{13}$$

For $k=1$ this operator agrees with the Yamabe operator, while for $k=2$ we recover the Paneitz operator.

Recently, Alexakis ([**Al2**], [**Al1**]) and Juhl [**Ju**] constructed new families of conformally invariant operators. Furthermore, Alexakis proved that, under some restrictions, his family of operators exhausts *all* conformally invariant differential operators.

2. Conformally Invariant ΨDOs

Let U be an open subset of $\mathbb{R}^n$. The (classical) symbols on $U\times\mathbb{R}^n$ are defined as follows.

DEFINITION 5. *1) $S_m(U\times\mathbb{R}^n)$, $m\in\mathbb{C}$, is the space of functions $p(x,\xi)$ contained in $C^\infty(U\times(\mathbb{R}^n\setminus\{0\}))$ such that $p(x,t\xi)=t^m p(x,\xi)$ for any $t>0$.*

2) $S^m(U\times\mathbb{R}^n)$, $m\in\mathbb{C}$, consists of functions $p\in C^\infty(U\times\mathbb{R}^n)$ with an asymptotic expansion $p\sim\sum_{j\geq 0}p_{m-j}$, $p_k\in S_k(U\times\mathbb{R}^n)$, in the sense that, for any integer N, any compact $K\subset U$ and any multi-orders α, β, there exists a constant $C_{NK\alpha\beta}>0$ such that, for any $x\in K$ and any $\xi\in\mathbb{R}^{d+1}$ so that $|\xi|\geq 1$, we have

$$|\partial_x^\alpha\partial_\xi^\beta(p-\sum_{j<N}p_{m-j})(x,\xi)|\leq C_{NK\alpha\beta}|\xi|^{\Re m-|\beta|-N}. \tag{14}$$

Given a symbol $p\in S^m(U\times\mathbb{R}^n)$ we let $p(x,D)$ be the continuous linear operator from $C_c^\infty(U)$ to $C^\infty(U)$ such that

$$p(x,D)u(x)=(2\pi)^{-n}\int e^{ix\cdot\xi}p(x,\xi)\hat{u}(\xi)d\xi \qquad \forall u\in C_c^\infty(U). \tag{15}$$

We define ΨDOs on the manifold M^n as follows.

DEFINITION 6. *$\Psi^m(M)$, $m\in\mathbb{C}$, consists of continuous operators P from $C_c^\infty(M)$ to $C^\infty(M)$ such that:*

(i) The Schwartz kernel of P is smooth off the diagonal;

(ii) In any local coordinates the operator P can be written as

$$P=p(x,D)+R, \tag{16}$$

where p is a symbol of order m and R is a smoothing operator.

Recall that the principal symbol of a ΨDO makes sense intrinsically as a function $p_m(x,\xi)\in C^\infty(T^*M\setminus\{0\})$ such that

$$p_m(x,\lambda\xi)=\lambda^m p_m(x,\xi) \qquad \forall(x,\xi)\in T^*M\setminus\{0\} \quad \forall\lambda>0. \tag{17}$$

Recall also that P is said to be *elliptic* if $p_m(x,\xi)\neq 0$ for all $(x,\xi)\in T^*M\setminus\{0\}$. This is equivalent to the existence of a parametrix in $\Psi^{-m}(M)$, i.e., an inverse modulo smoothing operators.

This said, in order to define Riemannian and conformally invariant ΨDOs, we need to consider the following class of symbols.

DEFINITION 7. *$S_m(M_n(\mathbb{R})_+\times\mathbb{R}^n)$, $m\in\mathbb{C}$, consists of functions $a(g,\xi)$ in $C^\infty(M_n(\mathbb{R})_+\times(\mathbb{R}^n\setminus\{0\}))$ such that $a(g,t\xi)=t^m a(g,\xi)$ $\forall t>0$.*

In the sequel we let $\Psi^{-\infty}(M)$ denote the space of smoothing operators on M.

Definition 8. *A Riemannian invariant ΨDO of order m and weight w is the datum for every Riemannian manifold (M^n,g) of an operator $P_g \in \Psi^m(M)$ in such a way that:*

(i) *For $j=0,1,\ldots$ there are finitely many $a_{j\alpha\beta} \in S_{m-j}(M_n(\mathbb{R})_+ \times \mathbb{R}^n)$ such that, in any local coordinates, P_g has symbol*

$$\sigma(P_g)(x,\xi) \sim \sum_{j\geq 0} \sum_{\alpha,\beta} (\partial^\alpha g(x))^\beta a_{j\alpha\beta}(g(x),\xi). \tag{18}$$

(ii) *For all $t>0$ we have*

$$P_{tg} = t^{-w} P_g \qquad \bmod \Psi^{-\infty}(M). \tag{19}$$

Remark. For differential operators this definition is equivalent to Definition 3, because two differential operators differing by a smoothing operator must agree.

Definition 9. *A conformally invariant ΨDO of order m and biweight (w,w') is a Riemannian invariant ΨDO of order m such that, for all $f \in C^\infty(M,\mathbb{R})$,*

$$P_{e^f g} = e^{w'f} P_g e^{-wf} \qquad \bmod \Psi^{-\infty}(M). \tag{20}$$

In the sequel we say that a Riemannian invariant is *admissible* if its principal symbol does not depend on the derivatives of the metric (i.e. in (18) we can take $a_{0\alpha\beta}=0$ for $(\alpha,\beta)\neq 0$).

Proposition 1. *Let P_g be a conformally invariant ΨDO of order m and biweight (w,w').*

(1) *Let Q_g be a conformally invariant ΨDO of order m' and biweight (w,w''), and assume that P_g or Q_g is properly supported. Then Q_gP_g is a conformally invariant ΨDO of order $m+m'$ and biweight (w,w'').*

(2) *Assume that P_g is elliptic and admissible. Then the datum on every Riemannian manifold (M^n,g) of a parametrix $Q_g \in \Psi^{-m}(M)$ for P_g gives rise to a conformally invariant ΨDO of biweight (w',w).*

For instance, if $Q_g^{(k)}$ is a parametrix for the kth order GJMS operator $\Box_g^{(k)}$, then $Q_g^{(k)}$ is a conformally invariant ΨDO of biweight $(\frac{n+2k}{4},\frac{n-2k}{4})$. By multiplying these operators with the operators of Alexakis and Juhl we obtain various examples of conformally invariant ΨDOs that are not differential operators or parametrices of elliptic differential operators

3. The Logarithmic Singularity of a ΨDO

We can give a precise description of the singularity of the Schwartz kernel of a ΨDO near the diagonal and, in fact, the general form of these singularities can be used to characterize ΨDOs (see, e.g., [**Hö**], [**Me**], [**BGr**]). In particular, if $P: C_c^\infty(M) \rightarrow C^\infty(M)$ if a ΨDO of integer order $m \geq -n$, then in local coordinates its Schwartz kernel $k_P(x,y)$ has a behavior near the diagonal $y=x$ of the form

$$k_P(x,y) = \sum_{-(m+n)\leq j \leq -1} a_j(x,x-y) - c_P(x)\log|x-y| + O(1), \tag{21}$$

where $a_j(x,y) \in C^\infty(U\times(\mathbb{R}^n\setminus\{0\}))$ is homogeneous of degree j in y and we have

$$c_P(x) = \frac{1}{(2\pi)^n}\int_{S^{n-1}} p_{-n}(x,\xi)d\sigma(\xi), \tag{22}$$

where $p_{-n}(x,\xi)$ is the symbol of degree $-n$ of P and we have denoted by $d\sigma(\xi)$ is the surface measure of S^{n-1}.

It seems to have been first observed by Connes-Moscovici [**CMo**] (see also [**GVF**], [**Po5**]) that the coefficient $c_P(x)$ makes sense globally on M as a 1-density.

In the sequel we refer to the density $c_P(x)$ as the *logarithmic singularity* of the Schwartz kernel of P.

If P is elliptic, then we shall call a *Green kernel for* P the Schwartz kernel of any parametrix $Q \in \Psi^{-m}(M,\mathcal{E})$ for P. Such a parametrix is uniquely defined only modulo smoothing operators, but the singularity near the diagonal of the Schwartz kernel of Q, including the logarithmic singularity $c_Q(x)$, does not depend on the choice of Q.

Definition 10. *If $P \in \Psi^m(M)$, $m \in \mathbb{Z}$, is elliptic, then the Green kernel logarithmic singularity of P is the density*

$$\gamma_P(x) := c_Q(x), \tag{23}$$

where $Q \in \Psi^{-m}(M)$ is any given parametrix for P.

Next, because of (22) the density $c_P(x)$ is related to the noncommutative residue trace of Wodzicki ([**Wo1**], [**Wo3**]) and Guillemin [**Gu1**] as follows.

Let $\Psi^{<-n}(M) = \bigcup_{\Re m<-n} \Psi^m(M)$ denote the class of ΨDOs whose symbols are integrable with respect to the ξ-variable. If P is a ΨDO in this class then the restriction to the diagonal of its Schwartz kernel $k_P(x,y)$ defines a smooth density $k_P(x,x)$. Therefore, if M is compact then P is trace-class on $L^2(M)$ and we have

$$\operatorname{Trace} P = \int_M k_P(x,x). \tag{24}$$

In fact, the map $P \rightarrow k_P(x,x)$ admits an analytic continuation $P \rightarrow t_P(x)$ to the class $\Psi^{\mathbb{C}\setminus\mathbb{Z}}(M)$ of non-integer ΨDOs, where analyticity is meant with respect to holomorphic families of ΨDOs as in [**Gu2**] and [**KV**]. Furthermore, if $P \in \Psi^{\mathbb{Z}}(M)$ and if $(P(z))_{z\in\mathbb{C}}$ is a holomorphic family of ΨDOs such that $\operatorname{ord} P(z) = \operatorname{ord} P + z$ and $P(0) = P$. Then, at $z = 0$, the map $z \rightarrow t_{P(z)}(x)$ has at worst a simple pole singularity with residue given by

$$\operatorname{Res}_{z=0} t_{P(z)}(x) = -c_P(x). \tag{25}$$

Suppose now that M is compact. Then the *noncommutative residue* is the linear functional on $\Psi^{\mathbb{Z}}(M)$ defined by

$$\operatorname{Res} P := \int_M c_P(x) \qquad \forall P \in \Psi^{\mathbb{C}\setminus\mathbb{Z}}(M). \tag{26}$$

Thanks to (22) this definition agrees with the usual definition of the noncommutative residue. Moreover, by using (25) we see that if $(P(z))_{z\in\mathbb{C}}$ is a holomorphic family of ΨDOs such that $\operatorname{ord} P(z) = \operatorname{ord} P + z$ and $P(0) = P$, then the map $z \rightarrow \operatorname{Trace} P(z)$ has an analytic extension to $\mathbb{C} \setminus \mathbb{Z}$ and, at $z = 0$, it has at worst a simple pole singularity with residue given by

$$\operatorname{Res} P = -\operatorname{Res}_{z=0} \operatorname{Trace} P(z). \tag{27}$$

Using this it is not difficult to see that the noncommutative residue is a trace on $\Psi^{\mathbb{Z}}(M)$. Wodzicki [**Wo2**] even proved that his is the unique trace up to constant multiple when M is connected and has dimension ≥ 2.

Finally, let $P : C^\infty(M) \to C^\infty(M)$ be a ΨDO of integer order $m \geq 0$ with a positive principal symbol. For $t > 0$ let $k_t(x,y)$ denote the Schwartz kernel of e^{-tP}. Then $k_t(x,y)$ is a smooth kernel and, as $t \to 0^+$,

$$k_t(x,x) \sim t^{-\frac{n}{m}} \sum_{j\geq 0} t^{\frac{j}{m}} a_j(P)(x) + \log t \sum_{j \geq 0} t^j b_j(P)(x), \tag{28}$$

where we further have $a_{2j+1}(P)(x) = b_j(P)(x) = 0$ for all $j \in \mathbb{N}_0$ when P is a differential operator (see, e.g., [**Gi**], [**Gr**]).

Using the Mellin Formula, we can explicitly relate the coefficients of the above heat kernel asymptotics to the singularities of the local zeta function $t_{P^{-s}}(x)$ (see, e.g., [**Wo3**, 3.23]). In particular, if for $j = 0, \ldots, n-1$ we set $\sigma_j = \frac{n-j}{m}$, then

$$mc_{P^{-\sigma_j}}(x) = \Gamma(\sigma_j)^{-1} a_j(P)(x). \tag{29}$$

The above equalities provide us with an immediate connection between the Green kernel logarithmic singularity of P and the heat kernel asymptotics (28). Indeed, as the partial inverse P^{-1} is a parametrix for P in $\Psi^{-m}(M)$, setting $j = n - m$ in (29) gives

$$a_{n-m}(P)(x) = mc_{P^{-1}}(x) = m\gamma_P(x). \tag{30}$$

4. Fefferman's Program in Conformal Geometry

In the sequel by *Green kernel* of an elliptic ΨDO we shall mean the Schwartz kernel of a parametrix, and by *null kernel* of a selfadjoint ΨDO we shall mean the Schwartz kernel of the orthogonal projection onto its null space.

The program of Fefferman in conformal geometry can be described as follows.

Fefferman's Program (Analytic Aspect). *Give a precise geometric description of the singularities of the Schwartz, Green and null kernels of conformally invariant operators in terms of local conformal invariants.*

As stated by Theorem 1, any local Riemannian invariant is a linear combination of Weyl Riemannian invariants. Is there a similar description for local conformal invariants? Establishing such a description is the aim of the geometric aspect of Fefferman's program:

Fefferman's Program (Geometric Aspect). *Determine all local invariants of a conformal structure.*

4.1. Ambient metric and Weyl conformal invariants. The analogues in conformal geometry of the Weyl Riemannian invariants are obtained via the ambient metric construction of Fefferman-Graham ([**FG1**], [**FG2**]).

In this section we denote by (M^n, g) a general Riemannian manifold of dimension n. Consider the metric ray-bundle,

$$\mathcal{G} := \{t^2 g(x); x \in M,\ t > 0\} \subset S^2T^*M \xrightarrow{\pi} M. \tag{31}$$

It carries the family of dilations,

$$\delta_s(x, \bar{g}) := s^2 \bar{g} \qquad \forall x \in M \quad \forall \bar{g} \in \mathcal{G}_x \quad \forall s > 0, \tag{32}$$

It also carries the (degenerate) tautological metric,

$$g_0(x, \bar{g}) := (d\pi(x))^* \, \bar{g} \qquad \forall (x, \bar{g}) \in \mathcal{G}. \tag{33}$$

Thus, if $\{x^j\}$ are local coordinates with respect to which $g(x) = g_{ij}dx^i \otimes dx^j$ and if we denote by t the fiber coordinate on $\mathcal{G}$ defined by the metric g, then in the local coordinates $\{x^j, t\}$ we have

$$g_0(x,t) = t^2 g_{ij} dx^i \otimes dx^j. \tag{34}$$

The *ambient space* is defined to be

$$\tilde{\mathcal{G}} := \mathcal{G} \times (-1,1). \tag{35}$$

In the sequel we shall use the letter ρ to denote the variable with values in $(-1,1)$. Then $\mathcal{G}$ can be identified with the hypersurface $\mathcal{G}_0 := \{\rho = 0\} \subset \tilde{\mathcal{G}}$.

Theorem 2 ([**FG1**], [**FG2**]). *There exists a unique Lorentzian metric $\tilde{g}$ on $\tilde{\mathcal{G}}$ defined formally near $\rho = 0$ such that:*

$$\delta_s^* \tilde{g} = s^2 g_0, \qquad \tilde{g}_{|\rho=0} = g_0, \tag{36}$$

$$\operatorname{Ric}(\tilde{g}) = \begin{cases} O(\rho^\infty) & \text{if } n \text{ is odd,} \\ O(\rho^{\frac{n}{2}}) & \text{if } n \text{ is even.} \end{cases} \tag{37}$$

The ambient metric depends only on the conformal class of g, so any local Riemannian invariant of $(\tilde{\mathcal{G}}, \tilde{g})$ gives rise to a local conformal invariant of (M^n, g).

Definition 11. *The Weyl conformal invariants are the local conformal invariants arising from the Weyl Riemannian invariants of $(\tilde{\mathcal{G}}, \tilde{g})$.*

For instance, the Weyl tensor is obtained by pushing down to M the curvature tensor $\tilde{R}$ of $\tilde{\mathcal{G}}$. Therefore, the invariants in (5)–(6) are Weyl conformal invariants.

In fact, if we use the Ricci-flatness of the ambient metric, then we see that there is no Weyl conformal invariant of weight 1 and the only of these invariants in weight 2 is $|W|^2$. In addition, in weight 3 we only have the invariants in (6) together with the invariant arising from $|\tilde{\nabla}\tilde{R}|^2$, namely, the Fefferman-Graham invariant,

$$\Phi_g := |V|^2 + 16\langle W, U\rangle + 16|C|^2, \tag{38}$$

where $C_{jkl} = \nabla_l A_{jk} - \nabla_k A_{jl}$ is the Cotton tensor and V and U are the tensors

$$V_{sijkl} = \nabla_s W_{ijkl} - g_{is}C_{jkl} + g_{js}C_{ikl} - g_{ks}C_{lij} + g_{ls}C_{kij}, \tag{39}$$

$$U_{sjkl} = \nabla_s C_{jkl} + g^{pq}A_{sp}W_{qjkl}. \tag{40}$$

Next, a very important result is the following.

Proposition 2 ([**BEG**]).

(1) *If n is odd, then any local conformal invariant is a linear combination of Weyl conformal invariants.*
(2) *If n is even, the same holds in weight $\leq \frac{n}{2}$.*

In even dimension a description of the scalar local conformal invariants of weight $w \geq \frac{n}{2} + 1$ was recently presented by Graham-Hirachi [**GH**]. More precisely, they modified the construction of the ambient metric in such way as to obtain a metric on the ambient space $\tilde{\mathcal{G}}$ which is smooth of any order near $\mathcal{G}_0$. There is an ambiguity on the choice of a smooth ambient metric, but such a metric agrees with the ambient metric of Fefferman-Graham up to order $< \frac{n}{2}$ near $\mathcal{G}_0$.

Using a smooth ambient metric we can construct Weyl conformal invariants in the same way as we do by using the ambient metric of Fefferman-Graham. If such an invariant does not depend on the choice of the smooth ambient metric we then say that it is an *ambiguity-independent* Weyl conformal invariant. Not every conformal invariant arises this way, since in dimension $n = 4m$ this construction does not encapsulate the exceptional local conformal invariants of [**BG**].

PROPOSITION 3 (Graham-Hirachi [**GH**]). *Let w be an integer $\geq \frac{n}{2}$.*

1) If $n \equiv 2 \mod 4$, or if $n \equiv 0 \mod 4$ and w is even, then every scalar local conformal invariant of weight w is a linear combination of ambiguity-independent Weyl conformal invariants.

2) If $n \equiv 0 \mod 4$ and w is odd, then every scalar local conformal invariant of weight w is a linear combination of ambiguity-independent Weyl conformal invariants and of exceptional conformal invariants.

5. Logarithmic Singularities of Conformally Invariant Operators

One aim of this paper is to look at the logarithmic singularities (as defined in (21)–(22)) of conformally invariant ΨDOs.

In the sequel we denote by $|v_g(x)|$ the volume density of (M^n, g), i.e., in local coordinates $|v_g(x)| = \sqrt{g(x)}|dx|$, where $|dx|$ is the Lebesgue density. We also denote by $[g]$ the conformal class of g.

PROPOSITION 4. *Consider a family $(P_{\hat{g}})_{\hat{g}\in[g]} \subset \Psi^m(M)$ for which there are real numbers w and w' such that, for all $f \in C^\infty(M, \mathbb{R})$, we have*

$$P_{e^f g} \equiv e^{w' f} P_g e^{-wf} \mod \Psi^{-\infty}(M). \tag{41}$$

Then, at the level of the logarithmic singularities,

$$c_{P_{e^f g}}(x) = e^{(w'-w)f(x)} c_{P_g}(x) \qquad \forall f \in C^\infty(M, \mathbb{R}). \tag{42}$$

This result generalizes a well-known result of Parker-Rosenberg [**PR**] about the logarithmic singularity of the Green kernel of the Yamabe operator. Moreover, using (22) and (30) this also allows us to recover and extend results of Gilkey [**Gi**] and Paycha-Rosenberg [**PRo**] on the noncommutative residue densities of elliptic ΨDOs satisfying (41). In particular, all the assumptions on the compactness of M or on the invertibility and the values of the principal symbol of P_g can be removed from those statements.

PROPOSITION 5 (see [**Po4**]). *Let P_g be a Riemannian invariant ΨDO of weight w and integer order. Then*

$$c_{P_g}(x) = \mathcal{I}_{P_g}(x)|v_g(x)| \tag{43}$$

where $\mathcal{I}_{P_g}(x)$ is a local Riemannian invariant of weight w.

Combining this with Proposition 4 allows us to prove the following.

THEOREM 3 ([**Po4**]). *Let P_g be a conformally invariant Riemannian ΨDO of integer order and biweight (w, w'). In odd dimension, as well as in even dimension when $w' > w$, the logarithmic singularity $c_{P_g}(x)$ is of the form*

$$c_{P_g}(x) = \mathcal{I}_{P_g}(x)|v_g(x)|, \tag{44}$$

where $\mathcal{I}_{P_g}(x)$ is a universal linear combination of Weyl conformal invariants of weight $\frac{n}{2} + w - w'$. If n is even and we have $w' \leq w$, then $c_{P_g}(x)$ still is of a similar form, but in this case $\mathcal{I}_{P_g}(x)$ is a local conformal invariant of weight $\frac{n}{2} + w - w'$ of the type described in Proposition 3.

As an application of this result we can obtain a precise description of the logarithmic singularities of the Green kernels of the GJMS operators.

THEOREM 4. *1) In odd dimension the Green kernel logarithmic singularity $\gamma_{\Box_g^{(k)}}(x)$ is always zero.*

2) In even dimension and for $k = 1, \ldots, \frac{n}{2}$ we have

$$\gamma_{\Box_g^{(k)}}(x) = c_g^{(k)}(x) d\nu_g(x), \tag{45}$$

where $c_g^{(k)}(x)$ is a linear combination of Weyl conformal invariants of weight $\frac{n}{2} - k$. In particular, we have

$$c_g^{(\frac{n}{2})}(x) = (4\pi)^{-\frac{n}{2}} \frac{n}{(n/2)!}, \qquad c_g^{(\frac{n}{2}-1)}(x) = 0, \qquad c_g^{(\frac{n}{2}-2)}(x) = \alpha_n |W(x)|_g^2, \tag{46}$$

$$c_g^{(\frac{n}{2}-3)}(x) = \beta_n W_{ij}{}^{kl} W_{lk}{}^{pq} W_{pq}{}^{ij} + \gamma_n W_i{}^{jk}{}_l W^i{}_{pk}{}^q W_j{}^{pl}{}_q + \delta_n \Phi_g, \tag{47}$$

where W is the Weyl curvature tensor, Φ_g is the Fefferman-Graham invariant (38) and α_n, β_n, γ_n and δ_n are universal constants depending only on n.

Finally, we can get an explicit expression for $c_g^{(1)}(x)$ in dimensions 6 and 8 by making use of the computations by Parker-Rosenberg [**PR**] of the coefficient $a_{n-2}(\Box_g)(x)$ of t^{-1} in the heat kernel asymptotics (28) for the Yamabe operator. Indeed, as by (30) we have $2\gamma_{\Box_g}(x) = a_{n-2}(\Box_g)(x)$, using [**PR**, Prop. 4.2] we see that, in dimension 6,

$$c_g^{(1)}(x) = \frac{1}{360} |W(x)|^2, \tag{48}$$

and, in dimension 8,

$$c_g^{(1)}(x) = \frac{1}{90720} (81\Phi_g + 352 W_{ij}{}^{kl} W_{lk}{}^{pq} W_{pq}{}^{ij} + 64 W_i{}^{jk}{}_l W^i{}_{pk}{}^q W_j{}^{pl}{}_q). \tag{49}$$

In order to use the results of [**PR**] the manifold M has to be compact. However, as $c_g^{(1)}(x)$ is a local Riemannian invariant which makes sense independently of whether M is compact or not, the above formulas for $c_g^{(1)}(x)$ remain valid when M is non-compact.

6. The Bergman Kernel of a Strictly Pseudoconvex Domain

Let $D = \{r(z) < 0\} \subset \mathbb{C}^{n+1}$ be a strictly pseudoconvex domain with boundary $\partial D = \{r(z) = 0\}$. The fact that D is strictly pseudoconvex means that the defining function $r(z)$ can be chosen so that $\bar{\partial}\partial r$ defines a positive definite Hermitian form on the holomorphic tangent space $T^{1,0}D$.

Let $\mathcal{O}(D)$ denote the space of holomorphic functions on D. The *Bergman projection*,

$$B : L^2(D) \longrightarrow \mathcal{O}(D) \cap L^2(D), \tag{50}$$

is the orthogonal projection of $L^2(D)$ onto the space of holomorphic L^2-functions on D. The *Bergman kernel*, denoted $B(z, w)$, is the Schwartz kernel of B defined so that

$$Bu(z) = \int B(z, w) u(w) dw \qquad \forall u \in L^2(D). \tag{51}$$

Equivalently, $B(z, w)$ is the reproducing kernel of the Hilbert space $\mathcal{O}(D) \cap L^2(D)$.

In the analysis of the Bergman kernel an important result is the following.

THEOREM 5 (Fefferman [**Fe1**]). *Near ∂D we have*

$$B(z,z) = \varphi(z) r(z)^{-(n+1)} - \psi(z) \log r(z), \tag{52}$$

where $\varphi(z)$ and $\psi(z)$ are smooth up to the boundary.

The original motivation for the program of Fefferman [**Fe2**] was to give a precise description of the singularity of the Bergman kernel near ∂D in terms of local geometric invariants of ∂D. In this case the complex structure of D induces on ∂D a *CR structure* and, as D is strictly pseudoconvex, the CR structure of ∂D is *strictly pseudoconvex*. Thus, the original goals of Fefferman were the following:

(i) Express the singularity in terms of local invariants of the strictly pseudoconvex CR structure of ∂D.

(ii) Determine *all* local invariants of a strictly pseudoconvex CR structure.

We refer to Section 9 for the precise definition of a local invariant of a strictly pseudoconvex CR structure. For now let us recall that, in general, a *CR structure* on an oriented manifold M^{2n+1} is given by the datum of a hyperplane bundle $H \subset TM$ equipped with an (integrable) complex structure J_H. For instance, the CR structure on the boundary ∂D above is given by the complex hyperplane bundle

$$H := T(\partial D) \cap iT(\partial D) \subset T(\partial D). \tag{53}$$

Let (M, H, J) be a CR manifold. Set $T_{1,0} = \ker(J - i) \subset T_{\mathbb{C}}M$ and $T_{0,1} = \ker(J + i)$, so that $H \otimes \mathbb{C} = T_{1,0} \otimes T_{0,1}$. Since M is orientable there is a non-vanishing 1-form θ on M annihilating H. The *Levi form* is the Hermitian form L_θ on $T_{1,0}$ defined by

$$L_\theta(Z, W) = -id\theta(Z, \overline{W}) \qquad \forall Z, W \in C^\infty(M, T_{1,0}). \tag{54}$$

When we can choose θ so that L_θ is positive definite we say that M is *strictly pseudoconvex*. Notice that this implies that θ is a contact form.

Examples of CR manifolds include:

- Boundaries of complex domains in $\mathbb{C}^{n+1}$, e.g., the sphere $S^{2n+1} \subset \mathbb{C}^{n+1}$ and the hyperquadric $Q^{2n+1} := \{z \in \mathbb{C}^{n+1}; \Im z_{n+1} = |z_1|^2 + \cdots + |z_n|^2\}$.
- The Heisenberg group $\mathbb{H}^{2n+1}$ and its quotients $\Gamma \backslash \mathbb{H}^{2n+1}$ by discrete cocompact subgroups.
- Circle bundles over complex manifolds.

Recall that the Heisenberg group $\mathbb{H}^{2n+1}$ can be realized as $\mathbb{R}^{n+1}$ equipped with the group law and dilations,

$$x.y = (x_0 + y_0 + \sum_{j=1}^{n} (x_{n+j} y_j - x_j y_{n+j}), x_1 + y_1, \ldots, x_{2n} + y_{2n}), \tag{55}$$

$$t.(x_0, \ldots, x_{2n}) = (t^2 x_0, tx_1, \ldots, tx_{2n}), \qquad t \in \mathbb{R}. \tag{56}$$

Notice that the group-law (55) is homogeneous with respect to the anisotropic dilations (56).

The Lie algebra $\mathfrak{h}^{2n+1}$ of $\mathbb{H}^{2n+1}$ is spanned by the left-invariant vector fields,

$$X_0 = \frac{\partial}{\partial x_0}, \qquad X_j = \frac{\partial}{\partial x_j} + x_{n+j} \frac{\partial}{\partial x_0}, \qquad X_{n+j} = \frac{\partial}{\partial x_{n+j}} - x_j \frac{\partial}{\partial x_0}, \tag{57}$$

where j ranges over $1, \ldots, n$. Notice that, with respect to the dilations (56), the vector field X_0 is homogeneous of degree -2, while $X_1, \ldots. X_{2n}$ are homogeneous of degree -1. Moreover, for $j, k = 1, \ldots, n$, we have the Heisenberg relations,

$$[X_j, X_{n+k}] = -2\delta_{jk} X_0, \qquad [X_j, X_k] = [X_{n+j}, X_{n+k}] = 0. \tag{58}$$

The CR structure of $\mathbb{H}^{2n+1}$ is defined by the hyperplane bundle

$$H = \operatorname{Span}\{X_1, \ldots, X_{2n}\} \tag{59}$$

equipped with the complex structure J defined by

$$JX_j = X_{n+j}, \qquad JX_{n+j} = -X_j, \qquad j = 1, \ldots, n. \tag{60}$$

The hyperplane H is the annihilator of the 1-form,

$$\theta_0 := dx_0 - \sum_{j=1}^{n} (x_{n+j} dx_j - x_j dx_{n+j}). \tag{61}$$

One can check that the associated Levi form is positive definite, so $\mathbb{H}^{2n+1}$ is a strictly pseudoconvex CR manifold. This is in fact the local model of such a manifold.

7. Heisenberg Calculus

In this section, we briefly recall the main facts about the Heisenberg calculus. This calculus was introduced by Beals-Greiner [**BGr**] and Taylor [**Tay**] (see also [**EM**], [**Po3**]). This is the most relevant calculus to study the main geometric operators on CR manifolds.

7.1. Overview of the Heisenberg calculus. The Heisenberg calculus holds in full generality for *Heisenberg manifolds*, that is, manifolds M^{d+1} together with a distinguished hyperplane bundle $H \subset TM$. This terminology stems from the fact that, for a Heisenberg manifold, the relevant notion of tangent bundle is that of a bundle of 2-step nilpotent Lie groups whose fibers are isomorphic to $\mathbb{H}^{2n+1} \times \mathbb{R}^d$ for some k and n such that $2n + k = d$ (see, e.g., [**BGr**], [**Po1**]). This tangent Lie group bundle can be described as follows.

First, there is an intrinsic Levi form obtained as the 2-form $\mathcal{L} : H \times H \to TM/H$ such that, for any point $a \in M$ and any sections X and Y of H near a, we have

$$\mathcal{L}_a(X(a), Y(a)) = [X, Y](a) \qquad \text{mod } H_a. \tag{62}$$

In other words the class of $[X, Y](a)$ modulo H_a depends only on $X(a)$ and $Y(a)$, not on the germs of X and Y near a (see [**Po1**]).

We define the tangent Lie algebra bundle $\mathfrak{g}M$ as the graded Lie algebra bundle consisting of $(TM/H) \oplus H$ together with the fields of Lie bracket and dilations such that, for sections X_0, Y_0 of TM/H and X', Y' of H and for $t \in \mathbb{R}$, we have

$$[X_0 + X', Y_0 + Y'] = \mathcal{L}(X', Y'), \qquad t.(X_0 + X') = t^2 X_0 + tX'. \tag{63}$$

Each fiber $\mathfrak{g}_a M$ is a two-step nilpotent Lie algebra so, by requiring the exponential map to be the identity, the associated tangent Lie group bundle GM appears as $(TM/H) \oplus H$ together with the grading above and the product law such that, for sections X_0, Y_0 of TM/H and X', Y' of H, we have

$$(X_0 + X').(Y_0 + Y') = X_0 + Y_0 + \frac{1}{2}\mathcal{L}(X', Y') + X' + Y'. \tag{64}$$

A motivating example for the Heisenberg calculus is the *horizontal sub-Laplacian* Δ_b on a Heisenberg manifold (M^{d+1}, H) equipped with a Riemannian metric. This is the operator $\Delta_b : C^\infty(M) \to C^\infty(M)$ defined by

$$\Delta_b = d_b^* d_b, \qquad d_b = \pi \circ d, \tag{65}$$

where π is the orthogonal projection onto H^* (identified with a subbundle of T^*M using the Riemannian metric).

An H-frame of TM is a frame $X_0, X_1, \ldots, X_d$ of TM such that $X_1, \ldots, X_d$ span H. Locally, we always can find an H-frame $X_0, X_1, \ldots, X_d$ such that Δ_b takes the form

$$\Delta_b = -(X_1^2 + \cdots + X_{2n}^2) + \sum_{j=1}^{d} a_j(x) X_j. \tag{66}$$

As the differentiation along X_0 is missing we see that Δ_b is not elliptic. However, whenever the Levi form (62) is everywhere non-zero, a celebrated theorem of Hörmander [**Hö2**] ensures us that Δ_b is hypoelliptic with gain of one derivative (i.e., if $\Delta_b u$ is in L^2_{loc} then u must be in the Sobolev space $W^{2,1}_{\text{loc}}$).

In the case of the Heisenberg group, we can explicitly construct a fundamental solution for Δ_b (see [**BGr**], [**FS1**]). This fundamental solution comes from a symbol of type $(\frac{1}{2}, \frac{1}{2})$ in the sense of Hörmander [**Hö**]. As the usual symbolic calculus does not hold anymore for ΨDOs of type $(\frac{1}{2}, \frac{1}{2})$, the full strength of the classical pseudodifferential calculus cannot be used to study natural operators on Heisenberg manifolds such as the horizontal sub-Laplacian Δ_b.

The relevant substitute for the classical pseudodifferential calculus is precisely provided by the Heisenberg calculus. The idea is to construct a class of pseudodifferential operators, called Ψ_HDOs, which near each point $a \in M$ are approximated (in a suitable sense) by left-invariant convolution operators on $G_a M$. This allows us to get a pseudodifferential calculus with a full symbolic calculus with inverses and which is invariant under changes of charts preserving the hyperplane bundle H.

The symbols that we consider in the Heisenberg calculus are the following.

Definition 12. *1) $S_m(U \times \mathbb{R}^{d+1})$, $m \in \mathbb{C}$, is the space of functions $p(x,\xi)$ in $C^\infty(U \times (\mathbb{R}^{d+1} \setminus \{0\}))$ such that $p(x, t.\xi) = t^m p(x,\xi)$ for any $t > 0$.*

2) $S^m(U \times \mathbb{R}^{d+1})$, $m \in \mathbb{C}$, consists of functions $p \in C^\infty(U \times \mathbb{R}^{d+1})$ with an asymptotic expansion $p \sim \sum_{j \geq 0} p_{m-j}$, $p_k \in S_k(U \times \mathbb{R}^{d+1})$, in the sense that, for any integer N, any compact $K \subset U$ and any multi-orders α, β, there exists a constant $C_{NK\alpha\beta} > 0$ such that, for any $x \in K$ and any $\xi \in \mathbb{R}^{d+1}$ so that $\|\xi\| \geq 1$, we have

$$|\partial_x^\alpha \partial_\xi^\beta (p - \sum_{j<N} p_{m-j})(x,\xi)| \leq C_{NK\alpha\beta} \|\xi\|^{\Re m - \langle\beta\rangle - N}, \tag{67}$$

where we have set $\langle\beta\rangle = 2\beta_0 + \beta_1 + \ldots + \beta_d$.

Next, for $j = 0, \ldots, d$ let $\sigma_j(x,\xi)$ denote the symbol (in the classical sense) of the vector field $\frac{1}{i} X_j$ and set $\sigma = (\sigma_0, \ldots, \sigma_d)$. Then for $p \in S^m(U \times \mathbb{R}^{d+1})$ we let $p(x, -iX)$ be the continuous linear operator from $C_c^\infty(U)$ to $C^\infty(U)$ such that

$$p(x, -iX)u(x) = (2\pi)^{-(d+1)} \int e^{ix.\xi} p(x, \sigma(x,\xi)) \hat{u}(\xi) d\xi \qquad \forall u \in C_c^\infty(U). \tag{68}$$

Let (M^{d+1}, H) be a Heisenberg manifold. We define the Ψ_HDOs on M as follows.

DEFINITION 13. *$\Psi_H^m(M)$, $m \in \mathbb{C}$, consists of continuous operators P from $C_c^\infty(M)$ to $C^\infty(M)$ such that:*

(i) The Schwartz kernel of P is smooth off the diagonal;

(ii) In any local coordinates equipped with an H-frame $X_0, \ldots, X_d$ the operator P can be written as

$$P = p(x, -iX) + R, \tag{69}$$

where $p(x,\xi)$ is a Heisenberg symbol of order m and R is a smoothing operator.

For any $a \in M$ the convolution on G_aM gives rise under the (linear) Fourier transform to a bilinear product for homogeneous symbols,

$$*^a : S_{m_1}(\mathfrak{g}_a^*M) \times S_{m_2}(\mathfrak{g}_a^*) \longrightarrow S_{m_1+m_2}(\mathfrak{g}_a^*M). \tag{70}$$

This product depends smoothly on a, so it gives rise to the product,

$$* : S_{m_1}(\mathfrak{g}^*M) \times S_{m_2}(\mathfrak{g}^*M) \longrightarrow S_{m_1+m_2}(\mathfrak{g}^*M), \tag{71}$$

$$p_1 * p_2(a,\xi) = [p_1(a,\cdot) *^a p_2(a,\cdot)](\xi). \tag{72}$$

This provides us with the right composition for principal symbols, since for any operators $P_1 \in \Psi_H^{m_1}(M)$ and $P_2 \in \Psi_H^{m_2}(M)$ such that P_1 or P_2 is properly supported we have

$$\sigma_{m_1+m_2}(P_1P_2) = \sigma_{m_1}(P_1) * \sigma_{m_2}(P_2). \tag{73}$$

Notice that when G_aM is not commutative, i.e., when $\mathcal{L}_a \neq 0$, the product $*^a$ is no longer the pointwise product of symbols and, in particular, it is not commutative. As a consequence, unless H is integrable, the product for Heisenberg symbols, while local, is not microlocal (see [**BGr**]).

When the principal symbol of $P \in \Psi_H^m(M)$ is invertible with respect to the product $*$, the symbolic calculus of [**BGr**] allows us to construct a parametrix for P in $\Psi_H^{-m}(M)$. In particular, although not elliptic, P is hypoelliptic with a controlled loss/gain of derivatives (see [**BGr**]).

In general, it may be difficult to determine whether the principal symbol of a given operator $P \in \Psi_H^m(M)$ is invertible with respect to the product $*$, but this can be completely determined in terms of a representation theoretic criterion on each tangent group G_aM, the so-called Rockland condition (see [**Po3**], Thm. 3.3.19). In particular, if $\sigma_m(P)(a,\cdot)$ is *pointwise* invertible with respect to the product $*^a$ for all $a \in M$.

7.2. The logarithmic singularity of a Ψ_HDO. It is possible to characterize the Ψ_HDOs in terms of their Schwartz kernels (see [**BGr**]). As a consequence we get the following description of the singularity near the diagonal of the Schwartz kernel of a Ψ_HDO.

In the sequel, given an open subset of local coordinates $U \subset \mathbb{R}^{d+1}$ equipped with an H-frame $X_0, \ldots, X_d$ of TU, for any $a \in U$ we let ψ_a denote the unique affine change of variables such that $\psi_a(a) = 0$ and $(\psi_{a*}X_j)(0) = \frac{\partial}{\partial x_j}$ for $j = 0, 1, \ldots, d+1$.

DEFINITION 14. *The local coordinates provided by ψ_a are called privileged coordinates centered at a.*

Throughout the rest of the paper the notion of homogeneity refers to homogeneity with respect to the anisotropic dilations (63).

PROPOSITION 6 ([**Po2**, Prop. 3.11]). *Let* $\Psi_H^m(M)$, $m \in \mathbb{Z}$.

1) In local coordinates equipped with an H*-frame the kernel* $k_P(x,y)$ *has a behavior near the diagonal* $y = x$ *of the form*

$$k_P(x,y) = \sum_{-(m+d+2)\leq j\leq -1} a_j(x, -\psi_x(y)) - c_P(x)\log\|\psi_x(y)\| + O(1), \tag{74}$$

where $a_j(x,y) \in C^\infty(U \times (\mathbb{R}^n \setminus \{0\}))$ *is homogeneous of degree* j *in* y*, and we have*

$$c_P(x) = (2\pi)^{-(d+1)} \int_{\|\xi\|=1} p_{-(d+2)}(x,\xi)\iota_E d\xi, \tag{75}$$

where $p_{-(d+2)}(x,\xi)$ *is the symbol of degree* $-(d+2)$ *of* P *and* E *denotes the anisotropic radial vector* $2x^0\partial_{x^0} + x^1\partial_{x^1} + \cdots + x^d\partial_{x^d}$.

2) The coefficient $c_P(x)$ *makes sense globally on* M *as a 1-density.*

Let $P \in \Psi_H^m(M)$ be such that its principal symbol is invertible in the Heisenberg calculus sense and let $Q \in \Psi_H^{-m}(M)$ be a parametrix for P. Then Q is uniquely defined modulo smoothing operators, so the logarithmic singularity $c_Q(x)$ does not depend on the particular choice of Q.

DEFINITION 15. *If* $P \in \Psi_H^m(M)$, $m \in \mathbb{Z}$*, has an invertible principal symbol, then its Green kernel logarithmic singularity is the density*

$$\gamma_P(x) := c_Q(x), \tag{76}$$

where $Q \in \Psi_H^{-m}(M)$ *is any given parametrix for* P.

In the same way as for classical ΨDOs, the logarithmic singularity densities are related to the construction of the noncommutative residue trace for the Heisenberg calculus (see [**Po2**]).

8. pseudo-Hermitian Invariants

8.1. pseudo-Hermitian geometry. Let (M^{2n+1}, H, J) be a strictly pseudoconvex CR manifold. In the terminology of [**We**] a *pseudo-Hermitian structure* on M is given by the datum of real 1-form on M such that θ annihilates H and the associated Levi form (62) is positive definite. Notice that θ is uniquely determined up to a conformal factor. Conversely, the conformal class of θ is uniquely determined by the strictly pseudoconvex CR structure of M.

Since θ is a contact form there exists a unique vector field X_0 on M, called the *Reeb field*, such that $\iota_{X_0}\theta = 1$ and $\iota_{X_0}d\theta = 0$. Let $\mathcal{N} \subset T_{\mathbb{C}}M$ be the complex line bundle spanned by X_0. We then have the splitting

$$T_{\mathbb{C}}M = \mathcal{N} \oplus T_{1,0} \oplus T_{0,1}. \tag{77}$$

The Levi metric h_θ is the unique Hermitian metric on $T_{\mathbb{C}}M$ such that:

- The splitting (77) is orthogonal with respect to h_θ;
- h_θ commutes with complex conjugation;
- We have $h(X_0, X_0) = 1$ and h_θ agrees with L_θ on $T_{1,0}$.

Notice that the volume form of h_θ is $\frac{1}{n!}(d\theta)^n \wedge \theta$.

As proved by Tanaka [**Ta**] and Webster [**We**], the datum of the pseudo-Hermitian contact form θ uniquely defines a connection, the *Tanaka-Webster connection*, which preserves the pseudo-Hermitian structure of M, i.e., such that $\nabla\theta = 0$ and $\nabla J = 0$. It can be defined as follows.

Let $\{Z_j\}$ be a frame of $T_{1,0}$. We set $Z_{\bar{j}} = \overline{Z_j}$. Then $\{X_0, Z_j, Z_{\bar{j}}\}$ forms a frame of $T_{\mathbb{C}}M$. In the sequel such a frame will be called an *admissible frame* of $T_{\mathbb{C}}M$. Let $\{\theta, \theta^j, \theta^{\bar{j}}\}$ be the coframe of $T^*_{\mathbb{C}}M$ dual to $\{X_0, Z_j, Z_{\bar{j}}\}$. With respect to this coframe we can write $d\theta = ih_{j\bar{k}}\theta^j \wedge \theta^{\bar{k}}$.

Using the matrix $(h_{j\bar{k}})$ and its inverse $(h^{j\bar{k}})$ to lower and raise indices, the connection 1-form $\omega = (\omega_j{}^k)$ and the torsion form $\tau_j = A_{jk}\theta^k$ of the Tanaka-Webster connection are uniquely determined by the relations

$$d\theta^k = \theta^j \wedge \omega_j{}^k + \theta \wedge \tau^k, \qquad \omega_{j\bar{k}} + \omega_{\bar{k}j} = dh_{j\bar{k}}, \qquad A_{jk} = A_{kj}. \tag{78}$$

In addition, we have the structure equations

$$d\omega_j{}^k - \omega_j{}^l \wedge \omega_l{}^k = R_j{}^k{}_{l\bar{m}}\theta^l \wedge \theta^{\bar{m}} + W_{j\bar{k}l}\theta^l \wedge \theta - W_{\bar{k}j\bar{l}}\theta^{\bar{l}} \wedge \theta + i\theta_j \wedge \tau_{\bar{k}} - i\tau_j \wedge \theta_{\bar{k}}. \tag{79}$$

The *pseudo-Hermitian curvature tensor* of the Tanaka-Webster connection is the tensor with components $R_{j\bar{k}l\bar{m}}$, its *Ricci tensor* is $\rho_{j\bar{k}} := R_l{}^l{}_{j\bar{k}}$ and its *scalar curvature* is $\kappa_\theta := \rho_j{}^j$.

8.2. Local pseudo-Hermitian invariants. Let us now define local pseudo-Hermitian invariants. The definition is more involved than that of local Riemannian invariants, because:

- The components of the Tanaka-Webster connection and its curvature and torsion tensors are defined with respect to the datum of a local frame $Z_1, \ldots, Z_n$ which never is a frame $\frac{\partial}{\partial z^1}, \ldots \frac{\partial}{\partial z^n}$ associated to local coordinates $z^1, \ldots, z^n$;

- In order to get local pseudo-Hermitian invariants from pseudo-Hermitian invariant Ψ_HDOs it is important to take into account the tangent group bundle of a CR manifold, in which the Heisenberg group comes into play.

Before defining local pseudo-Hermitian invariants, some notation needs to be introduced.

Let $U \subset \mathbb{R}^n$ be an open subset of local coordinates equipped with a frame $Z_1, \ldots, Z_n$ of $T_{1,0}$. Write $Z_j = X_j - iX_{n+j}$, where X_j and X_{n+j} are real vector fields. Then $X_0, \ldots, X_{2n}$ is a local H-frame of TM. We shall call this frame the *H-frame associated to* $Z_1, \ldots, Z_n$.

Let $\eta^0, \ldots, \eta^{2n}$ be the coframe of T^*M dual to $X_0, \ldots, X_{2n}$ (so that $\eta^0 = \theta$). We write $X_j = X_j{}^k\partial_{x^k}$ and $\eta^j = \eta^j{}_k dx^k$. We also write $Z_j = Z_j{}^k\partial_{x^k}$. It will be convenient to identify $X_0(x)$ with the vector $(X_0{}^k(x)) \in \mathbb{R}^{2n+1}$ and $Z(x) := (Z_1(x), \ldots, Z_n(x))$ with the matrix $(Z_j{}^k(x))$ in $M_{n,2n+1}(\mathbb{C})^\times$, where the latter denotes the open subset of $M_{n,2n+1}(\mathbb{C})$ consisting of regular matrices.

For $j, \bar{k} = 1, \ldots, n$ we set $h_{j\bar{k}} = h_\theta(Z_j, Z_k) = i\theta([Z_j, Z_{\bar{k}}])$, and for $j, k = 1, \ldots, 2n$ we set $L_{jk} = \theta([X_j, X_k])$. Let $M_n(\mathbb{C})_+$ denote the open cone of positive definite Hermitian $n \times n$ matrices. In the sequel it will also be convenient to identify h_θ with the matrix $h_\theta(x) := (h_{j\bar{k}}(x)) \in M_n(\mathbb{C})_+$.

Thanks to the integrability of $T_{1,0}$ we have $\theta([Z_j, Z_k]) = 0$. As we have $[Z_j, Z_k] = [X_j, X_k] - [X_{n+j}, X_{n+k}] - i([X_{n+j}, X_k] + [X_j, X_{n+k}])$ we see that

$$L_{n+j,n+k} = L_{j,k} \qquad \text{and} \qquad L_{j,n+k} = -L_{n+j,k}. \tag{80}$$

Since $[Z_j, Z_{\bar{k}}] = [X_j, X_k] + [X_{n+j}, X_{n+k}] + i([X_{n+j}, X_k] - [X_j, X_{n+k}])$ we get

(81) $$h_{j\bar{k}} = i\theta([Z_j, Z_{\bar{k}}]) = 2iL_{j,k} + 2L_{n+j,k}.$$

In other words, we have

(82) $$(L_{jk}) = \frac{1}{2}\begin{pmatrix} \Im h & -\Re h \\ \Re h & \Im h \end{pmatrix}.$$

For any $a \in U$ we let ψ_a be the affine change of variables to the privileged coordinates centered at a (cf. Definition 14). One checks that $\psi_a(x)^j = \eta^j{}_k(x^k - a^k)$, so we have

(83) $$\psi_{a*}X_j = X_j{}^k(\psi_a(x))\eta^l{}_k(a)\partial_l.$$

Given a vector field X defined near $x = 0$ let us denote by $X(0)_l$ the vector field obtained as the part in the Taylor expansion at $x = 0$ of X which is homogeneous of degree l with respect to the Heisenberg dilations (63). Then the Taylor expansions at $x = 0$ of the vector fields $\psi_{a*}X_0, \ldots, \psi_{a*}X_{2n}$ take the form

(84) $$X_0 = X_0^{(a)} + X_0(0)_{(-1)} + \cdots,$$

(85) $$X_j = X_j^{(a)} + X_j(0)_{(0)} + \cdots, \quad 1 \leq j \leq 2n,$$

with

(86) $$X_0^{(a)} = \partial_{x^0}, \qquad X_j^{(a)} = \partial_{x^j} + b_{jk}(a)x^k\partial_{x^0}, \quad 1 \leq j \leq 2n,$$

where we have set $b_{jk}(a) := \partial_k[X_j{}^l(\psi_a(x))]_{|x=0}\eta^0{}_l(a)$. Notice that $X_0^{(a)}$ is homogeneous of degree -2, while $X_1^{(a)}, \ldots, X_{2n}^{(a)}$ are homogeneous of degree -1.

The linear span of the vector fields $X_0^{(a)}, \ldots, X_{2n}^{(a)}$ is a 2-step nilpotent Lie algebra under the Lie bracket of vector fields. Therefore, this is the Lie algebra of left-invariant vector fields on a 2-step nilpotent Lie group $G^{(a)}$. The latter can be realized as $\mathbb{R}^{2n+1}$ equipped with the product

(87) $$x.y = (x^0 + y^0 + b_{kj}(a)x^j y^k, x^1 + y^1, \ldots, x^{2n} + y^{2n}).$$

Notice that $[X_j^{(a)}, X_k^{(a)}] = (b_{kj}(a) - b_{jk}(a))X_0^{(a)}$. In addition, we can check that $[\psi_{a*}X_j, \psi_{a*}X_k](0) = (b_{kj}(a) - b_{jk}(a))\partial_{x^0} \bmod H_0$. Thus,

(88) $$\begin{aligned} L_{jk}(a) = \theta(X_j, X_k)(a) &= (\psi_{a*}\theta)([\psi_{a*}X_j, \psi_{a*}X_k])(0) \\ &= \langle dx^0, [\psi_{a*}X_j, \psi_{a*}X_k](0)\rangle = b_{kj}(a) - b_{jk}(a). \end{aligned}$$

This shows that $G^{(a)}$ has the same structure constants as the tangent group G_aM, hence is isomorphic to it (see [**Po1**]). This also implies that $(-\frac{1}{2}L_{jk}(a))$ is the skew-symmetric part of $(b_{jk}(a))$. For $j, k = 1, \ldots, 2n$ set $\mu_{jk}(a) = b_{jk}(a) + \frac{1}{2}L_{jk}(a)$. The matrix $(\mu_{jk}(a))$ is the symmetric part of $(b_{jk}(a))$, so it belongs to the space $S_{2n}(\mathbb{R})$ of symmetric $2n \times 2n$ matrices with real coefficients.

In the sequel we set

(89) $$\Omega = M_n(\mathbb{C})_+ \times \mathbb{R}^{2n+1} \times M_{n,2n+1}(\mathbb{C})^\times \times S_{2n}(\mathbb{R}).$$

This is a manifold, and for any $x \in U$ the quadruple $(h(x), X_0(x), Z(x), \mu(x))$ is an element of Ω depending smoothly on x.

In addition, we let $\mathcal{P}$ be the set of monomials in the indeterminate variables $\partial^\alpha X_0{}^k$, $\partial^\alpha Z_j{}^k$ and $\partial^\alpha \overline{Z_j{}^k}$, where the integer j ranges over $\{1, \ldots, n\}$, the integer k ranges over $\{0, \ldots, 2n\}$, and α ranges over all multi-orders in $\mathbb{N}_0^{2n}$. Given the

Reeb field X_0 and a local frame $Z_0,\ldots,Z_n$ of $T_{1,0}$ by plugging $\partial_x^\alpha {X_0}^k(x)$, $\partial_x^\alpha {Z_j}^k(x)$ and $\partial^\alpha \overline{{Z_j}^k}(x)$ into a monomial $\mathfrak{p}\in\mathcal{P}$ we get a function which we shall denote by $\mathfrak{p}(X_0,Z,\overline{Z})(x)$.

Bearing all this mind we define local pseudo-Hermitian invariants as follows.

DEFINITION 16. *A local pseudo-Hermitian invariant of weight w is the datum on each pseudo-Hermitian manifold (M^{2n+1},θ) of a function $\mathcal{I}_\theta\in C^\infty(M)$ such that:*

(i) There exists a finite family $(a_{\mathfrak{p}})_{\mathfrak{p}\in\mathcal{P}}\subset C^\infty(\Omega)$ such that, in any local coordinates equipped with a frame $Z_1,\ldots,Z_n$ of $T_{1,0}$, we have

$$\mathcal{I}_\theta(x)=\sum_{\mathfrak{p}\in\mathcal{P}} a_{\mathfrak{p}}(h(x),X_0(x),Z(x),\mu(x))\mathfrak{p}(X_0,Z,\overline{Z})(x). \tag{90}$$

(ii) We have $\mathcal{I}_{t\theta}(x)=t^{-w}\mathcal{I}_\theta(x)$ for any $t>0$.

Any local Riemannian invariant of h_θ is a local pseudo-Hermitian invariant. However, the above notion of weight for pseudo-Hermitian invariant is anisotropic with respect to h_θ. For instance if we replace θ by $t\theta$ then h_θ is rescaled by t on $T_{1,0}\oplus T_{0,1}$ and by t^2 on the vertical line bundle $\mathcal{N}\otimes\mathbb{C}$.

On the other hand, as shown in [**JL2**, Prop. 2.3], by means of parallel translation along parabolic geodesics any orthonormal frame $Z_1(a),\ldots,Z_n(a)$ of $T_{1,0}$ at a point $a\in M$ can be extended to a local frame $Z_1,\ldots,Z_n$ of $T_{1,0}$ near a. Such a frame is called a *special orthonormal frame*.

Furthermore, as also shown in [**JL2**, Prop. 2.3] any special orthonormal frame $Z_1,\ldots,Z_n$ near a allows us to construct *pseudo-Hermitian normal coordinates* $x_0, z^1=x^1+ix^{n+1},\ldots,z^n=x^n+ix_{2n}$ centered at a in such way that in the notation of (84)–(85) we have

$$X_0(0)_{(-2)}=\partial_{x^0},\qquad Z_j(0)_{(-1)}=\partial_{z^j}+\frac{i}{2}\bar{z}^j\partial_{x^0},\qquad \omega_{j\bar{k}}(0)=0. \tag{91}$$

Write $Z_j=X_j-iX_{n+j}$, where X_j and X_{n+j} are real vector fields. Then we have $X_j(0)_{(-1)}=\partial_{x^j}-\frac{1}{2}x^{n+j}\partial_{x^0}$ and $X_{n+j}(0)_{(-1)}=\partial_{x^{n+j}}+\frac{1}{2}x^j\partial_{x^0}$. In particular, we have $X_j(0)=\partial_{x^j}$ for $j=0,\ldots,2n$. This implies that the affine change of variables ψ_0 to the privileged coordinates at 0 is just the identity. Moreover, in the notation of (86) for $j=1,\ldots,n$ we have

$$X_j^{(0)}=\partial_{x^j}-\frac{1}{2}x^{n+j}\partial_{x^0},\qquad X_{n+j}^{(0)}=\partial_{x^{n+j}}+\frac{1}{2}x^j\partial_{x^0}. \tag{92}$$

Incidentally, this shows that the matrix $(b_{jk}(0))$ is skew-symmetric, so its symmetric part vanishes, i.e., $\mu(0)=0$.

PROPOSITION 7 ([**Po4**]). *Assume each pseudo-Hermitian manifold (M^{2n+1},θ) gifted with a function $\mathcal{I}_\theta\in C^\infty(M)$ in such a way that $\mathcal{I}_{t\theta}(x)=t^{-w}\mathcal{I}_\theta(x)$ for any $t>0$. Then the following are equivalent:*

(i) $\mathcal{I}_\theta(x)$ is a local pseudo-Hermitian invariant;

(ii) There exists a finite family $(a_{\mathfrak{p}})_{\mathfrak{p}\in\mathcal{P}}\subset\mathbb{C}$ such that, for any pseudo-Hermitian manifold (M^{2n+1},θ) and any point $a\in M$, in any pseudo-Hermitian normal coordinates centered at a associated to any given special orthonormal frame $Z_1,\ldots,Z_n$

of $T_{1,0}$ near a, we have

(93)
$$\mathcal{I}_\theta(a) = \sum_{\mathfrak{p}\in\mathcal{P}} a_{\mathfrak{p}}\mathfrak{p}(X_0, Z, \overline{Z})(x)_{|x=0}.$$

(iii) $\mathcal{I}_\theta(x)$ is a universal linear combination of complete tensorial contractions of covariant derivatives of the pseudo-Hermitian curvature tensor and of the torsion tensor of the Tanaka-Webster connection.

8.3. pseudo-Hermitian invariant Ψ_HDOs. We define homogeneous symbols on $\Omega \times \mathbb{R}^{2n+1}$ as follows.

DEFINITION 17. *$S_m(\Omega \times \mathbb{R}^{2n+1})$, $m \in \mathbb{C}$, consists of functions $a(h, X_0, Z, \xi)$ in $C^\infty(\Omega \times (\mathbb{R}^{2n+1} \setminus \{0\}))$ such that $a(\theta, Z, t\xi) = t^m a(\theta, Z, \xi)$ $\forall t > 0$.*

In addition, recall that if $Z_1, \ldots, Z_n$ is a local frame of $T_{1,0}$ then its associated H-frame is the frame $X_0, \ldots, X_{2n}$ of TM such that $Z_j = X_j - iX_{n+j}$ for $j = 1, \ldots, n$.

DEFINITION 18. *A pseudo-Hermitian invariant Ψ_HDO of order m and weight w is the datum on each pseudo-Hermitian manifold (M^{2n+1}, θ) of an operator P_θ in $\Psi_H^m(M)$ such that:*

(i) For $j = 0, 1, \ldots$ there exists a finite family $(a_{j\mathfrak{p}})_{\mathfrak{p}\in\mathcal{P}} \subset S_{m-j}(\Omega \times \mathbb{R}^{2n+1})$ such that, in any local coordinates equipped with the H-frame associated to a frame $Z_1, \ldots, Z_n$ of $T_{1,0}$, the operator P_θ has symbol $p_\theta \sim \sum p_{\theta,m-j}$ with

(94)
$$p_{\theta,m-j}(x, \xi) = \sum_{\mathfrak{p}\in\mathcal{P}} \mathfrak{p}(X_0, Z, \overline{Z})(x) a_{j\mathfrak{p}}(h(x), X_0(x), Z(x), \mu(x), \xi).$$

(ii) For all $t > 0$ we have $P_{t\theta} = t^{-w} P_\theta$ modulo $\Psi^{-\infty}(M)$.

In addition, we will say that P_θ is admissible *if in (94) we can take $a_{0\mathfrak{p}}(h, X_0, Z, \mu, \xi)$ to be zero for $\mathfrak{p} \neq 1$.*

For instance, the horizontal sub-Laplacian Δ_b is an admissible pseudo-Hermitian invariant differential operator of weight 1.

We gather the main properties of pseudo-Hermitian invariant Ψ_HDOs in the following.

PROPOSITION 8 ([**Po4**]). *Let P_θ be a pseudo-Hermitian invariant Ψ_HDO of order m and weight w.*

1. *Let Q_θ be a pseudo-Hermitian invariant Ψ_HDO of order m' and weight w', and assume that P_θ or Q_θ is uniformly properly supported. Then $P_\theta Q_\theta$ is a pseudo-Hermitian invariant Ψ_HDO of order $m + m'$ and weight $w + w'$.*
2. *Assume that P_θ is admissible and its principal symbol is invertible in the Heisenberg calculus sense. Then the datum on every pseudo-Hermitian manifold (M^{2n+1}, θ) of a parametrix $Q_\theta \in \Psi^{-m}(M)$ gives rise to a pseudo-Hermitian invariant Ψ_HDO of order $-m$ and weight $-w$.*

Finally, concerning the logarithmic singularities of pseudo-Hermitian invariant Ψ_HDOs the following holds.

PROPOSITION 9 ([**Po4**]). *Let P_θ be a pseudo-Hermitian invariant Ψ_HDO of order m and weight w. Then the logarithmic singularity $c_{P_\theta}(x)$ takes the form*

(95)
$$c_{P_\theta}(x) = \mathcal{I}_{P_\theta}(x)|(d\theta)^n \wedge \theta|,$$

where $\mathcal{I}_\theta(x)$ is a local pseudo-Hermitian invariant of weight $n + 1 + w$.

9. CR Invariants and Fefferman's Program

9.1. Local CR Invariants. The local CR invariants can be defined as follows.

Definition 19. *A local scalar CR invariant of weight w is a local scalar pseudo-Hermitian invariant $\mathcal{I}_\theta(x)$ such that*

$$\mathcal{I}_{e^f\theta}(x) = e^{-wf(x)}\mathcal{I}_\theta(x) \qquad \forall f \in C^\infty(M,\mathbb{R}). \tag{96}$$

When M is a real hypersurface the above definition of a local CR invariant agrees with the definition in [**Fe2**] in terms of Chern-Moser invariants (with our convention about weight a local CR invariant that has weight w in the sense of (96) has weight $2w$ in [**Fe2**]).

The analogue of the Weyl curvature in CR geometry is the Chern-Moser tensor ([**CM**], [**We**]). Its components with respect to any local frame $Z_1, \ldots, Z_n$ of $T_{1,0}$ are

$$S_{j\bar{k}l\bar{m}} = R_{j\bar{k}l\bar{m}} - (P_{j\bar{k}}h_{l\bar{m}} + P_{l\bar{k}}h_{j\bar{m}} + P_{l\bar{m}}h_{j\bar{k}} + P_{j\bar{m}}h_{l\bar{k}}), \tag{97}$$

where $P_{j\bar{k}} = \frac{1}{n+2}(\rho_{j\bar{k}} - \frac{\kappa}{2(n+1)}h_{j\bar{k}})$ is the CR Schouten tensor. The Chern-Moser tensor is a CR invariant tensor of weight 1, so we get scalar local CR invariants by taking complete tensorial contractions. For instance, as a scalar invariant of weight 2 we have

$$|S|^2_\theta = S^{\bar{j}k\bar{l}m}S_{j\bar{k}l\bar{m}}, \tag{98}$$

and as scalar invariants of weight 3 we get

$$S_{i\bar{j}}{}^{\bar{k}l}S_{k\bar{l}}{}^{\bar{p}q}S_{p\bar{q}}{}^{\bar{i}j} \quad \text{and} \quad S_i{}^{j\bar{k}}{}_{\bar{l}}S^{\bar{i}}{}_{\bar{j}p}{}^{q}S^{\bar{p}}{}_{\bar{q}k}{}^{l}. \tag{99}$$

More generally, the Weyl CR invariants are obtained as follows. Let $\mathcal{K}$ be the canonical line bundle of M, i.e., the annihilator of $T_{1,0} \wedge \Lambda^n T^*_{\mathbb{C}}M$ in $\Lambda^{n+1}T^*_{\mathbb{C}}M$. The Fefferman bundle is the total space of the circle bundle,

$$\mathcal{F} := (\mathcal{K} \setminus \{0\})/\mathbb{R}^*_+. \tag{100}$$

It carries a natural S^1-invariant Lorentzian metric g_θ whose conformal class depends only the CR structure of M, for we have $g_{e^f\theta} = e^f g_\theta$ for any $f \in C^\infty(M,\mathbb{R})$ (see [**Fe1**], [**Le**]). Notice also that the Levi metric defines a Hermitian metric h^*_θ on $\mathcal{K}$, so we have a natural isomorphism of circle bundles $\iota_\theta : \mathcal{F} \to \Sigma_\theta$, where $\Sigma_\theta \subset \mathcal{K}$ denotes the unit sphere bundle of $\mathcal{K}$.

Lemma 1 ([**Fe2**]; see also [**Po4**]). *Any local scalar conformal invariant $\mathcal{I}_g(x)$ of weight w uniquely defines a local scalar CR invariant of weight w.*

9.2. CR invariant operators.

Definition 20. *A CR invariant $\Psi_H DO$ of order m and biweight (w, w') is a pseudo-Hermitian invariant $\Psi_H DO$ P_θ such that*

$$P_{e^f\theta} = e^{w'f}P_\theta e^{-wf} \qquad \forall f \in C^\infty(M,\mathbb{R}). \tag{101}$$

We summarize the algebraic properties of CR invariant Ψ_HDOs in the following.

Proposition 10 ([**Po4**]). *Let P_θ be a CR invariant $\Psi_H DO$ of order m and biweight (w, w').*

(1) *Let Q_θ be a CR invariant $\Psi_H DO$ of order m' and biweight (w'', w), and assume that P_θ or Q_θ is uniformly properly supported. Then $P_\theta Q_\theta$ is a CR invariant $\Psi_H DO$ of order $m+m'$ and biweight (w'', w').*

(2) *Assume that P_θ is admissible and its principal symbol is invertible in the Heisenberg calculus sense. Then the datum on every pseudo-Hermitian manifold (M^{2n+1}, θ) of a parametrix $Q_\theta \in \Psi^{-m}(M)$ gives rise to a CR invariant $\Psi_H DO$ of order $-m$ and biweight (w', w).*

Next, we have plenty of CR invariant operators thanks to the following result.

Proposition 11 ([**JL1**], [**GG**]; see also [**Po4**]). *Any conformally invariant Riemannian differential operator L_g of weight w uniquely defines a CR invariant differential operator L_θ of the same weight.*

When L_g is the Yamabe operator the corresponding CR invariant operator is the CR Yamabe operator introduced by Jerison-Lee [**JL1**] in their solution of the Yamabe problem on CR manifolds. Namely,

$$\boxdot_\theta = \Delta_b + \frac{n}{n+2}\kappa_\theta, \tag{102}$$

where κ_θ is the Tanaka-Webster scalar curvature. This is a CR invariant differential operator of biweight $(\frac{-n}{2}, -\frac{n+2}{2})$.

More generally, Gover-Graham [**GG**] proved that for $k = 1, \ldots, n+1$ the GJMS operator $\Box_g^{(k)}$ on the Fefferman bundle gives rise to a selfadjoint differential operator,

$$\boxdot_\theta^{(k)} : C^\infty(M) \longrightarrow C^\infty(M). \tag{103}$$

This is a CR invariant operator of biweight $(\frac{k-(n+1)}{2}, -\frac{k+n+1}{2})$ and it has the same principal symbol as

$$(\Delta_b + i(k-1)X_0)(\Delta_b + i(k-3)X_0)\cdots(\Delta_b - i(k-1)X_0). \tag{104}$$

In particular, except for the critical value $k = n+1$, the principal symbol of $\boxdot_\theta^{(k)}$ is invertible in the Heisenberg calculus sense (see [**Po3**, Prop. 3.5.7]). The operator $\boxdot_\theta^{(k)}$ is called the CR GJMS operator of order k. For $k = 1$ we recover the CR Yamabe operator. Notice that by making use of the CR tractor calculus we also can define CR GJMS operators of order $k \geq n+2$ (see [**GG**]). These operators can also be obtained by means of geometric scattering theory (see [**HPT**]).

9.3. Fefferman's program. In the same way as in conformal geometry, in the setting of CR geometry the program of Fefferman has two main aspects:

Fefferman's Program (Analytic Aspect). *Give a precise geometric description of the singularities of the Schwartz, Green and null kernels of CR invariant operators in terms of local conformal invariants.*

Fefferman's Program (Geometric Aspect). *Determine all local invariants of a strictly pseudoconvex CR structure.*

Concerning the latter aspect, the analogues of the Weyl conformal invariants are the *Weyl CR invariants* which are the local CR invariants arising from the Weyl conformal invariants of the Fefferman as described by Lemma 1. Notice that, for the Fefferman bundle, the ambient metric was constructed by Fefferman [**Fe2**] as a Kähler-Lorentz metric. Therefore, the Weyl CR invariants are the local CR invariants that arise from complete tensorial contractions of covariant derivatives of the curvature tensor of Fefferman's ambient Kähler-Lorentz metric.

Bearing this in mind the CR analogue of Proposition 2 is given by the following.

PROPOSITION 12 ([**Fe2**, Thm. 2], [**BEG**, Thm. 10.1]). *Every local CR invariant of weight $\leq n+1$ is a linear combination of local Weyl CR invariants.*

In particular, we recover the fact that there is no local CR invariant of weight 1. Furthermore, we see that every local CR invariant of weight 2 is a constant multiple of $|S|_\theta$. Similarly, the local CR invariants of weight 3 are linear combinations of the invariants (99) and of the invariant Φ_θ that arises from the Fefferman-Graham invariant Φ_{g_θ} of the Fefferman Lorentzian space $\mathcal{F}$.

10. Logarithmic singularities of CR invariant Ψ_HDOs

Let us now look at the logarithmic singularities of CR invariant Ψ_HDOs. To this end let us denote by $[\theta]$ the conformal class of θ.

PROPOSITION 13. *Consider a family $(P_{\hat{\theta}})_{\hat{\theta}\in[\theta]} \subset \Psi^m(M)$ such that*

$$P_{e^f\theta} = e^{w'f} P_\theta e^{-wf} \qquad \forall f \in C^\infty(M,\mathbb{R}). \tag{105}$$

Then

$$c_{P_{e^f\theta}}(x) = e^{(w'-w)f(x)} c_{P_\theta}(x) \qquad \forall f \in C^\infty(M,\mathbb{R}). \tag{106}$$

This result generalizes a previous result of N.K. Stanton [**St**]. Combining it with Proposition 9, and using Proposition 12 , we obtain the following.

THEOREM 6 ([**Po4**]). *Let P_θ be a CR invariant $\Psi_H DO$ of order m and biweight (w,w'). Then the logarithmic singularity $c_{P_\theta}(x)$ takes the form*

$$c_{P_\theta}(x) = \mathcal{I}_{P_\theta}(x)|(d\theta)^n \wedge \theta|, \tag{107}$$

where $\mathcal{I}_\theta(x)$ is a scalar local CR invariant of weight $n+1+w-w'$. If we further have $w \leq w'$, then $\mathcal{I}_\theta(x)$ is a linear combination of Weyl CR invariants of weight $n+1+w-w'$.

We can make use of this result to study the logarithmic singularities of the Green kernels of the CR GJMS operators.

THEOREM 7. *For $k=1,\ldots,n$ we have*

$$\gamma_{\square_\theta^{(k)}}(x) = c_\theta^k(x)|d\theta^n \wedge \theta|, \tag{108}$$

where $c_\theta^k(x)$ is a linear combination of scalar Weyl CR invariants of weight $n+1-k$. In particular,

$$c_\theta^{(n)}(x) = 0, \qquad c_\theta^{(n-1)}(x) = \alpha_n |S|_\theta^2, \tag{109}$$

$$c_\theta^{(n-2)}(x) = \beta_n S_{i\bar{j}}{}^{\bar{k}l} S_{k\bar{l}}{}^{\bar{p}q} S_{p\bar{q}}{}^{\bar{i}j} + \gamma_n S_i{}^{j\bar{k}}{}_{\bar{l}} S^{\bar{i}}{}_{\bar{j}p}{}^{q} S^{\bar{p}}{}_{\bar{q}k}{}^{l} + \delta_n \Phi_\theta, \tag{110}$$

where S is the Chern-Moser curvature tensor, Φ_θ is the CR Fefferman-Graham invariant, and the constants α_n, β_n, γ_n and δ_n depend only on n.

References

[Al1] Alexakis, S.: *On conformally invariant differential operators in odd dimension.* Proc. Nat. Acad. Sci. USA **100** (2003), no. 2, 4409–4410.

[Al2] Alexakis, S.: *On conformally invariant differential operators.* E-print, arXiv, Aug. 06, 50 pages.

[BEG] Bailey, T.N.; Eastwood, M.G.; Graham, C.R.: *Invariant theory for conformal and CR geometry.* Ann. Math. **139** (1994) 491–552.

[BG] Bailey, T.N.; Gover, A.R.: *Exceptional invariants in the parabolic invariant theory of conformal geometry* Proc. A.M.S. **123** (1995), 2535–2543.

[BGr] Beals, R.; Greiner, P.C.: *Calculus on Heisenberg manifolds.* Annals of Mathematics Studies, vol. 119. Princeton University Press, Princeton, NJ, 1988.

[CM] Chern, S. S.; Moser, J. K. *Real hypersurfaces in complex manifolds.* Acta Math. **133** (1974), 219–271.

[CMo] Connes, A.; Moscovici, H.: *The local index formula in noncommutative geometry.* Geom. Funct. Anal. **5** (1995), no. 2, 174–243.

[EM] Epstein, C.L.; Melrose, R.B.: *The Heisenberg algebra, index theory and homology.* Preprint, 2000. Available online at `http://www-math.mit.edu/~rbm/book.html`.

[Fe1] Fefferman, C.: *Monge-Ampère equations, the Bergman kernel, and geometry of pseudoconvex domains.* Ann. of Math. (2) **103** (1976), no. 2, 395–416.

[Fe2] Fefferman, C.: *Parabolic invariant theory in complex analysis.* Adv. in Math. **31** (1979), no. 2, 131–262.

[FG1] Fefferman, C.; Graham, C.R.: *Conformal invariants.* Élie Cartan et les Mathématiques d'Aujourd'hui, Astérisque, hors série, (1985), 95–116.

[FG2] Fefferman, C.; Graham, C.R.: *The ambient metric.* E-print, arXiv, Oct. 07.

[FS1] Folland, G.; Stein, E.: *Estimates for the $\bar\partial_b$ complex and analysis on the Heisenberg group.* Comm. Pure Appl. Math. **27** (1974) 429–522.

[Gi] Gilkey, P.B.: *Invariance theory, the heat equation, and the Atiyah-Singer index theorem.* 2nd edition. Studies in Advanced Mathematics. CRC Press, Boca Raton, FL, 1995.

[GG] Gover, A.R.; Graham, C.R.: *CR invariant powers of the sub-Laplacian.* J. Reine Angew. Math. **583** (2005), 1–27.

[GVF] Gracia-Bondía, J.M.; Várilly, J.C.; Figueroa, H.: *Elements of noncommutative geometry.* Birkhäuser Boston, Boston, MA, 2001.

[GJMS] Graham, C.R.; Jenne, R.; Mason, L.J.; Sparling, G.A.: *Conformally invariant powers of the Laplacian. I. Existence.* J. London Math. Soc. (2) **46** (1992), no. 3, 557–565.

[GH] Graham, C.R.; Hirachi, M.: *Inhomogeneous ambient metrics. Symmetries and overdetermined systems of partial differential equations*, 403–420, IMA Vol. Math. Appl., 144, Springer, New York, 2008.

[Gr] Greiner, P.: *An asymptotic expansion for the heat equation.* Arch. Rational Mech. Anal. **41** (1971) 163–218.

[Gu1] Guillemin, V.W.: *A new proof of Weyl's formula on the asymptotic distribution of eigenvalues.* Adv. in Math. **55** (1985), no. 2, 131–160.

[Gu2] Guillemin, V.W.: *Gauged Lagrangian distributions.* Adv. Math. **102** (1993), no. 2, 184–201.

[Hi1] Hirachi, K.: *Construction of boundary invariants and the logarithmic singularity of the Bergman kernel.* Ann. of Math. **151** (2000) 151–191.

[Hi2] Hirachi, K.: *Ambient metric construction of CR invariant differential operators. Symmetries and overdetermined systems of partial differential equations*, 61–75, IMA Vol. Math. Appl., 144, Springer, New York, 2008.

[HPT] Hislop, P.D.; Perry, P.A.; Tang, S.-H.: *CR-invariants and the scattering operator for complex manifolds with boundary.* Anal. PDE **1** (2008), no. 2, 197–227.

[Hö2] Hörmander, L.: *Hypoelliptic second order differential equations.* Acta Math. **119** (1967), 147–171.

[Hö] Hörmander, L.: *The analysis of linear partial differential operators. III. Pseudodifferential operators.* Grundlehren der Mathematischen Wissenschaften, 274. Springer-Verlag, Berlin, 1994.

[JL1] Jerison, D.; Lee, J.M.: *The Yamabe problem on CR manifolds.* J. Differential Geom. **25** (1987), no. 2, 167–197.

[JL2] Jerison, D.; Lee, J.M.: *Intrinsic CR normal coordinates and the CR Yamabe problem.* J. Differential Geom. **29** (1989), no. 2, 303–343.

[Ju] Juhl, A.: *Families of conformally covariant differential operators, Q-curvature and holography.* Progress in Mathematics, Birkhäuser, Vol. 275, 2009, 500 pages.

[KV] Kontsevich, M.; Vishik, S.: *Geometry of determinants of elliptic operators. Functional analysis on the eve of the 21st century*, Vol. 1 (New Brunswick, NJ, 1993), 173–197, Progr. Math., 131, Birkhäuser Boston, Boston, MA, 1995.

[Le] Lee, J.M.: *The Fefferman metric and pseudo-Hermitian invariants.* Trans. Amer. Math. Soc. **296** (1986), no. 1, 411–429.

[Me] Melrose, R.: *The Atiyah-Patodi-Singer index theorem.* A.K. Peters, Boston, 1993.

[PR] Parker, T; Rosenberg, S.: *Invariants of conformal Laplacians.* J. Differential Geom. **25** (1987), no. 2, 199–222.

[PRo] Paycha, S.; Rosenberg, S.: *Conformal anomalies via canonical traces. Analysis, geometry and topology of elliptic operators*, World Scientific, 2006.

[Po1] Ponge, R.: *The tangent groupoid of a Heisenberg manifold.* Pacific Math. J. **227** (2006) 151–175.

[Po2] Ponge, R.: *Noncommutative residue for Heisenberg manifolds and applications in CR and contact geometry.* J. Funct. Anal. **252** (2007), 399–463.

[Po3] Ponge, R.: *Heisenberg calculus and spectral theory of hypoelliptic operators on Heisenberg manifolds.* Mem. Amer. Math. Soc. **194** (2008), no. 906, viii+ 134 pp.

[Po4] Ponge, R.: *Logarithmic singularities of Schwartz kernels and local invariants of conformal and CR structures.* E-print, arXiv, Oct. 07, 44 pp. To appear in Proc. London Math. Soc..

[Po5] Ponge, R.: *Noncommutative residue and Dixmier trace.* E-print, arXiv, Oct. 09. To appear in the proceedings of the Noncommutative Geometry Workshop (Fields Institute, Toronto, Canada, May 27-31, 2008).

[Ro] Rockland, C.: *Intrinsic nilpotent approximation.* Acta Appl. Math. **8** (1987), no. 3, 213–270.

[St] Stanton, N.K.: *Spectral invariants of CR manifolds.* Michigan Math. J. **36** (1989), no. 2, 267–288.

[Ta] Tanaka, N.: *A differential geometric study on strongly pseudo-convex manifolds.* Lectures in Mathematics, Department of Mathematics, Kyoto University, No. 9. Kinokuniya Book-Store Co., Ltd., Tokyo, 1975.

[Tay] Taylor, M.E.: *Noncommutative microlocal analysis. I.* Mem. Amer. Math. Soc. 52 (1984), no. 313,

[We] Webster, S.: *Pseudo-Hermitian structures on a real hypersurface.* J. Differential Geom. **13** (1978), no. 1, 25–41.

[Wo1] Wodzicki, M.: *Local invariants of spectral asymmetry.* Invent. Math. **75** (1984), no. 1, 143–177.

[Wo2] Wodzicki, M.: *Spectral asymmetry and noncommutative residue* (in Russian), Habilitation Thesis, Steklov Institute, (former) Soviet Academy of Sciences, Moscow, 1984.

[Wo3] Wodzicki, M.: *Noncommutative residue. I. Fundamentals. K-theory, arithmetic and geometry* (Moscow, 1984–1986), 320–399, Lecture Notes in Math., 1289, Springer, Berlin-New York, 1987.

Department of Mathematics, University of Toronto, Canada.

(Current address) Graduate School of Mathematical Sciences, University of Tokyo, Japan

E-mail address: `ponge@ms.u-tokyo.ac.jp`