ON THE SECOND COEFFICIENT OF THE ASYMPTOTIC EXPANSION OF BOUTET DE MONVEL–SJÖSTRAND

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ABSTRACT. In this paper, we calculate the second coefficient of the asymptotic expansion of Boutet de Monvel–Sjöstrand.

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1. INTRODUCTION AND THE MAIN RESULT

Let \((X, T^{1,0}X)\) be a CR manifold and let \(\overline{\partial}_b\) be the tangential Cauchy–Riemann operator on \(X\). The orthogonal projection \(\Pi : L^2(X) \to \text{Ker} \overline{\partial}_b\) is called the Szegő projection, and we call its distribution kernel \(\Pi(x, y)\) the Szegő kernel. The study of the Szegő kernel is a classical subject in several complex variables and CR geometry. We recall the following classical result of Boutet de Monvel and Sjöstrand [2] about the description of the Szegő kernel:

**Theorem 1.1 (Boutet de Monvel–Sjöstrand).** Let \(X\) be a compact orientable strongly pseudovoncex CR manifold of real dimension \(2n + 1, n \geq 1\). Suppose that \(\overline{\partial}_b : \text{Dom} \overline{\partial}_b \subset L^2(X) \to L^2_{(0,1)}(X)\) has closed range. Let \(D \subset X\) be an open coordinate patch with local coordinates \(x = (x_1, \ldots, x_{2n+1})\). Then,

\[
\Pi(x, y) \equiv \int_0^{\infty} e^{it\phi(x,y)} a(x, y, t)dt \mod \mathcal{C}_\infty(D \times D),
\]

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where
\[
\phi(x, y) \in \mathcal{C}^\infty(D \times D), \quad \text{Im} \phi \geq 0,
\] (1.2)
\[
\phi(x, y) = 0 \text{ if and only if } x = y,
\]
\[
d_x \phi(x, y) = -d_y \phi(x, y) = -\omega_0(x), \text{ for every } x \in D,
\]
(1.3)
\[
a(x, y, t) \sim \sum_{j=0}^{+\infty} a_j(x, y) t^{n-j} \text{ in } S_{1,0}^n(D \times D \times \mathbb{R}_+),
\]
where \(\omega_0 \in \mathcal{C}^\infty(X, T^*X)\) is the global one form given by (1.6).

We refer the reader to Sections 2.1, 2.2 for the setup, notations and terminology used in Theorem 1.1. The Boutet de Monvel and Sjöstrand’s description of the Szegő kernel has profound impact in several complex variables, CR and complex geometry and geometric quantization theory, e.t.c. For example, Catlin [3] and Zelditch [20] established Bergman kernel asymptotic expansions for high power of positive holomorphic line bundles by using Theorem 1.1 (see also [11]). It should be mentioned that Tian [19] obtained the leading term of Bergman kernel asymptotics for high power of positive line bundles by using peak section method. The first few coefficients of Bergman kernel asymptotic expansion were calculated by Lu [14] (see also [5], [9] [10],[13],[15],[16]) and play an important role in Kähler geometry (see Donaldson [4]). On the other hand, the first coefficient at the diagonal of the expansion (1.3) is known, but the lower order terms of the expansion (1.3) were not yet known. Boutet de Monvel–Sjöstrand [2] (see also [8]) showed that

\[
a_0(x, x) = \frac{1}{2\pi^{n+1}} \det L_x, \quad \text{at every } x \in X,
\]
where \(\det L_x = \mu_1(x)\mu_2(x)\cdots\mu_n(x), \mu_j(x), j = 1, \ldots, n,\) are the eigenvalues of the Levi form with respect to the given Hermitian metric on \(CTX.\) If we take Levi metric on \(CTX\) (see (1.9)), then

\[
a_0(x, x) = \frac{1}{2\pi^{n+1}} \text{ on } D.
\]

It is a very natural question to calculate the lower order terms of the expansion (1.3). The goal of this paper is to calculate \(a_1(x, x)\) in (1.3). It should be mentioned that the explicit formula of \(a_1(x, x)\) has further applications in the study of CR Toeplitz quantization.

We now formulate our main result. For some standard notations and terminology, we refer the reader to Sections 2.1, 2.2. Let \((X, T^{1,0}X)\) be an orientable, compact strongly pseudoconvex CR manifold of dimension \(2n + 1, n \geq 1.\) Fix a global non-vanishing 1-form \(\omega_0(x) \in \mathcal{C}^\infty(X, T^*X)\) so that

\[
\omega_0(u) = 0, \text{ for every } u \in T^{1,0}X \oplus T^{0,1}X,
\]
(1.6)
\[
-\frac{1}{2i} d\omega_0|_{T^{1,0}X} \text{ is positive definite.}
\]

For every \(x \in X,\) the Levi form at \(x\) is the Hermitian quadratic form on \(T^{1,0}_xX\) given by

\[
L_x(u, \overline{v}) := \frac{1}{2} \langle d\omega_0(x), u \wedge \overline{v} \rangle, \quad \text{for all } u, v \in T^{1,0}_xX.
\]
(1.7)

Let \(T \in \mathcal{C}^\infty(X, TX)\) be the global real vector field given by

\[
\omega_0(T) = -1, \quad d\omega_0(T, \cdot) = 0.
\]
(1.8)
The Levi form $\mathcal{L}_x$ induces a Hermitian metric (called Levi metric) $\langle \cdot \mid \cdot \rangle$ on $\mathcal{C}X$ given by

\[
\langle u \mid v \rangle = \mathcal{L}_x(u, \partial), \quad \text{for every } u, v \in T^1_0X, \quad x \in X,
\]

\[
\langle \Pi \mid \overline{\Pi} \rangle = \langle u \mid \overline{v} \rangle, \quad \text{for every } u, v \in T^1_0X, \quad x \in X,
\]

\[
T^1_0X \perp T^{0,1}X, \quad T \perp (T^1_0X \oplus T^{0,1}X),
\]

\[
\langle T \mid T \rangle = 1.
\]

Let $\langle \cdot \mid \cdot \rangle$ be the $L^2$ inner product on $\Omega^{0,q}(X)$ induced by $\langle \cdot \mid \cdot \rangle$ and let $L^2\langle 0,q \rangle(X)$ be the completion of $\Omega^{0,q}(X)$ with respect to $\langle \cdot \mid \cdot \rangle$. We write $L^2(X) := L^2\langle 0,0 \rangle(X)$. Let

\[
\overline{\partial}_b : \mathcal{G}^\infty(X) \rightarrow \Omega^{0,1}(X)
\]

be the tangential Cauchy-Riemann operator (see (2.9)) and we extend $\overline{\partial}_b$ to $L^2$ space by

\[
\overline{\partial}_b : \text{Dom } \overline{\partial}_b \subset L^2(X) \rightarrow L^2\langle 0,1 \rangle(X),
\]

\[
\text{Dom } \overline{\partial}_b := \{ u \in L^2(X); \overline{\partial}_b u \in L^2\langle 0,1 \rangle(X) \}.
\]

Let

\[
\Pi : L^2(X) \rightarrow \ker \overline{\partial}_b
\]

be the orthogonal projection and let $\Pi(x, y) \in \mathcal{G}'(X \times X)$ be the distribution kernel of $\Pi$.

Let $D \subset X$ be any open open coordinate patch with local coordinates $x = (x_1, \ldots, x_{2n+1})$. For $b(x, y, t) \in S^1_0(D \times D \times \mathbb{R}^+)$, we write $b_0(x, y)$ and $b_1(x, y)$ to denote the first order term of $b$ and the second order term of $b$ respectively. Before we state our main result, it should be mentioned that the phase function $\phi$ in (1.1) is not unique and also the terms $a_0(x, y)$ and $a_1(x, y)$ are not unique. We can replace the phase function $\phi$ by $\hat{\phi} := f\phi$, where $f$ is a smooth function with $f(x, x) = 1$. Then, $\hat{\phi}$ satisfies (1.2) and $\phi$ and $\hat{\phi}$ are equivalent in the sense of Melin–Sjöstrand (see Melin–Sjöstrand [17, p. 172]). When we change $\phi$ to $\hat{\phi}$ in (1.1), the symbol $a(x, y, t)$ and $a_0(x, y)$ and $a_1(x, y)$ will also be changed. Hence, $a_0(x, y)$ and $a_1(x, y)$ depend on the phase function and are not unique. Even we fix $\phi$ in (1.1), the functions $a_0(x, y)$ and $a_1(x, x)$ are not unique. For example, we can take

\[
a_0(x, y) := a_0(x, y) + c(x, y)\phi(x, y), \quad c(x, y) \in \mathcal{G}^\infty(D \times D),
\]

\[
a_1(x, y) := a_1(x, y) - nic(x, y).
\]

Set

\[
\hat{a}(x, y, t) \sim t^n\hat{a}_0(x, y) + t^{n-1}\hat{a}_1(x, y) + \sum_{j=2}^{\infty} t^{n-j}\hat{a}_j(x, y) \text{ in } S^0_{1,0}(D \times D \times \mathbb{R}^+).
\]

It is not difficult to see that

\[
\int_0^\infty e^{it\phi(x, y)}\hat{a}(x, y, t)dt \equiv \int_0^\infty e^{it\phi(x, y)}a(x, y, t)dt \mod \mathcal{G}^\infty(D \times D).
\]

Hence, $a_0(x, y)$ and $a_1(x, x)$ are not unique.

To overcome the difficulty about the uniqueness for the symbols, we first look for some specific phase functions. Let $x = (x_1, \ldots, x_{2n+1})$ be local coordinates of $X$ defined on an open set $D$ of $X$ with $T = -\frac{\partial}{\partial x_{2n+1}}$ on $D$. By Malgrange preparation theorem [6, Theorem 7.5.5], we have

\[
\phi(x, y) = f(x, y)(-x_{2n+1} + g(x', y)) \text{ on } D,
\]
where $\phi$ is as in (1.1), $f, g \in C^\infty(D \times D)$, $f(x, x) = 1$, for every $x \in D$. Let
\[ \Phi := -x_{2n+1} + g(x', y). \]

It is not difficult to see that $\Phi$ satisfies (1.2), $\Phi$ and $\phi$ are equivalent in the sense of Melin–Sjöstrand. Moreover, we have
\[ (T^2 \Phi)(x, x) = 0, \text{ at every } x \in D. \tag{1.11} \]

Now we show that under supplementary conditions, we have uniqueness (see Lemma 3.2 for a proof)

**Lemma 1.1.** Let $D \subset X$ be any open coordinate patch with local coordinates $x = (x_1, \ldots, x_{2n+1})$. Let $\phi_1, \phi_2 \in C^\infty(D \times D)$. Suppose that $\phi_1, \phi_2$ satisfy (1.2), (1.11), $\phi_1$ and $\phi$ are equivalent in the sense of Melin–Sjöstrand, $\phi_2$ and $\phi$ are equivalent in the sense of Melin–Sjöstrand, where $\phi$ is as in (1.1). Suppose that
\[ \int_0^{+\infty} e^{i\phi_2(x,y)t} a(x, y, t) dt \equiv \int_0^{+\infty} e^{i\phi_1(x,y)t} \beta(x, y, t) dt \mod C^\infty(D \times D), \]
where $a(x, y, t), \beta(x, y, t) \in S^0_{cl}(D \times D \times \mathbb{R}_+)$ with
\[ a_0(x, x) = \beta_0(x, x), \text{ for all } x \in D, \tag{1.12} \]
\[ (T \alpha_0)(x, x) = (T \beta_0)(x, x) = 0, \text{ for all } x \in D. \]
Then, we have
\[ \alpha_1(x, x) = \beta_1(x, x), \text{ for every } x \in D. \tag{1.13} \]

From Lemma 1.1, we see that if we can choose the leading term in the expansion (1.3) satisfying (1.12) for all equivalent phase functions $\phi$ satisfying (1.2), (1.11), then the second coefficient of the expansion (1.3) at the diagonal is uniquely determined. This is possible by Lemma 3.3 below. Moreover, we will show in Lemma 3.3 that we can take the leading term in the expansion (1.3) as a function $\frac{1}{2\pi i} + r(x, y), r = O(|x - y|), \text{Tr} = 0$, for all equivalent phase functions $\phi$ satisfying (1.2), (1.11), and hence the second coefficient of the expansion (1.3) at the diagonal is well-defined. The main result of this work is the following

**Theorem 1.2.** With the notations and assumptions above, suppose that $\overline{\partial}_b : \text{Dom } \overline{\partial}_b \subset L^2(X) \to L^2_{(0,1)}(X)$ has closed range. Let $D \subset X$ be any open coordinate patch with local coordinates $x = (x_1, \ldots, x_{2n+1})$. Let $\hat{\phi} \in C^\infty(D \times D)$. Suppose that $\hat{\phi}$ satisfies (1.2), (1.11) and $\phi$ and $\hat{\phi}$ are equivalent in the sense of Melin–Sjöstrand, where $\phi$ is as in (1.1). Then, we can find $A(x, y, t) \in S^0_{cl}(D \times D \times \mathbb{R}_+)$ with
\[ A_0(x, x) = \frac{1}{2\pi i} + r(\text{scal})(x), \text{ for every } x \in D, \tag{1.14} \]
\[ TA_0 = 0 \text{ on } D, \]
\[ A_1(x, x) = \frac{1}{4\pi i} R_{\text{scal}}(x), \text{ for every } x \in D, \tag{1.15} \]
such that
\[ \Pi(x, y) \equiv \int_0^{+\infty} e^{i\phi(x,y)} A(x, y, t) dt \mod C^\infty(D \times D), \tag{1.16} \]
where $R_{\text{scal}}$ is the Tanaka–Webster scalar curvature on $X$ (see (2.11)).
2. Preliminaries

2.1. Standard notations and some background. We use the following notations through this article: \( \mathbb{N} = \{1, 2, \ldots\} \) is the set of natural numbers, \( \mathbb{N}_0 = \mathbb{N} \cup \{0\} \), \( \mathbb{R} \) is the set of real numbers, \( \mathbb{R}_+ = \{x \in \mathbb{R}; x \geq 0\} \). We write \( \alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}_0^n \) if \( \alpha_j \in \mathbb{N}_0 \), \( j = 1, \ldots, n \). For \( x = (x_1, \ldots, x_n) \in \mathbb{R}^n \), we write

\[
x^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n},
\]

\[
\partial_{\alpha} x_j = \frac{\partial}{\partial x_j}, \quad \partial^\alpha = \partial_{\alpha_1} \cdots \partial_{\alpha_n} = \frac{\partial^{\mid \alpha \mid}}{\partial x^\alpha}.
\]

Let \( z = (z_1, \ldots, z_n) \), \( z_j = x_{2j-1} + ix_{2j} \), \( j = 1, \ldots, n \), be coordinates of \( \mathbb{C}^n \). We write

\[
z^\alpha = z_1^{\alpha_1} \cdots z_n^{\alpha_n}, \quad \overline{z}^\alpha = \overline{z}_1^{\alpha_1} \cdots \overline{z}_n^{\alpha_n},
\]

\[
\partial_{\alpha} z_j = \frac{\partial}{\partial z_j} = \frac{1}{2} \left( \frac{\partial}{\partial x_{2j-1}} - i \frac{\partial}{\partial x_{2j}} \right), \quad \partial_{\alpha} \overline{z}_j = \frac{\partial}{\partial \overline{z}_j} = \frac{1}{2} \left( \frac{\partial}{\partial x_{2j-1}} + i \frac{\partial}{\partial x_{2j}} \right),
\]

\[
\partial^\alpha z = \partial_{\alpha_1} z_1 \cdots \partial_{\alpha_n} z_n = \frac{\partial^{\mid \alpha \mid}}{\partial z^\alpha}, \quad \partial^\alpha \overline{z} = \partial_{\alpha_1} \overline{z}_1 \cdots \partial_{\alpha_n} \overline{z}_n = \frac{\partial^{\mid \alpha \mid}}{\partial \overline{z}^\alpha}.
\]

For \( j, s \in \mathbb{Z} \), set \( \delta_{js} = 1 \) if \( j = s \), \( \delta_{js} = 0 \) if \( j \neq s \).

Let \( X \) be a \( \mathcal{C}^\infty \) paracompact manifold. We let \( TX \) and \( T^*X \) denote the tangent bundle of \( X \) and the cotangent bundle of \( X \) respectively. The complexified tangent bundle of \( X \) and the complexified cotangent bundle of \( X \) will be denoted by \( CTX \) and \( CT^*X \), respectively. Write \( \langle \cdot, \cdot \rangle \) to denote the pointwise duality between \( TX \) and \( T^*X \). We extend \( \langle \cdot, \cdot \rangle \) bilinearly to \( CTX \times CT^*X \).

Let \( D \subset X \) be an open set. The spaces of distributions of \( D \) and smooth functions of \( D \) will be denoted by \( \mathscr{D}'(D) \) and \( \mathcal{C}^\infty(D) \) respectively. Let \( \mathcal{E}'(D) \) be the subspace of \( \mathscr{D}'(D) \) whose elements have compact support in \( D \). Let \( \mathcal{E}^\infty_c(D) \) be the subspace of \( \mathcal{E}^\infty_c(D) \) whose elements have compact support in \( D \). Let \( A : \mathcal{E}^\infty_c(D) \to \mathscr{D}'(D) \) be a continuous operator. We write \( A(x, y) \) to denote the distribution kernel of \( A \). In this work, we will identify \( A \) with \( A(x, y) \). The following two statements are equivalent

(1) \( A \) is continuous: \( \mathcal{E}'(D) \to \mathcal{E}^\infty_c(D) \),

(2) \( A(x, y) \in \mathcal{E}^\infty_c(D \times D) \).

If \( A \) satisfies (1) or (2), we say that \( A \) is smoothing on \( D \). Let \( A, B : \mathcal{E}^\infty_c(D) \to \mathscr{D}'(D) \) be continuous operators. We write

\[
A \equiv B \text{ on } D
\]

or

\[
A(x, y) \equiv B(x, y) \mod \mathcal{E}^\infty_c(D \times D)
\]

if \( A - B \) is a smoothing operator. We sometimes will omit “on \( D \)” or “\( \mod \mathcal{E}^\infty_c(D \times D) \)” in (2.1) and (2.2) respectively. We say that \( A \) is properly supported if the restrictions of the two projections \((x, y) \to x, (x, y) \to y \) to \( \text{Supp } K_A \) are proper.

Let \( X \) be a smooth orientable manifold of real dimension \( 2n + 1 \). Let \( D \) be an open coordinate patch of \( X \) with local coordinates \( x \). We recall the following Hörmander symbol space...
Definition 2.1. For $m \in \mathbb{R}$, $S^m_{1,0}(D \times D \times \mathbb{R}_+) \subset \mathcal{C}^\infty(D \times D \times \mathbb{R}_+)$ is the space of all $a(x, y, t) \in \mathcal{C}^\infty(D \times D \times \mathbb{R}_+)$ such that for all compact $K \subset D \times D$ and all $\alpha, \beta, \gamma \in \mathbb{N}_0^{2n+1}$, there is a constant $C_{\alpha, \beta, \gamma} > 0$ such that

$$|\partial_x^\alpha \partial_y^\beta \partial_t^\gamma a(x, y, t)| \leq C_{\alpha, \beta, \gamma}(1 + |t|)^{m-|\gamma|}, \quad \text{for all } (x, y, t) \in K \times \mathbb{R}_+, \ t \geq 1.$$ 

Put

$$S^{-\infty}(D \times D \times \mathbb{R}_+) := \bigcap_{m \in \mathbb{R}} S^m_{1,0}(D \times D \times \mathbb{R}_+).$$

Let $a_j \in S^{m_j}_{1,0}(D \times D \times \mathbb{R}_+)$, $j = 0, 1, 2, \ldots$ with $m_j \to -\infty$, $j \to \infty$. Then there exists $a \in S^{m_0}_{1,0}(D \times D \times \mathbb{R}_+)$ unique modulo $S^{-\infty}$, such that $a - \sum_{j=0}^{k-1} a_j \in S^{m_k}_{1,0}(D \times D \times \mathbb{R}_+)$ for $k = 1, 2, \ldots$.

If $a$ and $a_j$ have the properties above, we write $a \sim \sum_{j=0}^{\infty} a_j$ in $S^{m_0}_{1,0}(D \times D \times \mathbb{R}_+)$. We write

$$s(x, y, t) \in S^m_{1,0}(D \times D \times \mathbb{R}_+)$$

if $s(x, y, t) \in S^m_{1,0}(D \times D \times \mathbb{R}_+)$ and

$$s(x, y, t) \sim \sum_{j=0}^{\infty} s_j(x, y) t^{m-j} \text{ in } S^m_{1,0}(D \times D \times \mathbb{R}_+),$$

$$s_j(x, y) \in \mathcal{C}^\infty(D \times D), \ j \in \mathbb{N}_0.$$

We sometimes omit "in $S^m_{1,0}(D \times D \times \mathbb{R}_+)$" in (2.4).

To calculate the first order term of Szegö kernel expansion explicitly, we also need the following version of stationary phase formula [6, Theorem 7.7.5]

Theorem 2.1. Let $D \subset \mathbb{R}^n$ be an open set, $K \subset D$ be a compact set, $F \in \mathcal{C}^\infty(D)$, $\text{Im} F \geq 0$ in $D$. Assume

$$\text{Im} F(0) = 0, \ F'(0) = 0, \ det \ F''(0) \neq 0, \ F' \neq 0 \text{ in } K \setminus \{0\}.$$ 

Let $u \in \mathcal{C}^\infty_c(D)$, $\text{Supp } u \subset K$, Then, for any $k > 0$,

$$\left| \int e^{ikF(x)} u(x) dx - e^{ikF(0)} \det \left( \frac{kF''(0)}{2\pi i} \right)^{-\frac{1}{2}} \sum_{j < N} k^{-j} P_j u \right| \leq C k^{-N} \sum_{|\alpha| \leq N} \sup_k |\partial_\alpha^x u|.$$ 

Here, $C$ is a bounded constant when $F$ is bounded in $\mathcal{C}^\infty(D)$, $\frac{|x|}{|F'(x)|}$ has a uniform bound and

$$P_j u := \sum_{\nu - \mu = j} \sum_{2^\nu \geq 3^\mu} i^{-j} 2^{-\nu} (F''(0)^{-1} D, D)^{\nu} (h^\nu u)(0) \frac{(h^\nu u)(0)}{\nu!}.$$ 

$$h(x) := F(x) - F(0) - \frac{1}{2}(F''(0) D, D) x, \ D = \begin{pmatrix} -i \partial_{x_1} \\ \vdots \\ -i \partial_{x_n} \end{pmatrix}.$$ 

2.2. Abstract CR manifolds. Let $X$ be a smooth orientable manifold of real dimension $2n + 1$ (at least three), we say $X$ is a Cauchy–Riemann manifold (CR manifold for short) if there is a subbundle $T^{1,0}_p X \subset CTX$, such that

1. dim$_{\mathbb{C}} T^{1,0}_p X = n$ for any $p \in X$.
2. $T^{1,0}_p X \cap T^{0,1}_p X = \{0\}$ for any $p \in X$, where $T^{0,1}_p X := \overline{T^{1,0}_p X}$. 

(3) For $V_1, V_2 \in \mathcal{C}^\infty(X, T^{1,0}X)$, then $[V_1, V_2] \in \mathcal{C}(X, T^{1,0}X)$, where $[\cdot, \cdot]$ stands for the Lie bracket between vector fields.

For such subbundle $T^{1,0}X$, we call it a CR structure of the CR manifold $X$. Let $(X, T^{1,0}X)$ be a smooth orientable CR manifold of dimension $2n + 1$. For dimension reason and the assumption that $X$ is orientable, there is a global real non-vanishing one form $\omega_0(x)$ such that
\[
\langle \omega_0(x), u \rangle = 0, \quad \text{for every } u \in T^{1,0}_x X \oplus T^{0,1}_x X.
\]

We define the Levi form (with respect to $\omega_0$) which is a globally defined $(1, 1)$-form, by
\[
\mathcal{L}_x(u, \overline{v}) := \frac{1}{2i} \langle \omega_0(x), \left[\hat{u}, \hat{v}\right] (x) \rangle,
\]
where $\hat{u}, \hat{v} \in \mathcal{C}^\infty(X, T^{1,0}X)$ such that $\hat{u}(x) = u \in T^{1,0}_x X$ and $\hat{v}(x) = v \in T^{0,1}_x X$. Note that by Cartan magic formula, we can also express the Levi form by
\[
\mathcal{L}_x(u, \overline{v}) = -\frac{1}{2i} (d\omega_0(x), u \wedge \overline{v}), \quad u, v \in T^{1,0}_x X.
\]

In other words,
\[
\mathcal{L}_x := -\frac{1}{2i} d\omega_0(x) \bigg|_{T^{1,0}_x X}.
\]

**Definition 2.2.** We say a CR manifold $X$ is strongly pseudoconvex if we can find $\omega_0$ so that $\mathcal{L}_x$ is positive definite for all $x \in X$.

From now on, we assume that $X$ is strongly pseudoconvex and we fix $\omega_0$ so that $\mathcal{L}_x$ is positive definite for all $x \in X$. Let $T \in \mathcal{C}^\infty(X, TX)$ be the global real vector field given by
\[
\omega_0(T) = -1, \quad d\omega_0(T, \cdot) = 0.
\]

The Levi form $\mathcal{L}_x$ induces a Hermitian metric (called Levi metric) $\langle \cdot \mid \cdot \rangle$ on $CTX$ given by
\[
\langle u \mid v \rangle = \mathcal{L}_x(u, \overline{v}), \quad \text{for every } u, v \in T^{1,0}_x X, x \in X,
\]
\[
\langle \overline{u} \mid \overline{v} \rangle = \langle u \mid v \rangle, \quad \text{for every } u, v \in T^{1,0}_x X, x \in X,
\]
\[
T^{1,0}X \perp T^{0,1}X, \quad T \perp (T^{1,0}X \oplus T^{0,1}X),
\]
\[
\langle T \mid T \rangle = 1.
\]

Let $\Gamma : CT^*_x X \to CT^*_x X$ be the anti-linear map given by $\langle u \mid v \rangle = \langle u, \Gamma v \rangle$ for $u, v \in CT^*_x X$, then we can take the induced Hermitian metric on $CT^*_X$ by $\langle u' \mid v' \rangle := \langle \overline{\Gamma^{-1} v} \mid \Gamma^{-1} u \rangle$ for $u, v \in CT^*_x X$. Put
\[
T^{*, 1,0} X := \Gamma(T^{1,0}X) = (T^{1,0}X \oplus CT)^\perp \subset CT^*_X, \quad T^{*, 0,1} X := T^{1,0}X.
\]

Take the Hermitian metric on $\Lambda^r(CT^*_X)$ by
\[
\langle u_1 \wedge \cdots \wedge u_r \mid v_1 \wedge \cdots \wedge v_r \rangle = \det \left( \langle (u_j)_{|u_k} \rangle_{j, k=1}^r \right), \quad \text{where } u_j, v_k \in CT^*_X, j, k = 1, \ldots, r.
\]

For every $q \in \{0, 1, \ldots, n\}$, the bundle of $(0, q)$ forms of $X$ is given by $T^{*, 0, q} X := \Lambda^q(T^{*, 0, 1} X)$ and let $\Omega^{0, q}(X)$ be the space of smooth $(0, q)$ forms on $X$. Let
\[
\pi^{(0, q)} : \Lambda^q(CT^*_X) \to T^{*, 0, q} X
\]
be the orthogonal projection with respect to $\langle \cdot | \cdot \rangle$. The tangential Cauchy–Riemann operator is defined by

$$\partial^b := \pi^{0,q+1} \circ d : \Omega^{0,q}(X) \to \Omega^{0,q+1}(X).$$

By Cartan magic formula, we can check that

$$\partial^2 b = 0.$$ 

Take the $L^2$-inner product $\langle \cdot | \cdot \rangle$ on $\Omega^{0,q}(X)$ induced by $\langle \cdot | \cdot \rangle$ via

$$(f|g) := \int_X \langle f | g \rangle dV_X, \quad f, g \in \Omega^{0,q}(X),$$

where $dV_X$ is the volume form with expression

$$dV_X(x) = \sqrt{\det \left( \left( \begin{array}{c|c} \frac{\partial}{\partial x_j} & \frac{\partial}{\partial x_k} \end{array} \right) \right)_{j,k=1}^{2n+1}} \ dx_1 \wedge \cdots \wedge dx_{2n+1}$$

in local coordinates $(x_1, \cdots, x_{2n+1})$. Let $\langle \cdot | \cdot \rangle$ be the $L^2$ inner product on $\Omega^{0,q}(X)$ induced by $\langle \cdot | \cdot \rangle$ and let $L^2_{(0,q)}(X)$ be the completion of $\Omega^{0,q}(X)$ with respect to $\langle \cdot | \cdot \rangle$. We write $L^2(X) := L^2_{(0,0)}(X)$. We extend $\partial_b$ to $L^2$ space by

$$\overline{\partial}_b : \text{Dom} \overline{\partial}_b \subset L^2(X) \to L^2_{(0,1)}(X),$$

$$\text{Dom} \overline{\partial}_b := \{ u \in L^2(X); \overline{\partial}_b u \in L^2_{(0,1)}(X) \}. $$

**Definition 2.3.** The orthogonal projection

$$\Pi : L^2(X) \to \text{Ker} \overline{\partial}_b := \{ u \in \text{Dom} \overline{\partial}_b; \overline{\partial}_b u = 0 \}$$

is called the Szegő projection, and we call its distributional kernel $\Pi(x, y)$ the Szegő kernel.

**2.3. Pseudohermitian geometry on strongly pseudoconvex CR manifolds.** We will use the same notations as before. We call

$$HX := \text{Re} \left( T^{1,0}X \oplus T^{0,1}X \right)$$

the contact structure of $X$, and let $J$ be the complex structure on $HX$ so that $T^{1,0}X$ is the eigenspace of $J$ corresponding to the eigenvalue $i$. Let

$$\theta_0 := -\omega_0.$$ 

The following is well-known:

**Proposition 2.1.** [[18, Proposition 3.1]] With the same notations and assumptions, there exists an unique affine connection, called Tanaka–Webster connection,

$$\nabla := \nabla^{\theta_0} : \mathcal{C}^\infty(X, TX) \to \mathcal{C}^\infty(X, T^*X \otimes TX)$$

such that

1. $\nabla U \mathcal{C}^\infty(X, HX) \subset \mathcal{C}^\infty(X, HX)$ for $U \in \mathcal{C}^\infty(X, TX).$
2. $\nabla T = \nabla J = \nabla d\theta_0 = 0.$
3. The torsion $\tau$ of $\nabla$ satisfies: $\tau(U, V) = d\theta_0(U, V)T$, $\tau(T, JU) = -J\tau(T, U)$, $U, V \in \mathcal{C}^\infty(X, HX).$
Recall that $\nabla J \in \mathcal{E}^\infty(X, T^*X \otimes \mathcal{L}(HX, HX))$, $\nabla d\theta_0 \in \mathcal{E}^\infty(T^*X \otimes \Lambda^2(CT^*X))$ are defined by $(\nabla_U J)W = \nabla_U (JW) - J\nabla_U W$ and $\nabla_U d\theta_0 (W, V) = Ud\theta_0 (W, V) - d\theta_0 (\nabla_U W, V) - d\theta_0 (W, \nabla_U V)$ for $U \in \mathcal{E}^\infty(X, TX)$, $W, V \in \mathcal{E}^\infty(X, HX)$. Moreover, $\nabla J = 0$ and $\nabla d\omega_0 = 0$ imply that the Tanaka-Webster connection is compatible with the Levi metric. By definition, the torsion of $\nabla$ is given by $\tau(W, U) = \nabla W U - \nabla U W - [W, U]$ for $U, V \in \mathcal{E}^\infty(X, TX)$ and $\tau(T, U)$ for $U \in \mathcal{E}^\infty(X, HX)$ is called pseudohermitian torsion.

Let $\{L_\alpha\}_{\alpha=1}^n$ be a local frame of $T^{1,0}X$ and $\{\theta^\alpha\}_{\alpha=1}^n$ be the dual frame of $\{L_\alpha\}_{\alpha=1}^n$. We use the notations $Z_\pi := L_\pi$ and $\theta^\pi = \overline{\theta^\alpha}$. Write

$$\nabla L_\alpha = \omega^\beta_\alpha \otimes L_\beta, \quad \nabla L_\pi = \omega_\pi^\beta \otimes L_\beta,$$

and recall that $\nabla T = 0$.

We call $\omega^\beta_\alpha$ the connection one form of Tanaka-Webster connection with respect to the frame $\{L_\alpha\}_{\alpha=1}^n$. We denote $\Theta^\beta_\alpha$ the Tanaka-Webster curvature two form, and it is known that

$$\Theta^\beta_\alpha = d\omega^\beta_\alpha - \omega^\gamma_\alpha \wedge \omega^\beta_\gamma.$$

By direct computation, we also have

$$\Theta^\beta_\alpha = R^\beta_{\alpha jk} \theta^j \wedge \theta^k + A^\beta_{\alpha jk} \theta^j \wedge \theta^k + B^\beta_{\alpha jk} \theta^j \wedge \theta^k + C_0 \wedge \theta_0,$$

where $C_0$ is an one form. The term $R^\beta_{\alpha jk}$ is called the pseudohermitian curvature tensor and the trace

$$R_\alpha := \sum_{j=1}^n R^j_{\alpha jk}$$

is called the pseudohermitian Ricci curvature. Also, write

$$d\theta_0 = i g_{\alpha \beta} \theta^\alpha \wedge \theta^\beta$$

and $g^{\alpha \beta}$ be the inverse matrix of $g_{\alpha \beta}$, then the Tanaka-Webster scalar curvature $R$ with respect to the pseudohermitian structure $\theta_0$ is given by

$$R_{\text{scal}} := g^{\alpha \beta} R_{\alpha \beta}.$$

### 3. THE CALCULATION OF THE SECOND COEFFICIENT OF THE SZEGŐ KERNEL ASYMPTOTIC EXPANSION

In this section, we will prove Theorem 1.2. We will first show that how to select a suitable phase function and the leading term of the Szegő kernel asymptotic expansion such that the second order term of the Szegő kernel asymptotic expansion is well-defined.

#### 3.1. Uniqueness of the coefficients

We first recall some facts from the theory of oscillatory integral and distributions: Notice that $\int_0^\infty e^{-tx} dt = x^{-1}$, for Re $x > 0$. Also notice that by partial
integration and dominated convergence theorem,

\[ \int_0^1 \frac{1 - e^{-t}}{t} dt + \int_1^\infty e^{-t} t^{-1} dt = \int_0^\infty e^{-t} \log t dt \]

\[ = \lim_{m \to \infty} \left( \int_0^m \left(1 - \frac{t}{m}\right)^{m-1} \log t dt \right) \]

\[ = \lim_{m \to \infty} \left( m \int_0^1 s^{m-1} \log (m-1) ds \right) \]

\[ = \lim_{m \to \infty} \left( m \log m \int_0^1 s^{m-1} ds + m \int_0^1 s^{m-1} \log (1-s) ds \right) \]

\[ = \lim_{m \to \infty} \left( \log m - m \int_0^1 \sum_{k=1}^\infty \frac{s^{k+m-1}}{k} ds \right) \]

\[ = \lim_{m \to \infty} \left( \log m - m \sum_{k=1}^\infty \int_0^1 \frac{s^{k+m-1}}{k} ds \right) \]

\[ = \lim_{m \to \infty} \left( \log m - \sum_{k=1}^\infty \left( \frac{1}{k} - \frac{1}{m+k} \right) \right) \]

\[ = \lim_{m \to \infty} \left( \log m - \sum_{k=1}^\infty \frac{1}{k} \right) \]

Accordingly, we can check that by partial integration, if \( x \neq 0 \) and \( \text{Re} \ x \geq 0 \), then

\[ (3.1) \quad \text{P.V.} \int_0^\infty e^{-tx} t^m dt = \left\{ \begin{array}{ll}
 m!x^{-m-1} : & m \in \mathbb{Z}, \ m \geq 0 \\
 (\frac{-1)^m}{(m-1)!} x^{-m-1} \left( \log x + \gamma - \sum_{j=0}^{m-1} \frac{1}{j} \right) : & m \in \mathbb{Z}, \ m < 0
\end{array} \right. \]

where \( \gamma := \lim_{m \to \infty} \left( \sum_{j=1}^m \frac{1}{j} - \log m \right) \) is the Euler constant. On the other hand, by choosing a suitable contour, we can check that for a smooth function \( f \in \mathcal{C}_c^\infty(\mathbb{R}^n) \), \( \text{Im} f \geq 0 \), and any \( \epsilon > 0 \),

\[ (3.2) \quad \frac{1}{(-i)(f(x) + i\epsilon)} = \int_0^\infty e^{i(f(x)+i\epsilon)} dt; \]

and if \( df(x) \neq 0 \) if \( \text{Im} f(x) = 0 \), with convergence in \( \mathcal{D}'(\mathbb{R}^n) \), we define

\[ \frac{1}{(-i)(f(x) + i\epsilon)} := \lim_{\epsilon \to 0} \frac{1}{(-i)(f(x) + i\epsilon)^{\prime}} \]

and we can check that

\[ \frac{1}{(-i)(f(x) + i\epsilon)} = \int_0^\infty e^{if(x)} dt \]

in the sense of oscillatory integral. Moreover, we have:

**Lemma 3.1.** Let \( D \subset \mathbb{R}^n \) be a small enough open set near 0. Assume

\[ F(x) \in \mathcal{C}_c^\infty(D), F(0) = 0, \ \text{Im} F \geq 0, \ df \neq 0 \ if \ \text{Im} F = 0, \]

and

\[ G(x) \in \mathcal{C}_c^\infty(D), G(0) \neq 0, \ \text{Im}(FG) \geq 0, \ d(FG) \neq 0 \ if \ \text{Im}(FG) = 0. \]
Lemma 3.2. Fix $p$. Proof. First of all, by continuity, we may assume that on $D$

\begin{equation}
|G| \geq \frac{1}{2}|G(0)| > 0.
\end{equation}

From the construction of oscillatory integral [6, Theorem 7.8.2], in the sense of distribution,

\begin{align*}
\int_0^\infty e^{itG(x)}F(x)t^m dt &= \lim_{\varepsilon \to 0} \int_0^\infty e^{it(G(x)+i\varepsilon)}t^m dt \\
&= \lim_{\varepsilon \to 0} m! (-iG(x)F(x) + \varepsilon)^{m+1} (x) \\
&= \frac{m!}{G(x)^{m+1}} \lim_{\varepsilon \to 0} (F(x) + \varepsilon)^{m+1} \\
&= \frac{m!}{(-iG(x))^{m+1}} (F(x) + i0)^{m+1} \\
&= \int_0^\infty e^{itF(x)} \frac{t^m}{G(x)^{m+1}} dt.
\end{align*}

\[\Box\]

We first need

Lemma 3.2. Fix $p \in X$. Let $D \subset X$ be any open coordinate patch of $X$ with local coordinates $x = (x_1, \ldots, x_{2n+1})$, $p \in D$. Let $\phi_1, \phi_2 \in S^\infty(D \times D)$. Suppose that $\phi_1, \phi_2$ satisfy (1.2), $\phi_1$ and $\phi$ are equivalent in the sense of Melin–Sjöstrand, $\phi_2$ and $\phi$ are equivalent in the sense of Melin–Sjöstrand, where $\phi$ is as in (1.1), and

\begin{equation}
(T^2 \phi_1)(p, p) = (T^2 \phi_2)(p, p) = 0.
\end{equation}

Suppose that

\begin{equation}
\int_0^{+\infty} e^{i\phi_2(x, y)t} \alpha(x, y, t) dt = \int_0^{+\infty} e^{i\phi_1(x, y)t} \beta(x, y, t) dt \quad \text{mod } S^\infty(D \times D),
\end{equation}

where $\alpha(x, y, t), \beta(x, y, t) \in S^\infty(D \times D \times \mathbb{R}_+)$ with

\begin{align*}
\alpha_0(p, p) &= \beta_0(p, p), \\
(T\alpha_0)(p, p) &= (T\beta_0)(p, p) = 0.
\end{align*}

Then, we have

\begin{equation}
\alpha_1(p, p) = \beta_1(p, p).
\end{equation}

Proof. We take local coordinates $x = (x_1, \ldots, x_{2n+1})$ of $X$ such that

\begin{equation}
T = -\frac{\partial}{\partial x_{2n+1}}.
\end{equation}

As in [12, Section 8], we have

\[\phi_2(x, y) = f(x, y)\phi_1(x, y) + O(|x-y|^\infty),\]
for some \( f(x, y) \in \mathcal{C}^\infty(D \times D) \), and we may assume that
\[
\phi_2(x, y) = f(x, y)\phi_1(x, y).
\]
From (3.4) and (3.8), we can check that
\[
f(x, x) = 1, \quad \frac{\partial f}{\partial x_{2n+1}}(0, 0) = 0,
\]
and hence
\[
f((0, x_{2n+1}), 0) = 1 + O\left(|x_{2n+1}|^2\right).
\]
Applying Lemma 3.1 and (3.1) to oscillatory integrals (3.5), we see that
\[
\sum_{j=0}^n (n - j)!\alpha_j(x, y)(-i\phi_1)^j(x, y) \mod \phi_1^{n+1} = \sum_{j=0}^n (n - j)!\beta_j(x, y)(-i\phi_1)^j(x, y) \mod \phi_1^{n+1}
\]
up to some log term singularities. In particular, when \( x \neq y \),
\[
\sum_{j=0}^n (n - j)!\alpha_j(x, y)(-i\phi_1)^j(x, y) = f^{n+1}(x, y)\sum_{j=0}^n (n - j)!\beta_j(x, y)(-i\phi_1)^j(x, y) + (-i\phi_1)^{n+1}(x, y)S(x, y).
\]
for some \( S \in \mathcal{C}^\infty(D \times D) \). Now, take \( x = (0, x_{2n+1}) \) and \( y = 0 \) in the above equation, then from (3.6), (3.9) and (3.10), it is straightforward to check that
\[
(\alpha_1 - \beta_1)((0, x_{2n+1}), 0) = O(|x_{2n+1}|).
\]
By taking \( x_{2n+1} \to 0 \), we see that
\[
\alpha_1(0, 0) = \beta_1(0, 0).
\]
We need

**Lemma 3.3.** With the notations and assumptions used in Theorem 1.1, we can take \( a(x, y, t) \) in (1.1) so that
\[
Ta_0 = 0 \quad \text{on } D,
\]
\[
a_0(x, x) = \frac{1}{2\pi^{n+1}} \quad \text{for every } x \in D.
\]

**Proof.** Take local coordinates \( x = (x_1, \ldots, x_{2n+1}) \) of \( X \) so that \( T = -\frac{\partial}{\partial x_{2n+1}} \) on \( D \). By the relation
\[
d_x \phi(x, x) = -\omega_0(x), \quad \text{for every } x \in D,
\]
we know that \( \frac{\partial \phi}{\partial x_{2n+1}}(x, x) = -1 \neq 0 \). Thus, applying the Malgrange preparation theorem [6, Theorem 7.5.5], we have
\[
\phi(x, y) = f_1(x, y)(-x_{2n+1} + g_1(x', y))
\]
for some smooth functions \( f_1(x, y), g_1(x', y) \) with \( f_1(x, x) = 1 \), for every \( x \in D \), where \( x' = (x_1, \ldots, x_{2n}) \). Note that \( g_1 \) is independent of \( x_{2n+1} \). By Taylor formula, we have
\[
a_0(x, y) = \tilde{a}_0(x, y) = \tilde{a}_0((x', g_1(x', y)), y) + (-x_{2n+1} + g_1(x', y)) R(x, y),
\]
where
where $\tilde{a}_0$ denotes an almost analytic extension of $a_0$ with respect to the real variable $x_{2n+1}$, $R(x, y) \in \mathcal{C}^\infty(D \times D)$. Let
\begin{equation}
\tilde{a}_0(x', y) := \tilde{a}_0((x', g_1(x', y)), y) \in \mathcal{C}^\infty(D \times D).
\end{equation}

Then, by using integration by parts, we get
\[
\int_0^\infty e^{it\phi(x,y)}a_0(x,y)t^n\,dt = \int_0^\infty e^{it\phi(x,y)}\tilde{a}_0(x',y)t^n\,dt - i \int_0^\infty \frac{d}{dt} \left( e^{itf_1(x,y)(-x_{2n+1}+g_1(x',y))} \right) \frac{R(x,y)}{f_1(x,y)} t^n\,dt
\]
\[
= \int_0^\infty e^{it\phi(x,y)}\tilde{a}_0(x',y)t^n\,dt + i \int_0^\infty e^{it\phi(x,y)}\frac{R(x,y)}{f_1(x,y)} nt^{n-1}\,dt.
\]

Hence, we can replace $a_0(x,y)$ by $\tilde{a}_0(x',y)$ in (1.1) and by (1.5), we see that
\[
\tilde{a}_0(x,x) = \frac{1}{2\pi^{n+1}}, \text{ for every } x \in D.
\]

The lemma follows. \hfill \square

From now on, we assume that $a_0(x,y)$ satisfies (3.13). We have

**Theorem 3.1.** With the notations and assumptions used in Theorem 1.1, we assume that
\begin{equation}
\overline{\partial}_b x(\phi(x,y)) \text{ vanishes to infinite order at } x = y,
\end{equation}
\begin{equation}
\overline{\partial}_b(-\overline{\phi}(y,x)) \text{ vanishes to infinite order at } x = y.
\end{equation}

We have
\begin{equation}
a_0(x,y) - \frac{1}{2\pi^{n+1}} = O(|x-y|^N), \text{ for every } (x,y) \in D \times D, \text{ for every } N \in \mathbb{N}.
\end{equation}

**Proof.** Fix $p \in X$, let $x = (x_1, \ldots, x_{2n+1})$ be local coordinates of $X$ defined on $D$ with $x(p) = 0$, $T = -\frac{\partial}{\partial x_{2n+1}}$ and
\begin{equation}
T^{1,0}X = \text{span} \{ L_j; j = 1, \ldots, n \},
\end{equation}
\begin{equation}
L_j = \frac{\partial}{\partial \overline{z}_j} + O(|x|), \quad \frac{\partial}{\partial \overline{z}_j} = \frac{1}{2} \left( \frac{\partial}{\partial x_{2j-1}} + i \frac{\partial}{\partial x_{2j}} \right), \quad j = 1, \ldots, n.
\end{equation}

From $\overline{\partial}_b \Pi = 0$ and $\overline{\partial}_b \phi$ vanishes to infinite order at $x = y$, applying Malgrange preparation theorem \cite[Theorem 7.5.6]{6}, partial integration, Lemma 3.1, Melin–Sjöstrand \cite[p. 172]{17} and \cite[Section 8]{12}, it is not difficult to check that
\begin{equation}
(L_j a_0)(x,y) = h_j(x,y)(-x_{2n+1}+g_1(x',y)) + O(|x-y|^N), \quad \text{for every } N \in \mathbb{N}, \quad h_j \in \mathcal{C}^\infty(D \times D), \quad j = 1, \ldots, n,
\end{equation}
where $g_1 \in \mathcal{C}^\infty(D \times D)$ is as in (3.14). We claim that
\begin{equation}
|a_0(x,y) - \frac{1}{2\pi^{n+1}}| = O(|(x,y)|^N), \text{ for every } N \in \mathbb{N}_0.
\end{equation}

It is clear that (3.21) holds for $N = 0$. Suppose that (3.21) holds for $N = N_0, N_0 \in \mathbb{N}_0$. We are going to prove that (3.21) holds for $N = N_0 + 1$. From (3.19), (3.20), (3.21) and induction assumption, we have
\begin{equation}
\frac{\partial a_0}{\partial \overline{z}_j}(x',y) = O(|(x,y)|^{N_0}), \quad j = 1, \ldots, n.
\end{equation}
Similarly, we have

\[(3.23) \quad \frac{\partial a_0}{\partial w_j}(x', y) = O((x, y)^{|N_0|}), \quad j = 1, \ldots, n,\]

where \(\frac{\partial}{\partial w_j} = \frac{1}{2}(\frac{\partial}{\partial y_{2j-1}} - i\frac{\partial}{\partial y_{2j}}), \quad j = 1, \ldots, n.\)

Fix \(j \in \{1, \ldots, n\}\) and fix \(a, \beta \in \mathbb{N}_0, a + \beta = N_0.\) From \(a_0(x, x) = \frac{1}{2\pi i} \text{e}^{x},\) we have

\[(3.24) \quad \left(\left(\frac{\partial}{\partial z_j} + \frac{\partial}{\partial w_j}\right)^a\left(\frac{\partial}{\partial z_j} + \frac{\partial}{\partial w_j}\right)^\beta\right)a_0(x, x) = 0.\]

From (3.24), we have

\[(3.25) \quad \left(\left(\frac{\partial}{\partial z_j}\right)^a\left(\frac{\partial}{\partial w_j}\right)^\beta a_0\right)(0, 0) = \sum_{a_1, a_2, \beta_1, \beta_2 \in \mathbb{N}_0, a_1 + a_2 = a, \beta_1 + \beta_2 = \beta} c_{a_1, a_2, \beta_1, \beta_2} \left(\left(\frac{\partial}{\partial z_j}\right)^{a_1}\left(\frac{\partial}{\partial w_j}\right)^{a_2}\left(\frac{\partial}{\partial z_j}\right)^{\beta_1}\left(\frac{\partial}{\partial w_j}\right)^{\beta_2}a_0\right)(0, 0),\]

where \(c_{a_1, a_2, \beta_1, \beta_2}\) is a constant, for every \(a_1, a_2, \beta_1, \beta_2 \in \mathbb{N}_0\) and \(a_1 + a_2 = a, \beta_1 + \beta_2 = \beta, a_2 + \beta_1 > 0.\)

Since \(a_2 + \beta_1 > 0,\) from (3.22) and (3.23), we get

\[(3.26) \quad \left(\left(\frac{\partial}{\partial z_j}\right)^a\left(\frac{\partial}{\partial w_j}\right)^\beta a_0\right)(0, 0) = 0, \quad \text{for every} \quad a, \beta \in \mathbb{N}_0, \quad a + \beta = N_0.\]

We can repeat the proof of (3.26) with minor change and deduce that

\[(3.27) \quad \left(\left(\frac{\partial}{\partial z_j}\right)^a\left(\frac{\partial}{\partial w_j}\right)^\beta a_0\right)(0, 0) = 0, \quad \text{for every} \quad a, \beta \in \mathbb{N}_0^\mu, \quad |a| + |\beta| = N_0.\]

Since \(a_0\) is independent of \(x_{2n+1}\) and \(a_0(x', x) = \frac{1}{2\pi i} \text{e}^{x'},\) we have

\[(3.28) \quad \left(\left(\frac{\partial}{\partial y_{2n+1}}\right)^Na_0\right)(x, x) = 0, \quad \text{for every} \quad N \in \mathbb{N}.\]

From (3.28), we can repeat the proof of (3.26) with minor change and deduce that

\[(3.29) \quad \left(\left(\frac{\partial}{\partial z_j}\right)^a\frac{\partial}{\partial w_j}\left(\frac{\partial}{\partial y_{2n+1}}\right)^\gamma a_0\right)(0, 0) = 0, \quad \text{for every} \quad a, \beta, \gamma \in \mathbb{N}_0^\mu, \quad |a| + |\beta| + |\gamma| = N_0.\]

From (3.22), (3.23), (3.27), (3.29), we get

\[|a_0(x, y) - \frac{1}{2\pi i} \text{e}^{x}| = O(|(x, y)|^{N_0+1}).\]

By induction, we get the claim (3.21). From (3.21), the theorem follows. □
3.2. **Calculation of the coefficients.** To calculate \( a_1(x, x) \) in (1.1), we need to choose some good coordinates. We will work with the assumptions as in Theorem 1.1. Fix \( p \in X \). Since \( \partial_b \) has closed range, from [1], we see that there is an open set \( U \) of \( p \) such that \( U \) can be CR embedded into \( \mathbb{C}^{n+1} \). From now on, we identify \( U \) with \( \partial M \), where

\[
\partial M := \{ z \in \mathbb{C}^{n+1}; \ r(z) = 0 \}, \quad \tau(z) \in \mathcal{C}^\infty(\mathbb{C}^{n+1}, \mathbb{R}),
\]

\( J(\partial r) = 1 \) on \( \partial M \), \( J \) is the standard complex structure on \( \mathbb{C}^{n+1} \),

\( \hat{D} \) is an open set of \( p \) in \( \mathbb{C}^{n+1} \).

From [7, Lemma 3.2], we can find local holomorphic coordinates \( x = (x_1, \ldots, x_{2n+2}) = z = (z_1, \ldots, z_{n+1}), z_j = x_{2j-1} + ix_{2j}, j = 1, \ldots, n+1 \), defined on \( \hat{D} \) (we assume that \( \hat{D} \) is small enough) such that

\[
z(p) = 0,
\]

\[
r(z) = 2 \text{Im} z_{n+1} + \sum_{j=1}^{n} |z_j|^2 + O((|z_1|, \cdots, z_{n+1})^4).
\]

From now on, we assume that (3.31) hold. It is well-known that (see [2, Proposition 1.1, Theorem 1.5]) we can take \( \phi \in \mathcal{C}^\infty(U \times U) \) in (1.1) so that \( \phi \) satisfies (1.2) and

\[
\phi(z, w) = \frac{1}{i} \sum_{\alpha, \beta \in \mathbb{N}_0^n, |\alpha| + |\beta| \leq N} \frac{\partial^{\alpha + \beta}_{\bar{r} \bar{r}}}{\partial z_\alpha \partial \bar{z}_\beta}(0) \frac{z_\alpha w^\beta}{\alpha! \beta!} + O((z, w)^{N+1}), \quad \text{for every } N \in \mathbb{N}.
\]

From (3.32), we can check that

\[
\overline{\partial}_{b,x}(\phi(x, y)) \text{ vanishes to infinite order at } x = y,
\]

\[
\overline{\partial}_{b,y}(-\phi(y, x)) \text{ vanishes to infinite order at } x = y.
\]

From now on, we assume that \( \phi \) satisfies (1.2) and (3.32).

From implicit function theorem, if \( \hat{D} \) is small enough, we can find \( R(x_1, \ldots, x_{2n+1}) \in \mathcal{C}^\infty(D) \) such that

\[
\text{for every } x \in \hat{D}, (x_1, \ldots, x_{2n+1}) \in D, x \in U \text{ if and only if } x_{2n+2} = R(x_1, \ldots, x_{2n+1}),
\]

where \( D \) is an open set of \( \mathbb{R}^{2n+1}, 0 \in D \). From now on, we assume that \( \hat{D} \) is small enough so that (3.34) holds. Let \( x = (x_1, \ldots, x_{2n+1}) \) be local coordinates of \( D \) given by the map

\[
(x_1, \ldots, x_{2n+1}) \in D \rightarrow (x_1, \ldots, x_{2n+1}, R(x_1, \ldots, x_{2n+1})) \in U.
\]

From now on, we identify \( U \) with \( D \) and we will work with local coordinates \( x = (x_1, \ldots, x_{2n+1}) \) as (3.35). The following follows from some straightforward calculation. We omit the details.

**Proposition 3.1.** With the notations used above, we have

\[
R(x) = -\frac{1}{2} \sum_{j=1}^{2n} x_j^2 + O(|x|^4),
\]

\[
\frac{\partial^2 R}{\partial z_j \partial \bar{z}_k}(0) = -\frac{1}{2} \delta_{j,k}, \quad j, k = 1, \ldots, n,
\]
Proof. From (3.32), we have

\[ \phi(x, y) = -x_{2n+1} + y_{2n+1} - i\sum_{j=1}^{n} \left( \frac{\partial R}{\partial z_j} dz_j - \frac{\partial R}{\partial \bar{z}_j} d\bar{z}_j \right) + O(|x|^4), \]

(3.37)

\[ d\omega_0(x) = 2i \sum_{j=k}^{n} \frac{\partial^2 R}{\partial z_j \partial \bar{z}_k} dz_j \wedge d\bar{z}_k + O(|x|^3), \]

(3.38)

\[ T_{x}^1 X = \text{span} \left\{ \frac{\partial}{\partial z_i} + i \frac{\partial R}{\partial z_i} \frac{\partial}{\partial x_{2n+1}} + O(|x|^4) \right\}, \]

(3.39)

\[ T(x) = -\frac{\partial}{\partial x_{2n+1}} + O(|x|^2). \]

(3.40)

In particular, the volume form on \( X \) given by

\[ \lambda(x) dx_1 \cdots dx_{2n+1} = \frac{1}{n!} \left( -\frac{d\omega_0}{2} \right)^n \wedge \omega_0 \]

satisfies

\[ \lambda(0) = 1, \]

(3.41)

\[ \frac{\partial \lambda}{\partial x_j}(0) = 0, \quad j = 1, \ldots, 2n+1. \]

(3.42)

We also need

Proposition 3.2. With the same notations above, we have

\[ \phi(x, y) = -x_{2n+1} + y_{2n+1} + \frac{i}{2} \sum_{j=1}^{n} \left[ |z_j - w_j|^2 + (\bar{z}_j w_j - z_j \bar{w}_j) \right] + O\left( |(x, y)|^4 \right), \]

(3.43)

\[ \frac{\partial^4 \phi}{\partial z_j \partial z_k \partial \bar{z}_l \partial \bar{z}_s}(0, 0) = -i \frac{\partial^4 R}{\partial z_j \partial z_k \partial \bar{z}_l \partial \bar{z}_s}(0), \quad j, k, l, s \in \{1, \ldots, n\}, \]

(3.44)

\[ \frac{\partial^4 \phi}{\partial w_l \partial w_k \partial \bar{w}_j \partial \bar{w}_s}(0, 0) = -i \frac{\partial^4 R}{\partial w_l \partial w_k \partial \bar{w}_j \partial \bar{w}_s}(0), \quad j, k, l, s \in \{1, \ldots, n\}, \]

where \( \frac{\partial}{\partial y_j} = \frac{1}{2} \left( \frac{\partial}{\partial y_{2j-1}} - i \frac{\partial}{\partial y_{2j}} \right), j = 1, \ldots, n \), and

(3.45)

\[ T^2 \phi(0, 0) = 0. \]

Proof. From (3.32), we have

\[ \phi(x, y) = -x_{2n+1} + y_{2n+1} - i[R(x) + R(y) + \sum_{j=1}^{n} z_j \bar{w}_j] + O\left( |(x, y)|^4 \right) \]

(3.46)

\[ = -x_{2n+1} + y_{2n+1} + \frac{i}{2} \sum_{j=1}^{n} \left[ |z_j - w_j|^2 - 2z_j \bar{w}_j + |w_j|^2 \right] + O\left( |(x, y)|^4 \right) \]

\[ = -x_{2n+1} + y_{2n+1} + \frac{i}{2} \sum_{j=1}^{n} \left[ |z_j - w_j|^2 + (\bar{z}_j w_j - z_j \bar{w}_j) \right] + O\left( |(x, y)|^4 \right) \]
and
\[
\phi(x, 0) = -x_{2n+1} - iR(x) \\
(3.47) + \frac{1}{i} \sum_{a_j \in \mathbb{N}_0, j=1, \ldots, n+1, a_1+\cdots+a_{n+1} = 0} \frac{1}{\partial z_1^{a_1} \cdots \partial z_n^{a_n} \partial z_{n+1}^{a_{n+1}}}(0)z_1^{a_1} \cdots z_n^{a_n} (x_{2n+1} + iR(x))^{a_{n+1}} + O(|x|^5).
\]
From (3.47), we get
\[
(3.48) \frac{\partial^4 \phi}{\partial z_j \partial z_k \partial z_{\ell} \partial z_s}(0, 0) = -i \frac{\partial^4 R}{\partial z_j \partial z_k \partial z_{\ell} \partial z_s}(0), \ j, k, \ell, s \in \{1, \ldots, n\}.
\]
Similarly,
\[
(3.49) \frac{\partial^4 \phi}{\partial w_j \partial w_k \partial w_{\ell} \partial w_s}(0, 0) = -i \frac{\partial^4 R}{\partial w_j \partial w_k \partial w_{\ell} \partial w_s}(0), \ j, k, \ell, s \in \{1, \ldots, n\}.
\]
From (3.46), (3.48) and (3.49), we get (3.43) and (3.44).
Finally, because for all \(x\) near \(p\),
\[
T(x) = -\frac{\partial}{\partial x_{2n+1}} + O(|x|^2),
\]
it is clear that
\[
(3.50) T^2 \phi(0, 0) = 0.
\]

By Malgrange preparation theorem [6, Theorem 7.5.5] again, we have
\[
(3.51) \phi(x, y) = f(x, y)\Phi(x, y) \text{ on } D, \\
\Phi(x, y) = -x_{2n+1} + g(x', y),
\]
where \(f(x, y), g(x', y) \in \mathcal{C}^\infty(D \times D), x' = (x_1, \ldots, x_{2n})\). From Proposition 3.2, it is straightforward to check that
\[
(3.52) f(x, y) = 1 + O(|(x, y)|^3), \\
\Phi(x, y) \text{ satisfies (3.43), (3.44) and (3.45)}.
\]
We write
\[
(3.53) \Pi(x, y) \equiv \int_0^\infty e^{it\phi(x, y)}a(x, y, t)dt \equiv \int e^{i\Phi(x, y)}A(x, y, t)dt,
\]
where \(a(x, y, t), A(x, y, t) \in S_\mathcal{D}^n(D \times D \times \mathbb{R}_+),\)
\[
a(x, y, t) \sim \sum_{j=0}^\infty a_j(x, y)t^{n-j} \text{ in } S_\mathcal{D}^n(D \times D \times \mathbb{R}_+), \ a_j(x, y) \in \mathcal{C}^\infty(D \times D) \text{ for all } j \in \mathbb{N}_0,
\]
\[
(3.54) A(x, y, t) \sim \sum_{j=0}^\infty A_j(x, y)t^{n-j} \text{ in } S_\mathcal{D}^n(D \times D \times \mathbb{R}_+), \ A_j(x, y) \in \mathcal{C}^\infty(D \times D) \text{ for all } j \in \mathbb{N}_0.
\]
We can repeat the proof of Lemma 3.3 and conclude that we can take \( a_j(x, y), A_j(x, y) \) are independent of \( x_{2n+1} \), for every \( j \). From now on, we assume that \( a_j(x, y), A_j(x, y) \) are independent of \( x_{2n+1} \), for every \( j \), and hence

\[
\begin{align*}
\phi(x, y) = \phi(x', y), \quad & j = 0, 1, \ldots, \\
A_j(x, y) = A_j(x', y), \quad & j = 0, 1, \ldots.
\end{align*}
\]

Since \( \phi \) satisfies (3.33), we can repeat the proof of Theorem 3.1 with minor change and deduce that

\[
a_0(x', y) = \frac{1}{2\pi n + 1} + O((|x, y|^N)) , \text{ for every } N \in \mathbb{N}.
\]

Moreover, from Lemma 3.1 and the proof of Lemma 3.3, we can take \( A_0(x', y) \) to be

\[
A_0(x', y) = \frac{1}{2\pi n + 1} + O((|x, y|^N)) , \text{ for every } N \in \mathbb{N}.
\]

From Lemma 3.2, we see that to prove Theorem 1.2, we only need to calculate \( a_1(0, 0) \). Note \((T^2 \phi)(0, 0) = 0, (T^2 \Phi)(0, 0) = 0\). From this observation, we can repeat the proof of Lemma 3.2 and deduce that

\[
a_1(0, 0) = A_1(0, 0).
\]

Hence, to prove Theorem 1.2, we only need to calculate \( A_1(0, 0) \). Now, we are going to calculate \( A_1(0, 0) \). We apply the projection relation

\[
\Pi = \Pi^2,
\]

or equivalently, in the sense of oscillatory integral

\[
\Pi(x, y) \equiv \int_D \Pi(x, w)\Pi(w, y)\lambda(w)dw \mod \mathcal{C}^{\infty}(D \times D),
\]

to compute \( A_1(0, 0) = a_1(0, 0) \), where \( \lambda(w)dw \) is the volume form on \( X \). Now, shrink \( D \) if necessary. From

\[
\Pi(x, y) \in \mathcal{C}^{\infty}(X \times X \setminus \text{diag}X \times X),
\]

we may assume that all the base variables \( x, y, w \in D \) are within a compact set. Then, in the sense of oscillatory integral,

\[
\begin{align*}
\int_0^\infty e^{i\Phi(x, y)} A(x, y, t)dt \\
\equiv \int_D \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} e^{i\Phi(x, w) + i\Phi(w, y)} A(x, w, t)A(w, y, s)\lambda(w)dwdsdt \\
\equiv \int_0^\infty \left( \int_D \int_{\mathbb{R}^+} e^{i\Phi(x, w) + i\Phi(w, y)} A(x, w, t)A(w, y, t\sigma)\lambda(w)dw\sigma \right) dt \\
\equiv \int_0^\infty \left( \int_D \int_{\mathbb{R}^+} e^{i(-x_{2n+1} + g(x', w) + \sigma(w_{2n+1} + g(w', y))) A(x, w, t)A(w, y, t\sigma)\lambda(w)dw\sigma \right) dt.
\end{align*}
\]

Consider the phase function

\[
\Psi(w, \sigma, x, y) := -x_{2n+1} + g(x', w) + \sigma(-w_{2n+1} + g(w', y)).
\]
It is clear that \( \text{Im} \Psi \geq 0 \) for \( \sigma \geq 0 \). Also,

\[
d_w \Psi = d_w g(x', w) + \sigma(-dw_{2n+1} + d_x g(w', y)), \quad \frac{\partial \psi}{\partial \sigma} = -w_{2n+1} + g(w', y),
\]

and with respect to \((w, \sigma)\), \(\text{Hess}(\Psi)\) is a matrix of the form

\[
\text{Hess}(\Psi) = \begin{bmatrix}
\frac{\partial^2}{\partial x^2} (g(x', w) + \sigma g(w', y)) & \left( \frac{\partial^2}{\partial w_{2n+1}} (-w_{2n+1} + g(w', y)) \right) \\
-\frac{\partial^2}{\partial w_{2n+1}} (-w_{2n+1} + g(w', y)) & 0
\end{bmatrix}.
\]

Directly, at \((w, \sigma; x, y) = (0, 1, 0, 0) \in \mathbb{R}^{n+1} \times \mathbb{R}_+ \times \mathbb{R}^{2n+1} \times \mathbb{R}^{2n+1}\),

\[
\Psi = 0 \quad \text{and} \quad d_{w, \sigma} \Psi = 0
\]

and notice that \(\Phi:\) satisfies (3.43), (3.44) and (3.45) (see (3.52)), we can compute that at \((w, \sigma; x, y) = (0, 1, 0, 0) \in \mathbb{R}^{n+1} \times \mathbb{R}_+ \times \mathbb{R}^{2n+1} \times \mathbb{R}^{2n+1}\),

\[
(3.62) \quad \det \text{Hess}(\Psi) = \det \begin{bmatrix} 2i I_{2n} & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix} = -\det \begin{bmatrix} 2i I_{2n} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = (-1)^{n+1} 2^n,
\]

Hence, we can find a solution \(\tilde{W}(x', y)\) and \(\tilde{\Sigma}(x', y)\) near \(0 \in \mathbb{R}^{2n+1}\) and \(1 \in \mathbb{R}_+\) such that

\[
(3.63) \quad \frac{\partial \tilde{\Psi}}{\partial w}(\tilde{W}, \tilde{\Sigma}, x, y) = \frac{\partial \tilde{\Psi}}{\partial \sigma}(\tilde{W}, \tilde{\Sigma}, x, y) = 0.
\]

Note that \(\tilde{W}(x, y) = \tilde{W}(x', y)\) and \(\tilde{W}(x, y) = \tilde{\Sigma}(x', y)\) are independent of \(x_{2n+1}\). So by the stationary phase theorem of Melin–Sjöstrand, we get

\[
(3.64) \quad \int_0^\infty e^{it\Phi(x, y)} A(x, y, t)dt = \int_{D \times \mathbb{R}_+} e^{it\Psi(w, \sigma, x, y)} A(x, w, t)A(w, y, t\sigma)\lambda(w)dwd\sigma dt = \int_0^{+\infty} e^{it(-x_{2n+1}+\delta(x', \tilde{W}(x', y)))} B(x, y, t)dt,
\]

where

\[
(3.65) \quad B(x, y, t) \sim \sum_{j=0}^{\infty} B_j(x, y)t^{n-1} \quad \text{in} \quad S^m_{cl}(D \times D \times \mathbb{R}_+), \quad B_j(x, y) \in \mathcal{C}^\infty(D \times D), \quad \text{for every} \quad j \in \mathbb{N}_0.
\]

Since \(\tilde{W}(x', y), \tilde{\Sigma}(x', y)\) and \(A_j(x', y)\) are independent of \(x_{2n+1}\), for every \(j \in \mathbb{N}_0\), it is straightforward to see that up to \(O(|x - y|^N)\), for every \(N \in \mathbb{N}_0\), \(B_j(x, y)\) to be independent of \(x_{2n+1}\), for every \(j \in \mathbb{N}_0\). Hence,

\[
(3.66) \quad B_j(x, y) = B_j(x', y) + O(|x - y|^N), \quad \text{for every} \quad N \in \mathbb{N}, j \in \mathbb{N}_0.
\]
Also, observe that
\[
B_0(0, 0) = \det \left( \frac{\text{Hess}(\psi)}{2\pi i} \right)^{-\frac{1}{2}} A_0(0, 0)^2 \lambda(0)
\]
\[
= 2\pi^{n+1} \left( \frac{1}{2\pi^{n+1}} \right)^2 = \frac{1}{2\pi^{n+1}} = A_0(0, 0).
\]
(3.67)

For now \( \Pi = \Pi^2 \), we have
\[
\int_0^\infty e^{it(-x_{2n+1} + g(x', y))} A(x, y, t)dt \equiv \int_0^\infty e^{it(-x_{2n+1} + \tilde{g}(x', \tilde{W}(x', y)))} B(x, y, t)dt.
\]
Because of
\[
A_0(x, y)B_0(x, y) \neq 0,
\]
as in [12, Section 8], we can show that
\[
\tilde{g}(x', \tilde{W}(x', y)) = g(x', y) + O(|x - y|^N), \quad \text{for every } N \in \mathbb{N}_0.
\]
We may replace \( \tilde{g}(x', \tilde{W}(x', y)) \) by \( g(x', y) \) and we have
\[
\int_0^\infty e^{it\Phi(x, y)} A(x, y, t)dt \equiv \int_0^\infty e^{it\Phi(x, y)} B(x, y, t)dt \mod \mathcal{C}^\infty(D \times D).
\]

**Lemma 3.4.** With the notations used above, we have
\[
B_j(x, y) = A_j(x, y) + O(|x - y|^N), \quad \text{for every } N \in \mathbb{N}, j \in \mathbb{N}_0.
\]

**Proof.** We can repeat the procedure as in the discussion before (3.12) and conclude that
\[
B_0(x, y) - A_0(x, y) = h(x, y)(-x_{2n+1} + g(x', y)) + O(|x - y|^N), \quad \text{for every } N \in \mathbb{N}, j \in \mathbb{N}_0,
\]
where \( h(x, y) \in \mathcal{C}^\infty(D \times D) \). Take almost analytic extension and \( \hat{x}_{2n+1} = g(x', y) \) in (3.70), and notice that up to \( O(|x - y|^N) \), for every \( N \in \mathbb{N}_0 \), \( B_0(x, y) - A_0(x, y) \) is independent of \( x_{2n+1} \), we conclude that
\[
B_0(x, y) - A_0(x, y) = O(|x - y|^N), \quad \text{for every } N \in \mathbb{N}, j \in \mathbb{N}_0.
\]
(3.71)

From (3.71), we can repeat the procedure as in the discussion before (3.12) again and conclude that
\[
B_1(x, y) - A_1(x, y) = h_1(x, y)(-x_{2n+1} + g(x', y)) + O(|x - y|^N), \quad \text{for every } N \in \mathbb{N}, j \in \mathbb{N}_0,
\]
where \( h_1(x, y) \in \mathcal{C}^\infty(D \times D) \). Take almost analytic extension and \( \hat{x}_{2n+1} = g(x', y) \) in (3.72), and notice that up to \( O(|x - y|^N) \), for every \( N \in \mathbb{N}_0 \), \( B_1(x, y) - A_1(x, y) \) is independent of \( x_{2n+1} \), we conclude that
\[
B_1(x, y) - A_1(x, y) = O(|x - y|^N), \quad \text{for every } N \in \mathbb{N}, j \in \mathbb{N}_0.
\]
(3.72)

Continuing in this way, the lemma follows. \( \Box \)
3.3. Recursive formula between the first and the second coefficient. From (3.64), we see that
\[ t \int_{D \times \mathbb{R}_+} e^{it(\Phi(0,w) + \sigma \Phi(w,0))} A(0, w, t) A(w, 0, t\sigma) \lambda(w) dw d\sigma \]
\[ \sim B_0(0, 0) t^n + B_1(0, 0) t^{n-1} + \cdots. \]  
(3.73)

In this section, we will from the the asymptotic expansion (3.73) and Lemma 3.4 to get recursive formula between the first and the second coefficient.

Now, let
\[ F(\sigma, \sigma) := \Phi(0, w) + \sigma \Phi(w, 0) = g(0', w) + \sigma(-w_{2n+1} + g(w', 0)). \]
As (3.62) and the discussion before (3.62), we have \( (d_w F)(0, 1) = 0, (d_\sigma F)(0, 1) = 0 \) and
\[ \det \text{Hess}(F)(0, 1) = \det \begin{bmatrix} 2i l_{2n} & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix} = (-1)^{n+1} 2^n \]
(3.74)
and
\[ \text{Hess}(F)^{-1}(0, 1) = \begin{bmatrix} \frac{1}{2} l_{2n} & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix} \]
(3.75)
and
\[ \langle \text{Hess}(F)(0, 1)^{-1} D, D \rangle = 2i \sum_{j=1}^n \frac{\partial^2}{\partial z_j \partial \bar{z}_j} + 2 \frac{\partial^2}{\partial x_{2n+1} \partial \sigma} \]
(3.76)
where \( D := (-i \partial_{x_1}, \ldots, -i \partial_{x_{2n+1}}, -i \partial_{\sigma}) \). By Hörmander stationary phase formula Theorem 2.1,
\[ B_0(0, 0) t^n + B_1(0, 0) t^{n-1} + \cdots \sim t \int_{D \times \mathbb{R}_+} e^{iF(w, \sigma)} A(0, w, t) A(w, 0, t\sigma) \lambda(w) dw d\sigma \]
\[ \sim e^{iF(0, 1)} \det \left( \frac{i \text{Hess}(F)(0, 1)}{2 \pi i} \right)^{-\frac{3}{2}} \sum_{j=0}^{\infty} t^{-j} P_j \]
(3.77)
\[ \sim 2\pi^{n+1} (t^n P_0 + t^{n-1} P_1 + \cdots), \]
(3.78)
where
\[ P_0 = A_0(0, 0)^2 \lambda(0) \]
(3.79)
and
\[ P_1 = \sum_{0 \leq \mu \leq 2} \frac{i^{-1}}{\mu!(\mu + 1)!} \left( i \sum_{j=1}^n \frac{\partial^2}{\partial z_j \partial \bar{z}_j} + \frac{\partial^2}{\partial x_{2n+1} \partial \sigma} \right)^{\mu+1} (G^{\mu}(x, \sigma) A_0(0, x) A_0(x, 0) \lambda(x) \sigma^n) (0, 1) \]
\[ + 2 A_0(0, 0) A_1(0, 0) \lambda(0), \]
(3.80)
and
\[ G(x, \sigma) := F(x, \sigma) - F(0, 1) - \frac{1}{2} \left< \text{Hess}(F)(0, 1) \begin{pmatrix} x \\ \sigma - 1 \end{pmatrix}, \begin{pmatrix} x \\ \sigma - 1 \end{pmatrix} \right> \]
\[ = F(x, \sigma) - \frac{1}{2} \left< \text{Hess}(F)(0, 1) \begin{pmatrix} x \\ \sigma - 1 \end{pmatrix}, \begin{pmatrix} x \\ \sigma - 1 \end{pmatrix} \right> \]
(3.81)
satisfying
\begin{equation}
\frac{\partial^{\alpha} G}{\partial x^{\alpha_1} \partial \sigma^{\alpha_2}}(0, 1) = 0 \quad \text{for all } \alpha_1 \in \mathbb{N}_0^{2n+1}, \alpha_2 \in \mathbb{N}_0, |\alpha| = |\alpha_1| + |\alpha_2| \leq 2.
\end{equation}

Also, from Proposition 3.2 and (3.52), we can find that
\begin{equation}
\frac{\partial^{\alpha} G}{\partial x^{\alpha}}(0, 1) = \frac{\partial^{\alpha}}{\partial x^{\alpha}} (\Phi(0, x) + \Phi(x, 0)) \bigg|_{x=0} = 0, \quad \text{for all } \alpha \in \mathbb{N}_0^{2n+1}, |\alpha| = 3.
\end{equation}

Also, observe that
\begin{equation}
\frac{\partial^{\alpha} G}{\partial \sigma^{\alpha}}(0, 1) = 0, \quad \text{for all } \alpha \in \mathbb{N}_0, |\alpha| \geq 2.
\end{equation}

We now calculate each terms in $P_1$: For $\mu = 0$ in the summation, the summand is
\begin{equation}
\frac{1}{i} \left( \sum_{j=1}^{n} \frac{\partial^2}{\partial z_j \partial \bar{z}_j} + \frac{\partial^2}{\partial x_{2n+1} \partial \sigma} \right) (A_0(0, x) A_0(x, 0) \lambda(x) \sigma^n) (0, 1);
\end{equation}
for $\mu = 1$ in the summation, the summand is
\begin{equation}
\frac{1}{2i} \left( - \sum_{j,k=1}^{n} \frac{\partial^4}{\partial z_j \partial \bar{z}_j \partial z_k \partial \bar{z}_k} + 2i \sum_{j,k=1}^{n} \frac{\partial^4}{\partial z_j \partial \bar{z}_j \partial x_{2n+1} \partial \sigma} + \frac{\partial^4}{\partial x_{2n+1}^2 \partial \sigma^2} \right)
\end{equation}
acting on
\begin{equation}
G(x, \sigma) A_0(0, x) A_0(x, 0) \lambda(x) \sigma^n
\end{equation}
valuing at $(x, \sigma) = (0, 1)$; and for $\mu = 2$, the summand is
\begin{equation}
\frac{1}{12i} \left( -i \sum_{j,k,l=1}^{n} \frac{\partial^6}{\partial z_j \partial \bar{z}_j \partial z_k \partial \bar{z}_k \partial z_l \partial \bar{z}_l} - 3 \sum_{j,k,l=1}^{n} \frac{\partial^6}{\partial z_j \partial \bar{z}_j \partial z_k \partial \bar{z}_k \partial x_{2n+1} \partial \sigma} + 3i \sum_{j,k,l=1}^{n} \frac{\partial^6}{\partial z_j \partial \bar{z}_j \partial x_{2n+1}^2 \partial \sigma^2} + \frac{\partial^6}{\partial x_{2n+1}^3 \partial \sigma^3} \right)
\end{equation}
acting on
\begin{equation}
G^2(x, \sigma) A_0(0, x) A_0(x, 0) \lambda(x) \sigma^n
\end{equation}
valuing at $(x, \sigma) = (0, 1)$. Thus, by Proposition 3.1, Proposition 3.2, (3.52), (3.82), (3.83) and (3.84), also with (3.58) and Lemma 3.4, it is straightforward to check that
\begin{equation}
P_1 = A_0(0, 0)^2 \left[ \left( \sum_{j=1}^{n} \frac{\partial^2 \lambda}{\partial z_j \partial \bar{z}_j} \right)(0) + \frac{i}{2} \lambda(0) \sum_{j,k=1}^{n} \frac{\partial^4 (g(z, 0) + g(0, z))}{\partial z_j \partial \bar{z}_j \partial z_k \partial \bar{z}_k} (0, 0) \right]
+ 2A_0(0, 0) A_1(0, 0) \lambda(0).
\end{equation}

From (3.42), (3.44), (3.52) and notice that $A_0(0, 0) = \frac{1}{2\pi^{n+1}}$, we can rewrite (3.85):
\begin{equation}
P_1 = \frac{1}{(2\pi^{n+1})^2} \left[ \sum_{j=1}^{n} \left( \frac{\partial^2 \lambda}{\partial z_j \partial \bar{z}_j} \right)(0) + \sum_{j,k=1}^{n} \frac{\partial^4 R}{\partial z_j \partial \bar{z}_j \partial z_k \partial \bar{z}_k}(0) \right] + \frac{1}{\pi^{n+1}} A_1(0, 0),
\end{equation}
where $R$ is as in (3.44). From Lemma 3.4 and (3.77), we get
\begin{equation}
A_1(0, 0) = B_1(0, 0) = 2\pi^{n+1} P_1.
\end{equation}
From this observation and (3.86), we get
\[ A_1(0, 0) = B_1(0, 0) \]
\[ = 2\pi r^{n+1} P_1 \]
(3.87)
\[ = \frac{1}{2\pi r^{n+1}} \left[ \sum_{j=1}^{n} \left( \frac{\partial^2 \lambda}{\partial z_j \partial\bar{z}_j} \right)(0) + \sum_{j,k=1}^{n} \frac{\partial^4 R}{\partial z_j \partial\bar{z}_j \partial z_k \partial\bar{z}_k}(0) \right] + 2A_1(0, 0). \]
So we need to calculate
(3.88)
\[ A_1(0, 0) = -\frac{1}{2\pi r^{n+1}} \left[ \sum_{j=1}^{n} \left( \frac{\partial^2 \lambda}{\partial z_j \partial\bar{z}_j} \right)(0) + \sum_{j,k=1}^{n} \frac{\partial^4 R}{\partial z_j \partial\bar{z}_j \partial z_k \partial\bar{z}_k}(0) \right] \]
in the final subsection.

3.4. Calculation by geometric invariance. In this section, we calculate each term in (3.88) by the geometric invariance on X. We will continue work with local coordinates \( x = (x_1, \ldots, x_{2n+1}) \) as (3.35). We first calculate the Tanaka–Webster scalar curvature in terms of the coordinates \( x = (x_1, \ldots, x_{2n+1}) \). Recall that from Proposition 3.1
(3.89)
\[ \omega_0(x) = dx_{2n+1} - i \sum_{j=1}^{n} \left( \frac{\partial R}{\partial z_j} dz_j - \frac{\partial R}{\partial\bar{z}_j} d\bar{z}_j \right) + O(|x|^4), \]

(3.90)
\[ d\omega_0(x) = 2i \sum_{j,k=1}^{n} \frac{\partial^2 R}{\partial z_j \partial\bar{z}_k} dz_j \wedge d\bar{z}_k + O(|x|^3), \]

(3.91)
\[ T(x) = -\frac{\partial}{\partial x_{2n+1}} + O(|x|^2), \]

(3.92)
\[ T^1 X = \text{span} \{ L_j \}_{j=1}^n := \text{span} \left\{ \frac{\partial}{\partial z_j} + i \frac{\partial R}{\partial z_j} \frac{\partial}{\partial x_{2n+1}} + O(|x|^4) \right\}, \]

Write \( \nabla L_j = \Gamma^i_{ij} L_i \), where \( \nabla \) denotes the Tanaka–Webster connection (see Proposition 2.1). Recall that from [18, Lemma 3.2],
(3.93)
\[ d\omega_0 (\nabla L_j, L_k) = L_i (d\omega_0 (L_j, L_k)) - d\omega_0 (L_i, [L_j, L_k]_{T^1 X}). \]

Directly,
(3.94)
\[ d\omega_0 (\nabla L_j, L_k) = d\omega_0 (\Gamma^i_{ij} L_i, L_k) = 2\Gamma^i_{ij} \frac{\partial^2 R}{\partial z_i \partial\bar{z}_j} + O\left(|x|^3\right), \]

(3.95)
\[ L_i (d\omega_0 (L_j, L_k)) = 2 \left( i \frac{\partial^3 R}{\partial z_i \partial z_j \partial\bar{z}_k} - \frac{\partial R}{\partial z_i} \frac{\partial^3 R}{\partial x_{2n+1} \partial z_j \partial\bar{z}_k} \right) + O\left(|x|^3\right), \]

\[ [L_i, L_k] = \left[ \frac{\partial}{\partial z_i} + i \frac{\partial R}{\partial z_i} \frac{\partial}{\partial x_{2n+1}} + O(|x|^4), \frac{\partial}{\partial\bar{z}_k} - i \frac{\partial R}{\partial\bar{z}_k} \frac{\partial}{\partial x_{2n+1}} + O(|x|^4) \right] \]
\[ = \left( \frac{\partial R}{\partial z_i} \frac{\partial^2 R}{\partial\bar{z}_k \partial x_{2n+1}} - \frac{\partial R}{\partial\bar{z}_k} \frac{\partial^2 R}{\partial z_i \partial x_{2n+1}} - 2i \frac{\partial^2 R}{\partial z_i \partial\bar{z}_k} \right) \frac{\partial}{\partial x_{2n+1}} + O(|x|^3), \]
and hence
\begin{equation}
\tag{3.96}
d\omega_0 \left( L_j, [L_j, T_k] \right)_{\mathcal{T}^0} = O(|x|^3).
\end{equation}
Accordingly, by (3.36), for all $i, j, k = 1, \cdots, n$,
\begin{equation}
\tag{3.97}
\Gamma^k_{ij}(0) = 0.
\end{equation}
Moreover, by taking $\frac{\partial}{\partial z_h}$ both sides in (3.93), from (3.36), (3.94), (3.95) and (3.96), it is not difficult to check that
\begin{equation}
\tag{3.98}
\frac{\partial \Gamma^k_{ij}}{\partial z_h}(0) = -2 \frac{\partial^4 R}{\partial z_l \partial z_l \partial z_k \partial z_h}(0).
\end{equation}
Now, let $\{\theta^a\}_{j=1}^n$ and $\{\theta^{b\bar{\alpha}}\}_{j=1}^n$ be the dual frame of $\{L_{\alpha}\}_{j=1}^n$ and $\{T_{\beta}\}_{j=1}^n$, respectively. Denote
\begin{equation*}
\nabla L_{\alpha} = \omega^\beta_{\alpha} \otimes L_{\beta},
\end{equation*}
and we can check that the (1, 1) part of $d\omega^\beta_{\alpha}$ is
\begin{equation*}
- \sum_{k,l=1}^n \left( L_l \Gamma^\beta_{k\alpha} \right) \theta^k \wedge \theta^l + O(|x|),
\end{equation*}
and the (1, 1) part of $\Theta^\beta_{\alpha} = d\omega^\beta_{\alpha} - \omega^\gamma_{\alpha} \wedge \omega^\beta_{\gamma}$ denoted by
\begin{equation*}
\sum_{k,l=1}^n R^{\beta}_{\alpha kl} \theta^k \wedge \theta^l
\end{equation*}
equals the (1, 1) part of $d\omega^\beta_{\alpha}$. Hence the pseudohermitian Ricci curvature tensor at origin is
\begin{equation}
R_{\alpha l}(0) = \sum_{k=\beta=1}^n R^{\beta}_{\alpha kl}(0) = - \sum_{k=\beta=1}^n \frac{\partial \Gamma^\beta_{k\alpha}}{\partial z_l}(0) = 2 \sum_{k=1}^n \frac{\partial^4 R}{\partial z_k \partial z_k \partial z_{\alpha} \partial z_l}(0).
\end{equation}
Also, for
\begin{equation*}
-d\omega_0 = ig_{\alpha \bar{\beta}} \theta^\alpha \wedge \theta^{\bar{\beta}},
\end{equation*}
we can find that $\theta^\alpha(0) = dz_{\alpha}$ and $\theta^{\bar{\beta}}(0) = d\bar{z}_{\bar{\beta}}$, and
\begin{equation*}
g_{\alpha \bar{\beta}}(0) = \delta_{\alpha \bar{\beta}}.
\end{equation*}
Let $g^{cd}$ be the inverse matrix of $g_{ab}$. We have $g^{cd}(0) = \delta_{cd}$ and the Tanaka–Webster scalar curvature at the origin is
\begin{equation}
\tag{3.99}
R_{\text{scal}}(0) = g^{\alpha \bar{\beta}} R_{\alpha \bar{\beta}}(0) = 2 \sum_{l=1}^n \sum_{k=1}^n \frac{\partial^4 R}{\partial z_l \partial z_l \partial z_k \partial z_k}(0).
\end{equation}
Finally, for the volume form
\begin{equation*}
\lambda(x) dx := \frac{1}{n!} \left( \frac{-d\omega_0}{2} \right)^n \wedge \omega_0,
\end{equation*}
we have the expression

\[ (3.100) \]
\[
\frac{1}{n!} \left( \sum_{j,k=1}^{n} i \frac{\partial^2 R}{\partial z_j \partial \bar{z}_k} dz_j \wedge d\bar{z}_k + O(|x|^3) \right)^n \wedge \left( dx_{2n+1} - i \sum_{j=1}^{n} \left( \frac{\partial R}{\partial z_j} dz_j - \frac{\partial R}{\partial \bar{z}_j} d\bar{z}_j \right) + O(|x|^4) \right)
\]
\[
= \frac{1}{n!} \left( \sum_{j,k=1}^{n} -2 \frac{\partial^2 R}{\partial z_j \partial \bar{z}_k} - 2i + O(|x|^3) \right)^n \wedge \left( dx_{2n+1} - i \sum_{j=1}^{n} \left( \frac{\partial R}{\partial z_j} dz_j - \frac{\partial R}{\partial \bar{z}_j} d\bar{z}_j \right) + O(|x|^4) \right).
\]

From Proposition 3.1, we can check that

\[ (3.101) \]
\[
\frac{\partial^2 \lambda}{\partial z_i \partial \bar{z}_j}(0) = (-2)^n \left( -\frac{1}{2} \right)^{n-1} \sum_{j=1}^{n} \frac{\partial^4 R}{\partial z_j \partial \bar{z}_j \partial \bar{z}_j \partial z_j}(0) = -2 \sum_{j=1}^{n} \frac{\partial^4 R}{\partial z_j \partial \bar{z}_j \partial \bar{z}_j \partial z_j}(0).
\]

From (3.88), (3.99) and (3.101), we conclude that

\[ (3.102) \]
\[
A_1(0,0) = \frac{1}{4\pi^{n+1}} R_{\text{scal}}(0).
\]

Thus, the proof for (2) in Theorem 1.2 is completed for the point-wise equation (3.102) holds for all \( x_0 \in D \) and \( R_{\text{scal}} \) is globally well-defined on whole \( X \), and in particular on \( D \).

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