EXTREMAL METRICS FOR THE Q'-CURVATURE IN THREE DIMENSIONS

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Abstract. We construct contact forms with constant Q'-curvature on compact three-dimensional CR manifolds which admit a pseudo-Einstein contact form and satisfy some natural positivity conditions. These contact forms are obtained by minimizing the CR analogue of the II-functional from conformal geometry. Two crucial steps are to show that the P'-operator can be regarded as an elliptic pseudodifferential operator and to compute the leading order terms of the asymptotic expansion of the Greens function for $\sqrt{P'}$.

1. Introduction

The geometry of CR manifolds is studied via a choice of contact form and the induced Levi form. A natural question is whether there are preferred choices of contact form. One such choice is a CR Yamabe contact form, which has the property that the pseudohermitian scalar curvature is constant. Such contact forms exist on all compact CR manifolds [10, 13, 14, 24, 25]. Another such choice is a pseudo-Einstein contact form with constant Q'-curvature [6, 17]. The primary goal of this article is to show that the latter class of contact forms always exist in dimension three under natural positivity assumptions.

The idea of the Q'-curvature arose in the work of Branson, Fontana and Morpurgo [4] on Moser–Trudinger and Beckner–Onofri inequalities on the CR spheres. On any even-dimensional Riemannian manifold (M^n, g), the critical GJMS operator P_n is a conformally covariant differential operator P_n with leading order term $(-\Delta)^{n/2}$ which controls the behavior of the critical Q-curvature Q_n within a conformal class (cf. [3]). Specializing to the case of the standard n-sphere (S^n, g_0) in even dimensions, Beckner [1] and, via different techniques, Chang and the third-named author [8], used these objects to establish the Beckner–Onofri inequality:

$$\int_{S^n} w\, P_n w + 2\int_{S^n} Q_n w - \frac{2}{n}\left(\int_{S^n} Q_n\right)\log \fint_{S^n} e^{nw} \geq 0 \tag{1.1}$$

for all $w \in W^{n/2,2}$ and for Q_n an explicit (nonzero) dimensional constant, where $\fint$ denotes the average operator. Moreover, equality holds in (1.1) if and only if $e^{2w}g_0$ is Einstein, or equivalently, if and only if $e^{2w}g_0 = \Phi^* g_0$ for Φ an element of the conformal transformation group of S^n.

Branson, Fontana and Morpurgo investigated to what extent the above discussion holds on the standard CR spheres (S^{2n+1}, θ_0). While it has long been known that there is a CR covariant operator P_n with leading order term $(-\Delta_b)^{n+1}$, this

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operator has an infinite-dimensional kernel, namely the space $\mathcal{P}$ of CR pluriharmonic functions [15]. For this reason one does not expect P_n to give rise to a CR analogue of the sharp Beckner–Onofri inequality (1.1). Instead, Branson, Fontana and Morpurgo [4] observed that there is another operator P_n', defined only on $\mathcal{P}$, with all of the desired properties. That is, P_n' has leading term $(-\Delta_b)^{n+1}$, is CR covariant, and there is a (nonzero) dimensional constant Q_n' such that

$$\int_{S^{2n+1}} w\,P_n'w + 2\int_{S^{2n+1}} Q_n'w - \frac{2}{n+1}\left(\int_{S^{2n+1}} Q_n'\right)\log ⨍_{S^{2n+1}} e^{(n+1)w} \geq 0 \tag{1.2}$$

for all $w \in W^{n+1,2}\cap\mathcal{P}$. Moreover, equality holds in (1.2) if and only if $e^{2w}\theta_0$ is pseudo-Einstein and torsion-free, or equivalently, if and only if $e^{2w}\theta_0 = \Phi^*\theta_0$ for Φ a CR automorphism of S^{2n+1}.

In light of (1.1), it is natural to seek metrics of constant Q-curvature within a given conformal class on an even-dimensional Riemannian manifold. This question has been intensively studied in four dimensions. In particular, Chang and the third-named author [8] showed that on any compact Riemannian four-manifold (M^4,g) for which the Paneitz operator P_4 is nonnegative with trivial kernel and for which $\int Q_4 < 16\pi^2$, one can construct a metric $\hat{g} := e^{2w}g$ for which $\hat{Q}_4$ is constant by minimizing the functional

$$II(w) := \int_M w\,P_4w + 2\int_M Q_4w - \frac{1}{2}\left(\int_M Q_4\right)\log ⨍_M e^{4w}.$$

This construction, and various modifications of it, have played an important role in studying the geometry of four-manifolds; see [7] for further discussion.

The purpose of this article is to show that one can similarly construct contact forms with constant Q'-curvature on a compact three-dimensional CR manifold under natural positivity assumptions. To explain this, let us first recall the essential features of the Q'-curvature [6]. On any pseudohermitian three-manifold (M^3,θ), there is a differential operator $P_4'\colon\mathcal{P}\to C^\infty(M)$ defined on the space $\mathcal{P}$ of CR pluriharmonic functions with the properties that P_4' has leading term Δ_b^2, is symmetric in the sense that the pairing $(u,v)\mapsto\int u\,P_4'v$ is symmetric on $\mathcal{P}$, and satisfies the transformation formula

$$e^{2w}\hat{P}_4'(u) = P_4'(u) \mod \mathcal{P}^\perp$$

for all $u\in\mathcal{P}$, where $w\in C^\infty(M)$ and $\hat{P}_4'$ is defined in terms of $\hat{\theta}=e^w\theta$. The analytic properties of the P'-operator are improved by projecting onto $\mathcal{P}$. As we will see, if $\tau\colon C^\infty(M)\to\mathcal{P}$ is the orthogonal projection, then the operator $\overline{P}_4' := \tau P_4'\colon\mathcal{P}\to\mathcal{P}$ is a formally self-adjoint elliptic pseudodifferential operator. Most of the work of this article is dedicated to proving this fact and establishing asymptotic estimates for the Green function of $\overline{P}_4'$. Once this is accomplished, the argument [8] showing existence of a smooth minimizer of the II-functional on four-manifolds can be adapted to CR manifolds.

In general, one cannot associate an analogue of the Q-curvature to P_4'. However, one can do so when restricting to pseudo-Einstein contact forms. A contact form θ on M^3 is pseudo-Einstein if its scalar curvature R and torsion A_{11} satisfy the relation $\nabla_1R = i\nabla^1A_{11}$. This is equivalent to requiring that θ is locally volume-normalized with respect to a nonvanishing closed $(2,0)$-form [16]; such contact forms always exist on boundaries of domains in $\mathbb{C}^2$ [11]. For pseudo-Einstein contact forms, one can define a scalar invariant Q_4' which satisfies a simple transformation rule in terms of P_4' and the CR Paneitz operator P_4 upon changing the choice of pseudo-Einstein contact forms. In particular, $\int Q_4'$ is an invariant of the class of pseudo-Einstein contact forms. For boundaries of domains, it is a biholomorphic invariant; indeed, it is the Burns–Epstein invariant [5, 6].

Suppose that θ is a pseudo-Einstein contact form on M^3. Then $\hat{\theta} = e^w\theta$ is pseudo-Einstein if and only if w is a CR pluriharmonic function [16]. In particular, it makes sense to consider the transformation formula for the Q'-curvature, and one obtains

$$e^{2w}\hat{Q}_4' = Q_4' + P_4'(w) \mod \mathcal{P}^\perp$$

(see [6]). It is thus natural to consider the scalar quantity $\overline{Q}_4' := \tau Q_4'$. In particular, on the standard CR three-sphere, $\overline{P}_4'$ is precisely the operator considered by Branson, Fontana and Morpurgo [4] and $\overline{Q}_4'$ is precisely the constant in (1.2).

We construct contact forms for which $\overline{Q}_4'$ is constant by constructing minimizers of the II-functional $II\colon \mathcal{P} \to \mathbb{R}$ given by

$$II(w) = \int_M w\, P_4' w + 2\int_M Q_4' w - \left(\int_M Q_4'\right)\log \fint_M e^{2w} \tag{1.3}$$

on a pseudo-Einstein three-manifold (M^3, θ). In general the II-functional is not bounded below. However, under natural positivity conditions it is bounded below and coercive, in which case we can construct the desired minimizers.

Theorem 1.1. *Let (M^3, θ) be a compact, embeddable pseudo-Einstein three-manifold such that the P'-operator $\overline{P}_4'$ is nonnegative and $\ker \overline{P}_4' = \mathbb{R}$. Suppose additionally that*

$$\int_M \overline{Q}_4' < 16\pi^2. \tag{1.4}$$

Then there exists a function $w \in \mathcal{P}$ which minimizes the II-functional (1.3)*. Moreover, the contact form $\hat{\theta} := e^w\theta$ is such that $\hat{\overline{Q}}_4'$ is constant.*

The assumptions of Theorem 1.1 can be replaced by the assumptions that the CR Paneitz operator is nonnegative and there exists a pseudo-Einstein contact form with scalar curvature nonnegative but not identically zero. Note that this last assumption implies that the CR Yamabe constant is positive; it would be interesting to know if these conditions are equivalent. Chanillo, Chiu and the third-named author proved [9] that these assumptions imply that M^3 is embeddable. The first- and third-named authors proved [6] that these assumptions imply both that $\overline{P}_4' \geq 0$ with $\ker \overline{P}_4' = \mathbb{R}$ and that $\int \overline{Q}_4' \leq 16\pi^2$ with equality if and only if M^3 is CR equivalent to the standard CR three-sphere. Branson, Fontana and Morpurgo proved [4] Theorem 1.1 on the standard CR three-sphere. In summary, Theorem 1.1 implies the following result.

Corollary 1.2. *Let (M^3, θ) be a compact pseudo-Einstein manifold with nonnegative CR Paneitz operator which admits a pseudo-Einstein contact form with positive scalar curvature. Then there exists a function $w \in \mathcal{P}$ which minimizes the II-functional* (1.3)*. Moreover, the contact form $\hat{\theta} := e^w\theta$ is such that $\hat{\overline{Q}}_4'$ is constant.*

Note that the assumptions of Theorem 1.1 are all CR invariant; in particular, if M^3 is the boundary of a domain in $\mathbb{C}^2$, the assumptions are biholomorphic invariants. Note also that the conclusion that $\hat{\overline{Q}}_4'$ is constant cannot be strengthened to the conclusion that $\hat{Q}_4'$ is constant: In Section 5, we classify the contact forms on $S^1 \times S^2$ with its flat CR structure which have $\overline{Q}_4'$ constant, and observe that Q_4' is nonconstant for all of them.

The proof of Theorem 1.1 is analogous to the corresponding result in four-dimensional conformal geometry [8], though there are many new difficulties we must overcome. Since we are minimizing within $\mathcal{P}$, there is a Lagrange multiplier in the Euler equation for the II-functional which lives in the orthogonal complement $\mathcal{P}^\perp$ to $\mathcal{P}$. This is avoided by working with $\overline{P}_4'$. The greater difficulty is to show that minimizers for the II-functional exist in $W^{2,2} \cap \mathcal{P}$ under the hypotheses of Theorem 1.1. This is achieved by showing that $\overline{P}_4'$ satisfies a Moser–Trudinger-type inequality with the same constant as on the standard CR three-sphere under the positive assumption on $\overline{P}_4'$ and (1.4).

To prove that $\overline{P}_4'$ satisfies the above Moser–Trudinger-type inequality, we study the asymptotics of the Green function of $\left(\overline{P}_4'\right)^{1/2}$ in enough detail to apply the general results of Fontana and Morpurgo [12]. To make this precise, we require some more notation. Fix $\zeta \in M$ and let (z,t) be CR normal coordinates [25] in a neighborhood of ζ such that $(z(\zeta), t(\zeta)) = (0,0)$. Define $\rho^4(z,t) = |z|^4 + t^2$. For $m \in \mathbb{R}$, let

$$\mathcal{E}(\rho^m) = \left\{ g \in C^\infty(M \setminus \{\zeta\}) \colon |\partial_z^p \partial_{\bar z}^q \partial_t^r g(z,t)| \leq \rho(z,t)^{m-p-q-2r} \text{ near } \zeta \right\}.$$

The asymptotics of the Green function of $\left(\overline{P}_4'\right)^{1/2}$ are as follows.

Theorem 1.3. *Let (M^3, θ) be a compact embeddable pseudohermitian manifold such that P_4' is nonnegative. Fix $\zeta \in M$ and let G_ζ be the Green function for $\left(\overline{P}_4'\right)^{1/2}$ with pole at ζ. Then there is a function $B_\zeta \in C^\infty(M \setminus \{\zeta\})$ such that*

$$B_\zeta - \rho^{-2} \in \mathcal{E}\left(\rho^{-1-\varepsilon}\right)$$

for all $0 < \varepsilon < 1$ and

$$G_\zeta = \tau B_\zeta \tau.$$

We now outline the main argument used in the proof of Theorem 1.3. Fix a point $\zeta \in M$, the Green function of $\left(\overline{P}_4'\right)^{1/2}$ at ζ is given by

$$G_\zeta = \left(\overline{P}_4'\right)^{-\frac{1}{2}} \tau \delta_\zeta \tau.$$

Using standard argument in spectral theory, we observe that

$$\left(\overline{P}_4'\right)^{-\frac{1}{2}} = c \int_0^\infty t^{-\frac{1}{2}} \left(\overline{P}_4' + t + \pi\right)^{-1} dt \tag{1.5}$$

on $(\ker \overline{P}_4')^\perp \cap \hat{\mathcal{P}}$, where $\hat{\mathcal{P}}$ is the space of L^2 CR pluriharmonic functions, $\pi \colon \hat{\mathcal{P}} \to \ker \overline{P}_4'$ is the orthogonal projection, and $c^{-1} = \int_0^\infty t^{-\frac{1}{2}}(1+t)^{-1} dt$. Theorem 1.3 then follows from asymptotic expansions for $t^{-\frac{1}{2}}\left(\overline{P}_4' + t + \pi\right)^{-1}$. By using Boutet de Monvel–Sjöstrand's classical theorem for the Szegő kernel [2], we first show that $\overline{P}_4' = \tau E_2$ for E_2 a classical elliptic pseudodifferential operator on M of order 2. This allows us to apply classical theory of pseudodifferential operators to find a pseudodifferential operator G_t of order -2 depending continuously on t such that $(E_2 + t)G_t = I + F_t$, where F_t is a smoothing operator depending continuously on t and $|F_t(x,y)|_{C^m(M\times M)} \lesssim \frac{1}{1+t}$ for all $m\in\mathbb{N}$. Roughly speaking, $\tau G_t\tau$ is the leading term of the operator $\left(\overline{P}_4'+t+\pi\right)^{-1}$. By carefully studying the principal symbol and t-behavior of G_t, we can show that $G:=c\int_0^\infty t^{-\frac{1}{2}}\tau G_t\tau$ is a smoothing operator of order 2 with $G\tau\delta_\zeta\tau=\rho^{-2} \mod \mathcal{E}\left(\rho^{-1-\varepsilon}\right)$, for every $\varepsilon>0$.

This article is organized as follows. In Section 2 we review some basic concepts from pseudohermitian geometry and the definitions of the P'-operator and the Q'-curvature. In Section 3 we use Theorem 1.3 to show that $\left(\overline{P}_4'\right)^{1/2}$ satisfies a sharp Moser–Trudinger-type inequality. In Section 4 we prove Theorem 1.1. In Section 5 we show that there is no pseudo-Einstein contact form on $S^1\times S^2$ for which Q_4' is constant. The remaining sections are devoted to the proof of Theorem 1.3. In Section 6 we review some basic concepts about pseudodifferential operators and Fourier integral operators. In Section 7 we recall some properties of the orthogonal projection τ established in [21]. In Section 8 we establish some properties of the principal symbol of $\tau\Delta_b\tau$. The remaining sections focus on developing the tools to prove Theorem 1.3. In Section 9 we establish some properties of $\left(\overline{P}_4'\right)^{-1/2}$, in particular (1.5). In Section 10 we establish some smoothing properties of compositions SP_t of the Szegő projection with a t-dependent family of pseudodifferential operators. In Section 10 we identify the leading order term of $\left(\overline{P}_4'\right)^{-1/2}$. In Section 12 we prove Theorem 1.3.

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2. Preliminaries from pseudohermitian geometry

In this section we summarize some important concepts in pseudohermitian geometry as are needed to study the P'-operator and the Q'-curvature in dimension three.

Let M^3 be a smooth, oriented (real) three-dimensional manifold. A *CR structure* on M is a one-dimensional complex subbundle $T^{1,0}M=T^{1,0}\subset T_{\mathbb{C}}M:=TM\otimes\mathbb{C}$ such that $T^{1,0}\cap T^{0,1}=\{0\}$ for $T^{0,1}:=\overline{T^{1,0}}$. Let $H=\operatorname{Re}T^{1,0}$ and let $J\colon H\to H$ be the almost complex structure defined by $J(V+\bar{V})=i(V-\bar{V})$. Put $H_{\mathbb{C}}=H\times\mathbb{C}$.

Let θ be a *contact form* for $(M^3$; i.e. θ is a nonvanishing real one-form such that $\ker\theta=H$. Since M is oriented, a contact form always exists, and is determined up to multiplication by a positive real-valued smooth function. We say that $(M^3,T^{1,0}M)$ is *strictly pseudoconvex* if the *Levi form* $d\theta(\cdot,J\cdot)$ on $H\otimes H$ is positive definite for some, and hence any, choice of contact form θ. We shall always assume that our CR manifolds are strictly pseudoconvex. Take $\theta\wedge d\theta$ to be the volume form on M, we then get natural L^2 inner product $(\,\cdot\,,\cdot\,)$ on $C^\infty(M)$.

A *pseudohermitian manifold* is a pair (M^3,θ) consisting of a CR manifold and a contact form. The *Reeb vector field* T is the vector field such that $\theta(T)=1$ and $d\theta(T,\cdot)=0$. A $(1,0)$*-form* is a section of $T^*_{\mathbb{C}}M$ which annihilates $T^{0,1}$. An *admissible coframe* is a nonvanishing $(1,0)$-form θ^1 in an open set $U\subset M$ such that $\theta^1(T)=0$. Let $\theta^{\bar{1}}:=\overline{\theta^1}$ be its conjugate. Then $d\theta=ih_{1\bar{1}}\theta^1\wedge\theta^{\bar{1}}$ for some positive function $h_{1\bar{1}}$. The function $h_{1\bar{1}}$ is equivalent to the Levi form.

The *connection form* ${\omega_1}^1$ and the *torsion form* $\tau_1 = A_{11}\theta^1$ determined by an admissible coframe θ^1 are uniquely determined by

$$d\theta^1 = \theta^1 \wedge {\omega_1}^1 + \theta \wedge \tau^1,$$
$$\omega_{1\bar{1}} + \omega_{\bar{1}1} = dh_{1\bar{1}},$$

where we use $h_{1\bar{1}}$ to raise and lower indices as normal; e.g. $\tau^1 = h^{1\bar{1}}\tau_{\bar{1}}$ for $h^{1\bar{1}} = (h_{1\bar{1}})^{-1}$. The connection forms determine the *pseudohermitian connection* ∇ by

$$\nabla Z_1 := {\omega_1}^1 \otimes Z_1$$

and $\nabla T = 0$, where $\{Z_1, Z_{\bar{1}}, T\}$ is the dual basis to $\{\theta^1, \theta^{\bar{1}}, \theta\}$. The *scalar curvature* R of θ is given by the expression

$$d{\omega_1}^1 = R\theta^1 \wedge \theta^{\bar{1}} \mod \theta.$$

A (real-valued) function $w \in C^\infty(M)$ is *CR pluriharmonic* if locally $w = \operatorname{Re} f$ for some (complex-valued) function $f \in C^\infty(M, \mathbb{C})$ satisfying $Z_{\bar{1}} f = 0$. Equivalently, w is a CR pluriharmonic function if

$$\nabla_1\nabla_1\nabla^1 w + iA_{11}\nabla^1 w = 0$$

for $\nabla_1 := \nabla_{Z_1}$ (cf. [26]). We denote by $\mathcal{P}$ the space of all CR pluriharmonic functions.

Take $\theta \wedge d\theta$ to be the volume form on M. This induces a natural inner product $(\cdot,\cdot)$ on $C^\infty(M)$. Let $L^2(M)$ and $\hat{\mathcal{P}}$ denote the completions of $C^\infty(M)$ and $\mathcal{P}$, respectively, with respect to this inner product.

The *Paneitz operator* P_4 is the differential operator

$$\begin{aligned} P_4(f) &:= 4\nabla^1\left(\nabla_1\nabla_1\nabla^1 f + iA_{11}\nabla^1 f\right) \\ &= \Delta_b^2 f + T^2 f - 4\operatorname{Im}\nabla^1\left(A_{11}\nabla^1 f\right) \end{aligned}$$

for $\Delta_b := \nabla^1\nabla_1 + \nabla^{\bar{1}}\nabla_{\bar{1}}$ the *sublaplacian*. Note in particular that $\mathcal{P} \subset \ker P_4$. A key property of the Paneitz operator is that it is CR covariant; if $\hat{\theta} = e^w\theta$, then $e^{2w}\hat{P}_4 = P_4$ (cf. [16]).

Definition 2.1. Let (M^3, θ) be a pseudohermitian manifold. The *P'-operator* $P' \colon \mathcal{P} \to C^\infty(M)$ is defined by

$$\begin{aligned} P_4' w &= 4\Delta_b^2 w - 8\operatorname{Im}\left(\nabla^1(A_{11}\nabla^1 w)\right) - 4\operatorname{Re}\left(\nabla^1(R\nabla_1 w)\right) \\ &\quad + \frac{8}{3}\operatorname{Re} W_1\nabla^1 w - \frac{4}{3} w\nabla^1 W_1 \end{aligned} \tag{2.1}$$

for $w \in \mathcal{P}$, where $W_1 := \nabla_1 R - i\nabla^1 A_{11}$.

In particular,

$$\begin{aligned} &P_4' w = 4\Delta_b^2 w - R\Delta_b w - \Delta_b R w + (L_1L_2 + \overline{L}_1\overline{L}_2)w + (L_3 + \overline{L}_3)w + rw, \\ &L_1, L_2, L_3 \in C^\infty(M, T^{1,0}M), \quad r \in C^\infty(M), \quad w \in \mathcal{P}. \end{aligned} \tag{2.2}$$

A key property of the P'-operator is its conformal covariance: Let (M^3, θ) be a pseudohermitian manifold, let $w \in C^\infty(M)$, and set $\hat{\theta} = e^w\theta$. Then

$$e^{2w}\hat{P}_4'(u) = P_4'(u) + P_4(uw) \tag{2.3}$$

for all $u \in \mathcal{P}$. In particular, since P_4 is self-adjoint and annihilates CR pluriharmonic functions, (2.3) implies that the P'-operator is conformally covariant, mod $\mathcal{P}^\perp$.

A pseudohermitian manifold (M^3, θ) is *pseudo-Einstein* if $W_1 = 0$ for W_1 as in Definition 2.1.

Definition 2.2. Let (M^3, θ) be a pseudo-Einstein manifold. The *Q'-curvature* is

$$Q_4' = -2\Delta_b R - 4|A|^2 + R^2.$$

A key property of the Q'-curvature is its conformal covariance: Let (M^3, θ) be a pseudo-Einstein manifold, let $w \in \mathcal{P}$, and set $\hat{\theta} = e^w \theta$. Hence $\hat{\theta}$ is pseudo-Einstein [16]. Then

$$e^{2w} \hat{Q}_4' = Q_4' + P_4'(w) + \frac{1}{2} P_4\left(w^2\right). \tag{2.4}$$

In particular, Q_4' behaves as the Q-curvature for P_4', mod $\mathcal{P}^\perp$.

3. The Moser–Trudinger inequality for the P'-operator

A key step in our proof of Theorem 1.1 is to show that the P'-operator satisfies the same sharp Moser–Trudinger-type inequality as its counterpart on the sphere. This follows from the asymptotic expansion for the Green function of $\left(\overline{P}_4'\right)^{1/2}$ given in Theorem 1.3 and the general Adams-type theorem of Fontana and Morpurgo [12].

Given $k \in \mathbb{N}$ and $q > 0$, let $W^{k,q}$ denote the non-isotropic Sobolev space, given by the set of all functions u such that $Z_1 Z_2 \cdots Z_j u \in L^q(M)$ for all $Z_j \in C^\infty(M, H_{\mathbb{C}})$, $j = 0, 1, 2, \ldots, k$. For simplicity and readability, from now on, we write $W^{k,2} \cap \mathcal{P}$ to denote $W^{k,2} \cap \hat{\mathcal{P}}$.

Theorem 3.1. *Let (M^3, θ) be a compact pseudo-Einstein three-manifold for which the P'-operator is nonnegative with trivial kernel. Then there exists a constant C such that*

$$\log \fint_M e^{2(w - w_0)} \leq C + \frac{1}{16\pi^2}(w, P_4' w) \tag{3.1}$$

for all $w \in W^{2,2} \cap \mathcal{P}$.

Proof. From Theorem 1.3 we see that the leading order term of the Green function for $\overline{P}_4'$ is independent of (M^3, θ); in particular, it has exactly the same leading order term as the Green function for the P'-operator on the standard CR three-sphere. Furthermore, the next term in the asymptotic expansion of the Green function involves a definite loss of power in the asymptotic coordination ρ. Thus, by arguing analogously to the proof of [4, Theorem 2.1], we may apply the main result [12, Theorem 1] to conclude that there is a constant $C > 0$ such that

$$\int_M \exp\left(16\pi^2 \frac{(w - w_0)^2}{(w, P_4' w)}\right) \leq C \tag{3.2}$$

for all $f \in W^{2,2} \cap \mathcal{P}$. The desired inequality (3.1) is an immediate consequence of (3.2) and the elementary estimate

$$0 \leq 16\pi^2 \frac{(w - w_0)^2}{(w, P_4' w)} - 2\left(w - w_0\right) + \frac{1}{16\pi^2}(w, P_4' w). \qquad \square$$

Remark 3.2. A few comments are in order to explain the above constants. The convention used in [4] is that the sublaplacian is given by $-\operatorname{Re} \nabla^\gamma \nabla_\gamma$, which shows that our definition is -2 times theirs. With this in mind, their formula [4, (1.30)] for the P'-operator shows that our definition is 4 times theirs. Finally, they integrate with respect to the Riemannian volume element on S^3, regarded as the unit ball in $\mathbb{R}^4$, while we integrate with respect to $\theta \wedge d\theta$ for $\theta = \operatorname{Im} \overline{\partial}\left(|z|^2 - 1\right)$; in particular, our volume form is 2 times theirs. Together, these normalizations account for the apparent difference between our constant in (3.2) and the constant appearing in [4, (2.11)]. Note that θ has scalar curvature $R = 2$, and hence $\overline{Q}_4' = 4$.

4. Minimizing the functional II

Assuming the results of Section 1.3, we prove that smooth minimizers of the II-functional exist under natural positivity assumptions. We first construct weak minimizers.

Theorem 4.1. *Let (M^3, θ) be a compact pseudo-Einstein three-manifold such that $\int \overline{Q}_4' < 16\pi^2$. Suppose additionally that the P_4'-operator is nonnegative with $\ker \overline{P}_4' = \mathbb{R}$. Then*

$$\inf_{w \in W^{2,2} \cap \mathcal{P}} II[w]$$

is obtained by some function $w \in W^{2,2} \cap \mathcal{P}$.

Proof. Denote $K = \int \overline{Q}_4'$. Recall that

$$II[w] = (P_4' w, w) + 2 \int_M Q_4'(w - w_0) - K \log \fint_M e^{2(w - w_0)}$$

for $w_0 = \fint w$ the average value of M. If $K \leq 0$, it follows immediately that

$$II[w] \geq (P_4' w, w) + 2 \int_M Q_4'(w - w_0),$$

while if $K > 0$, Theorem 3.1 implies that

$$II[w] \geq \left(1 - \frac{K}{16\pi^2}\right)(P_4' w, w) + 2 \int_M Q_4'(w - w_0) - KC.$$

Together, these estimates imply that

$$II(w) \geq \left(1 - \frac{K^+}{16\pi^2}\right)(P_4' w, w) + 2 \int_M Q_4'(w - w_0) - KC \tag{4.1}$$

for $K^+ = \max\{0, K\}$ and C a positive constant independent of w.

Denote by $\lambda_1 = \lambda_1(P_4')$ the first nonzero eigenvalue

$$\lambda_1(P_4') = \inf\left\{ \frac{(P_4' w, w)}{\|w\|^2} : w \in W^{2,2} \cap \mathcal{P}, \quad \int_M w = 0 \right\}$$

of $\overline{P}_4'$, where $\|w\|^2 = (w, w)$. By assumption, $\lambda_1 > 0$. Together with (4.1), this shows that there are positive constants c_1, c_2 depending only on $(M^3, T^{1,0}M, \theta)$ such that

$$II[w] \geq c_1 \|w - w_0\|^2 - c_2. \tag{4.2}$$

In particular, II is bounded below.

Let $\{w_k\} \subset \mathcal{P}$ be a minimizing sequence of II, normalized so that $\|w_k\| = 1$ for all $k \in \mathbb{N}$. Using (4.1) and the local formula (2.1) for P'_4, it is easily seen that there is a positive constant c_3, independent of w, such that

$$\begin{aligned}\left(1 - \frac{K^+}{16\pi^2}\right) \int_M (\Delta_b w_k)^2 \leq c_3 \left| \int_M R |\nabla_b w_k|^2 \right| + c_3 \left| \int_M \operatorname{Im} A_{11} \nabla^1 w_k \nabla^1 w_k \right| \\ + 2 \left| \int_M Q'_4 \left(w_k - (w_k)_0\right) \right| + c_3.\end{aligned} \tag{4.3}$$

On the other hand, given any $\varepsilon > 0$, it holds that

$$\int_M |\nabla_b w_k|^2 = -\int_M w_k \Delta_b w_k \leq \varepsilon \int_M (\Delta_b w_k)^2 + \frac{1}{4\varepsilon} \|w_k - (w_k)_0\|_2^2.$$

We may thus combine (4.2) and (4.3) to conclude that $\{w_k\}$ is uniformly bounded in $W^{2,2} \cap \mathcal{P}$. Thus, by choosing a subsequence if necessary, we see that w_k converges weakly in $W^{2,2} \cap \mathcal{P}$ to a minimizer $w \in W^{2,2} \cap \mathcal{P}$ of II. $\square$

We need the following results:

Theorem 4.2. *For every $\ell \in \mathbb{N}_0$, we have*

$$\tau B_\ell \tau \overline{P}'_4 = \tau + \tau C_\ell \tau \quad \text{on } \hat{\mathcal{P}},$$

where $B_\ell, C_\ell \colon C^\infty(M) \to \mathscr{D}'(M)$ are continuous operators, B_ℓ is a smoothing operator of order $4 - \varepsilon$ for all $0 < \varepsilon < 1$, and $(\tau C_\ell \tau)(x, y) \in C^\ell(M \times M)$, where $\mathscr{D}'(M)$ denotes the space of distributions on M.

We refer the reader to the discussion after (10.1) for precise meaning of "smoothing operator of order $4 - \varepsilon$".

Theorem 4.3. *Let $w \in L^2(M)$. If $\Delta_b w \in L^2(M)$, then there is a constant $c > 0$ such that $e^{c|w|^2} \in L^1(M)$.*

We will prove Theorem 4.2 and Theorem 4.3 at the end of Section 1.3. These results allow us to prove that weak critical points of the II-functional are smooth.

Theorem 4.4. *Let (M^3, θ) be a compact three-dimensional pseudo-Einstein manifold. Suppose that $w \in W^{2,2} \cap \mathcal{P}$ is a critical point of the II-functional. Then w is smooth, and moreover, the contact form $\hat{\theta} := e^w \theta$ is such that $\hat{\overline{Q}}'_4$ is constant.*

Proof. It is readily seen that w is a critical point of the II-functional if and only if w is a weak solution to

$$P'_4 w + Q'_4 = \lambda e^{2w} \mod \mathcal{P}^\perp. \tag{4.4}$$

In particular, if w is smooth, then (2.4) implies that $\hat{\overline{Q}}'_4$ is constant. Now, we prove that w is smooth. Fix $\ell \in \mathbb{N}$ sufficiently large and let B_ℓ and C_ℓ be as in Theorem 4.2. From (4.4), we have

$$\tau B_\ell \tau(\lambda e^{2w}) = \tau B_\ell \overline{P}'_4 w + \tau B_\ell \tau Q'_4 = w + \tau C_\ell w + \tau B_\ell \tau Q'_4. \tag{4.5}$$

Note that

$$\tau C_\ell w + \tau B_\ell \tau Q'_4 \in C^\ell(M).$$

Since $w \in W^{2,2}$, we have $\Delta_b w \in L^2(M)$. From Theorem 4.3, we conclude that there exists a constant $c > 0$ such that

$$e^{c|w|^2} \in L^1(M),$$

and hence

$$\lambda e^{2w} \in L^q(M), \quad \text{for all } q > 1. \tag{4.6}$$

Since $\tau B_\ell \tau$ is a smoothing operator of order $4-\varepsilon$ for all $0<\varepsilon<1$, it holds that (see [23, Proposition 2.7])

$$\tau B_\ell \tau : W^{k,q} \to W^{k+1,q}, \quad \text{for all } q>1 \text{ and all } k \in \mathbb{N}_0. \tag{4.7}$$

From (4.5), (4.6) and (4.7), we obtain that

$$w \in W^{1,q}, \quad \text{for all } q>1. \tag{4.8}$$

From (4.6) and (4.8) it is easy to see that $\lambda e^{2w} \in W^{1,q}$ for all $q>1$. From this, (4.5) and (4.7) we conclude that $w+\tau C_\ell w + \tau B_\ell \tau Q_4' \in W^{2,q}$ for all $q>1$. Continuing in this way, we deduce that $w+\tau C_\ell w+\tau B_\ell \tau Q_4' \in W^{k,q}$ for all $q>1$ and all $k\in\mathbb{N}_0$ with $k\leq \ell$. Thus, $w\in W^{\ell,q}$, for all $q>1$. Since ℓ is arbitrary, we deduce that w is smooth. □

Proof of Theorem 1.1. By Theorem 4.1, there is a minimizer $w\in W^{2,2}\cap\mathcal{P}$ of the II-functional. By Theorem 4.4, w is smooth and the contact form $\hat\theta := e^w\theta$ is such that $\overline{\hat{Q}}_4'$ is constant, as desired. □

5. An example

Here we provide an example to show that minimizers of the II-functional, while they have $\overline{Q}_4'$ constant, need not have Q_4'-constant. Let $\mathbb{H}^1 := \mathbb{C}\times\mathbb{R}$ be the Heisenberg group. We write $(z,t)\in\mathbb{C}\times\mathbb{R}$ to denote the coordinates of $\mathbb{H}^1$ and let $\rho(z,t) = \left(|z|^4+t^2\right)^{1/4}$ be the usual pseudo-distance on $\mathbb{H}^1$. Put $\theta_0 = dt + iz d\overline{z} - i\overline{z}dz$ and let $T^{1,0}\mathbb{H}^1 = \left\{\lambda\left(\frac{\partial}{\partial z} + i\overline{z}\frac{\partial}{\partial t}\right) \,\middle|\, \lambda\in\mathbb{C}\right\}$. Let $\theta_1 = \rho^{-4}\theta_0$ be the contact form on $\mathbb{H}^1\setminus\{0\}$. Let

$$\Phi(z,t)\colon \mathbb{H}^1\to\mathbb{H}^1, \qquad (z,t)\mapsto \Big(\frac{z}{i\,|z|^2+t}, -\frac{t}{|z|^4+t^2}\Big),$$

be the CR inversion through the pseudo-sphere $\rho^{-1}(1)$. It is straightforward to check that the contact form $\theta_1 = \Phi^*\theta_0$ on $\mathbb{H}^1\setminus\{0\}$.

We will prove the following theorem.

Theorem 5.1. *Let Γ be a nontrivial dilation of the Heisenberg group $\mathbb{H}^1$ which fixes the origin $0\in\mathbb{H}^1$; i.e.*

$$\Gamma(z,t) = (\lambda z, \lambda^2 t)$$

for some $\lambda>0$. Then $S^1\times S^2 = (\mathbb{H}^1\setminus\{0\})/\Gamma$ with its standard CR structure is such that the minimizer of the II-functional is unique up to an additive constant, and moreover, the corresponding contact form $\hat\theta$ has $\overline{\hat{Q}}_4'\equiv 0$ but $\hat{Q}_4'\not\equiv 0$.

Proof. It is easy to check that $2\log\rho$ is the real part of the CR function $\log(|z|^2+it)$ on $\mathbb{H}^1\setminus\{0\}$ and hence $\log\rho$ is in $\mathcal{P}$ the space of CR pluriharmonic functions on $\mathbb{H}^1\setminus\{0\}$. From (2.4) it follows that

$$P_4'\log\rho^{-4} + \frac{1}{2}P_4\log^2\rho^{-4} = 0. \tag{5.1}$$

Consider now the contact form $\theta := \rho^{-2}\theta_0$. It is clear that θ is invariant under the action of Γ, and hence θ descends to a well-defined contact form on $S^1\times S^2$.

Since $\log\rho \in \mathcal{P}$, we know that θ is pseudo-Einstein. From (2.4) we see that the Q'-curvature Q_4' of θ is

$$\rho^{-4}Q_4' = P_4'\log\rho^{-2} + \frac{1}{2}P_4\log^2\rho^{-2} = -\frac{1}{2}P_4\log^2\rho^{-2}, \tag{5.2}$$

where the second equality uses (5.1). Since the Paneitz operator P_4 is self-adjoint and $\mathcal{P} \subset \ker P_4$, it follows that Q_4' is orthogonal, with respect to $\theta\wedge d\theta$, to the CR pluriharmonic functions. In particular, $\overline{Q}_4' \equiv 0$. Furthermore, one can compute directly from (5.2) that

$$Q_4' = 8\frac{|z|^4 - t^2}{|z|^4 + t^2},$$

which is clearly not identically zero.

Finally, using Lee's formula for the change of the scalar curvature under a conformal change of contact form [26, Lemma 2.4], we compute that the scalar curvature R of θ is

$$R = 2\frac{|z|^2}{\rho^2}.$$

Since this is nonnegative and θ is pseudo-Einstein, $\overline{P}_4'$ is nonnegative with trivial kernel [6, Proposition 4.9]. Now, if $\hat{\theta} = e^u\theta$ is a pseudo-Einstein contact form on $S^1\times S^2$ for which $\hat{\overline{Q}}_4' \equiv 0$, the transformation formula (2.4) implies that $\overline{P}_4'u \equiv 0$, whence u is constant, as desired. ☐

6. Preliminaries for pseudodifferential operators

We shall use the following notations: $\mathbb{R}_+ := \{x\in\mathbb{R} \,|\, x>0\}$ and $\mathbb{N}_0 = \mathbb{N}\cup\{0\}$. The *size* of a *multi-index* $\alpha = (\alpha_1,\ldots,\alpha_n)\in\mathbb{N}_0^n$ is $|a| := \alpha_1+\cdots+\alpha_n$. Given a multi-index α, we write $x^\alpha = x_1^{\alpha_1}\cdots x_n^{\alpha_n}$ for $x = (x_1,\ldots,x_n)$. Similarly, we write $\partial_x^\alpha = \partial_{x_1}^{\alpha_1}\cdots\partial_{x_n}^{\alpha_n}$ for $\partial_{x_j} = \frac{\partial}{\partial x_j}$ and $\partial_x^\alpha = \frac{\partial^{|\alpha|}}{\partial x^\alpha}$.

Let M be a smooth manifold. We denote by $\langle\,\cdot\,,\cdot\,\rangle$ the pointwise duality between TM and T^*M. We extend $\langle\,\cdot\,,\cdot\,\rangle$ bilinearly to $T_{\mathbb{C}}M\times T_{\mathbb{C}}^*M$. Let E be a C^∞ vector bundle over M. The fiber of E at $x\in M$ are denoted by E_x. Let $Y\subset M$ be an open set. The spaces of smooth sections of E over Y and distributional sections of E over Y are denoted by $C^\infty(Y,E)$ and $\mathscr{D}'(Y,E)$, respectively. Let $\mathscr{E}'(Y,E)$ be the subspace of $\mathscr{D}'(Y,E)$ whose elements have compact support in Y. For $m\in\mathbb{R}$, let $H^m(Y,E)$ denote the Sobolev space of order m of sections of E over Y. Put

$$\begin{aligned} H^m_{\mathrm{loc}}(Y,E) &= \left\{u\in\mathscr{D}'(Y,E) \,\middle|\, \varphi u\in H^m(Y,E) \text{ for all } \varphi\in C_0^\infty(Y)\right\}, \\ H^m_{\mathrm{comp}}(Y,E) &= H^m_{\mathrm{loc}}(Y,E)\cap\mathscr{E}'(Y,E). \end{aligned}$$

Fix a smooth density of integration on M. Let F be a smooth vector bundle over M. If $A\colon C_0^\infty(M,E)\to\mathscr{D}'(M,F)$ is continuous, we write $A(x,y)$ to denote the distributional kernel of A. The following two statements are equivalent:

(a) A is continuous as a mapping from $\mathscr{E}'(M,E)$ to $C^\infty(M,F)$.
(b) $A(x,y)\in C^\infty(M\times M, E_y\boxtimes F_x)$.

If A satisfies (a) or (b), we say that A is smoothing. Let $B\colon C_0^\infty(M,E)\to\mathscr{D}'(M,F)$ be a continuous operator. We write $A\equiv B$ if $A-B$ is a smoothing operator.

Let $H(x,y)\in\mathscr{D}'(M\times M, E_y\boxtimes F_x)$. We also denote by H the unique continuous operator $H\colon C_0^\infty(M,E)\to\mathscr{D}'(M,F)$ with distribution kernel $H(x,y)$. We henceforth identify H with $H(x,y)$.

Recall the Hörmander symbol spaces:

Definition 6.1. Let $M \subset \mathbb{R}^N$ be an open set. Let $m \in \mathbb{R}$ and let $0 \leq \rho \leq 1$, $0 \leq \delta \leq 1$. $S^m_{\rho,\delta}(M \times \mathbb{R}^{N_1})$ is the space of all $a \in C^\infty(M \times \mathbb{R}^{N_1})$ such that for all compact $K \Subset M$ and all $\alpha \in \mathbb{N}_0^N$, $\beta \in \mathbb{N}_0^{N_1}$, there is a constant $C > 0$ such that

$$\left|\partial_x^\alpha \partial_\xi^\beta a(x,\xi)\right| \leq C(1+|\xi|)^{m-\rho|\beta|+\delta|\alpha|} \quad \text{for all} \quad (x,\xi) \in K \times \mathbb{R}^{N_1}.$$

Denote

$$S^{-\infty}(M \times \mathbb{R}^{N_1}) := \bigcap_{m \in \mathbb{R}} S^m_{\rho,\delta}(M \times \mathbb{R}^{N_1}).$$

Let $a_j \in S^{m_j}_{\rho,\delta}(M \times \mathbb{R}^{N_1})$ for $j \in \mathbb{N}_0$ with $m_j \to -\infty$ as $j \to \infty$. Then there exists $a \in S^{m_0}_{\rho,\delta}(M \times \mathbb{R}^{N_1})$, unique modulo $S^{-\infty}(M \times \mathbb{R}^{N_1})$, such that $a - \sum_{j=0}^{k-1} a_j \in S^{m_k}_{\rho,\delta}(M \times \mathbb{R}^{N_1})$ for all $k \in \{0,1,2,\dots\}$.

If a and a_j have the properties above, we write $a \sim \sum_{j=0}^\infty a_j$ in $S^{m_0}_{\rho,\delta}(M \times \mathbb{R}^{N_1})$.

Let $S^m_{\mathrm{cl}}(M \times \mathbb{R}^{N_1})$ be the space of all symbols $a(x,\xi) \in S^m_{1,0}(M \times \mathbb{R}^{N_1})$ with

$$a(x,\xi) \sim \sum_{j=0}^\infty a_{m-j}(x,\xi) \text{ in } S^m_{1,0}(M \times \mathbb{R}^{N_1}),$$

with $a_k(x,\xi) \in C^\infty(M \times \mathbb{R}^{N_1})$ positively homogeneous of degree k in ξ; that is, $a_k(x,\lambda\xi) = \lambda^k a_k(x,\xi)$ for all $\lambda \geq 1$ and all $|\xi| \geq 1$.

By using partition of unity, we extend the definitions above to the cases when M is a smooth manifold and when we replace $M \times \mathbb{R}^{N_1}$ by T^*M.

Let $\Omega \subset M^3$ be an open coordinate patch. Let $a(x,y,\xi) \in S^m_{\rho,\delta}(T^*\Omega)$. We define

$$A(x,y) = \frac{1}{(2\pi)^3} \int e^{i<x-y,\xi>} a(x,\xi) d\xi$$

as an oscillatory integral. One can show that

$$A \colon C_0^\infty(\Omega) \to C^\infty(\Omega)$$

is continuous and has a unique continuous extension $A \colon \mathscr{E}'(\Omega) \to \mathscr{D}'(\Omega)$.

Definition 6.2. Let $m \in \mathbb{R}$. A pseudodifferential operator of order m type (ρ,δ) on M is a continuous linear map $A \colon C^\infty(M) \to \mathscr{D}'(M)$ such that on every open coordinate patch Ω, if we consider A as a continuous operator

$$A \colon C_0^\infty(\Omega) \to C^\infty(\Omega),$$

then the distributional kernel of A is

$$A(x,y) = \frac{1}{(2\pi)^3} \int e^{i<x-y,\xi>} a(x,\xi) d\xi$$

with $a \in S^m_{\rho,\delta}(T^*\Omega)$. We call $a(x,\xi)$ the symbol of A. We write $L^m_{\rho,\delta}(M)$ to denote the space of classical pseudodifferential operators of order m type (ρ,δ) on M. If $a(x,\xi) \in S^m_{\mathrm{cl}}(T^*\Omega)$, we call A a classical pseudodifferential operator of order m. We write $L^m_{\mathrm{cl}}(M)$ to denote the space of classical pseudodifferential operators of order m on M.

7. The distributional kernel of τ

In this section, we review some results in [21] about the orthogonal projection $\tau\colon L^2 \to L^2 \cap \mathcal{P}$ which are needed in the proof of our main result.

Let $\langle \cdot | \cdot \rangle$ be the Hermitian inner product on $T_{\mathbb{C}}M$ given by

$$\begin{aligned}
&\langle Z_1 | Z_2 \rangle = -\frac{1}{2i}\langle\, d\theta\,,\, Z_1 \wedge \overline{Z}_2\,\rangle \quad \text{for all } Z_1, Z_2 \in T^{1,0}M,\\
&\langle Z | W \rangle = 0 \quad \text{for all } Z \in T^{1,0}M,\, W \in T^{0,1}M,\\
&\langle T | T \rangle = 1, \quad \langle T | U \rangle = 0 \;\; \text{for all } U \in H_{\mathbb{C}}.
\end{aligned}$$

The Hermitian metric $\langle \cdot | \cdot \rangle$ on $T_{\mathbb{C}}M$ induces a Hermitian metric $\langle \cdot | \cdot \rangle$ on $T^*_{\mathbb{C}}M$. Take $\theta \wedge d\theta$ to be the volume form on M, we then get natural inner product on $\Omega^{0,1}(M) := C^\infty(M, T^{*0,1}M)$ induced by $\theta\wedge d\theta$ and $\langle \cdot | \cdot \rangle$, where $T^{*0,1}M$ denotes the bundle of $(0,1)$ forms of M. We denote this inner product by $(\,\cdot\,,\cdot\,)$ and denote the corresponding norm by $\|\cdot\|$. Let $L^2_{(0,1)}(M)$ denote the completion of $\Omega^{0,1}(M)$ with respect to $(\,\cdot\,,\cdot\,)$. Let $\overline{\partial}_b\colon C^\infty(M) \to \Omega^{0,1}(M)$ be the tangential Cauchy-Riemann operator. We extend $\overline{\partial}_b$ to L^2 by $\overline{\partial}_b\colon \operatorname{Dom}\overline{\partial}_b \to L^2_{(0,1)}(M)$, where

$$\operatorname{Dom}\overline{\partial}_b := \left\{ u \in L^2(M) \;\middle|\; \overline{\partial}_b u \in L^2_{(0,1)}(M) \right\}.$$

Let $\overline{\partial}_b^*\colon \operatorname{Dom}\overline{\partial}_b^* \to L^2(M)$ be the L^2 adjoint of $\overline{\partial}_b$. The Kohn Laplacian is given by

$$\begin{aligned}
\Box_b &:= \overline{\partial}_b^*\overline{\partial}_b\colon \operatorname{Dom}\Box_b \to L^2(M),\\
\operatorname{Dom}\Box_b &= \left\{ u \in L^2(M) \;\middle|\; u \in \operatorname{Dom}\overline{\partial}_b, \overline{\partial}_b u \in \operatorname{Dom}\overline{\partial}_b^* \right\}.
\end{aligned}$$

Note that $\Box_b$ is self-adjoint.

We pause and introduce some notations. Take $\chi(s) \in C^\infty(\mathbb{R})$ with $\chi(s) = 1$ if $s \geq \frac{1}{2}$ and $\chi(s) = 0$ if $s \leq \frac{1}{2}$. For $m \in \mathbb{R}$, $S^m_{1,0}(M \times M \times \mathbb{R}_+)$ is the space of all $a(x,y,s) \in C^\infty(M \times M \times \mathbb{R}_+)$ such that $\chi(s)a(x,y,s) \in S^m_{1,0}(M \times M \times \mathbb{R})$. Similarly, $S^m_{\mathrm{cl}}(M \times M \times \mathbb{R}_+)$ is the space of $a(x,y,s) \in C^\infty(M \times M \times \mathbb{R}_+)$ such that $\chi(s)a(x,y,s) \in S^m_{\mathrm{cl}}(M \times M \times \mathbb{R})$. As in Definition 6.1, let $a_j \in S^{m_j}_{1,0}(M \times M \times \mathbb{R}_+)$ for $j \in \mathbb{N}_0$ with $m_j \to -\infty$ as $j \to \infty$. Then there exists $a \in S^{m_0}_{1,0}(M \times M \times \mathbb{R}_+)$, unique modulo $S^{-\infty}(M \times M \times \mathbb{R}_+) := \bigcap_{m\in\mathbb{R}} S^m_{1,0}(M \times M \times \mathbb{R}_+)$, such that $a - \sum_{j=0}^{k-1} a_j \in S^{m_k}_{1,0}(M \times M \times \mathbb{R}_+)$ for all $k \in \{0,1,2,\dots\}$. If a and a_j have the properties above, we write $a \sim \sum_{j=0}^\infty a_j$ in $S^{m_0}_{1,0}(M \times M \times \mathbb{R}_+)$.

We return to our situation. The orthogonal projection $S\colon L^2(M) \to \ker\overline{\partial}_b = \ker\Box_b$ is the *Szegő projection*. From now on, we assume that M is embeddable. The follow facts are shown by the second-named author; see [21, Theorem 1.2 and Remark 1.4].

Theorem 7.1. *With the assumptions and notations above, we have*

$$\tau \equiv S + \overline{S}, \tag{7.1}$$

where $\overline{S}$ is the conjugate of S. Moreover, the kernel $\tau(x,y) \in \mathscr{D}'(M \times M)$ of τ satisfies

$$\tau(x,y) \equiv \int_0^\infty e^{i\varphi(x,y)s} a(x,y,s)ds + \int_0^\infty e^{-i\overline{\varphi}(x,y)s} \overline{a}(x,y,s)ds,$$

where

$$\begin{aligned}
&a(x,y,s)\in S^1_{\mathrm{cl}}(M\times M\times\mathbb{R}_+),\\
&a(x,y,s)\sim\sum_{j=0}^{\infty}a_j(x,y)s^{1-j}\ \textit{in}\ S^1_{1,0}(M\times M\times\mathbb{R}_+),\\
&a_j(x,y)\in C^\infty(M\times M)\quad\textit{for all}\ j\in\mathbb{N}_0,\\
&a_0(x,x)=\frac{1}{2}\pi^{-2}\quad\textit{for all}\ x\in M,
\end{aligned}$$

and

$$\begin{aligned}
&\varphi\in C^\infty(M\times M),\quad \operatorname{Im}\varphi(x,y)\geq 0,\quad d_x\varphi|_{x=y}=-\theta(x),\\
&\varphi(x,y)=-\overline{\varphi}(y,x),\\
&\varphi(x,y)=0\ \textit{if and only if}\ x=y,\\
&\sigma_{\Box_b}(x,\varphi'_x(x,y))\ \textit{vanishes to infinite order on}\ x=y.
\end{aligned}\tag{7.2}$$

Here $\sigma_{\Box_b}$ *denotes the principal symbol of* $\Box_b$.

We explain the last condition in (7.2). Let $x=(x_1,x_2,x_3)$ be local coordinates of X defined on an open set D of X and let $\xi=(\xi_1,\xi_2,\xi_3)$ be the dual coordinates. On D, the principal symbol of $\Box_b$ has the form

$$\sigma_{\Box_b}(x,\xi)=\sum_{\alpha\in\{0,1,2\}^3,|\alpha|\leq 2}a_\alpha(x)\xi^\alpha,$$

where $a_\alpha(x)\in C^\infty(D)$, for every multi-index α. The last condition in (7.2) means that for all $\gamma_1,\gamma_2\in\mathbb{N}_0^3$, we have

$$\frac{\partial^{|\gamma_1|+|\gamma_2|}}{\partial x^{\gamma_1}\partial y^{\gamma_2}}\Big(\sum_{\substack{\alpha\in\{0,1,2\}^3\\|\alpha|\leq 2}}a_\alpha(x)(\varphi'_x(x,y))^\alpha\Big)\Big|_{x=y}=0,\quad\forall x\in D.$$

We need the following fact about the Szegő kernel (cf. [2, 20]).

Theorem 7.2. *With the assumptions and notations above, the distributional kernel of* S *satisfies*

$$S(x,y)\equiv\int_0^\infty e^{i\varphi(x,y)s}a(x,y,s)ds$$

where $\varphi(x,y)\in C^\infty(M\times M)$ *and* $a(x,y,s)\in S^1_{\mathrm{cl}}(M\times M\times\mathbb{R}_+)$ *are as in Theorem 7.1.*

8. The principal symbol of $\tau\Delta_b$ on $\mathcal{P}$

It is well-known that Δ_b is a subelliptic operator. However, if we restrict Δ_b to $\mathcal{P}$, it is equivalent to an elliptic pseudodifferential operator.

Theorem 8.1. *There is a classical elliptic pseudodifferential operator* $E_1\in L^1_{\mathrm{cl}}(M)$ *with real-valued principal symbol such that*

$$-\tau\Delta_b\tau=\tau E_1\tau\quad\textit{on}\ \mathscr{D}'(M).$$

In particular, $-\tau\Delta_b=\tau E_1$ *on* $\mathcal{P}$.

The proof of Theorem 8.1 requires many ingredients. First, we have the following immediate consequence of the commutator formulae proven by Lee [26].

Lemma 8.2. *It holds that* $\overline{\Box}_b = \Box_b - iT + L$ *for some* $L \in C^\infty(M, H_{\mathbb{C}})$.

We need the following result given in [22, Lemma 5.7]

Lemma 8.3. *Let* $A, B\colon C_0^\infty(M) \to \mathscr{D}'(M)$ *be continuous operators such that the kernels of* A *and* B *satisfy*

$$A(x,y) = \int_0^\infty e^{i\varphi(x,y)s}\alpha(x,y,s)ds, \quad \alpha(x,y,s) \in S^k_{\mathrm{cl}}(M \times M \times \overline{\mathbb{R}}_+),$$
$$B(x,y) = \int_0^\infty e^{-i\overline{\varphi}(x,y)s}\beta(x,y,s)ds, \quad \beta(x,y,s) \in S^\ell_{\mathrm{cl}}(M \times M \times \overline{\mathbb{R}}_+)$$

for some $k, \ell \in \mathbb{Z}$, *where* $\varphi(x,y) \in C^\infty(M \times M)$ *is as in Theorem 7.1. Then,*

$$A \circ B \equiv 0, \quad B \circ A \equiv 0.$$

To proceed, set

$$\Sigma^- = \{(x, \lambda\theta(x)) \in T^*M;\, \lambda < 0\}, \quad \Sigma^+ = \{(x, \lambda\theta(x)) \in T^*M;\, \lambda > 0\}.$$

Let $\sigma_{\Box_b}(x,\xi)$ and $\sigma_{iT}(x,\xi)$ be the principal symbols of $\Box_b$ and iT, respectively. It is easy to see that $\sigma_{\Box_b}(x,\xi) = 0$ for all $(x,\xi) \in \Sigma^- \cup \Sigma^+$; that $\sigma_{iT}(x,\xi) > 0$ for all $(x,\xi) \in \Sigma^-$; and that $\sigma_{iT}(x,\xi) < 0$ for all $(x,\xi) \in \Sigma^+$. For $(x,\xi) \in T^*M$, we write $|\xi|$ to denote the point norm of the cotangent vector $\xi \in T^*_xM$. Take $\chi_0, \chi_1 \in C^\infty(T^*M, [0,1])$ such that

1. $\chi_0 = 1$ in a small neighbourhood of $\Sigma^- \cap \{(x,\xi) \in T^*M;\, |\xi| \geq 1\}$,
2. $\chi_1 = 1$ in a small neighbourhood of $\Sigma^+ \cap \{(x,\xi) \in T^*M;\, |\xi| \geq 1\}$,
3. $\operatorname{supp}\chi_0 \cap \operatorname{supp}\chi_1 = \emptyset$,
4. $\sigma_{iT}(x,\xi) > 0$ for all $(x,\xi) \in \operatorname{supp}\chi_0$,
5. $\sigma_{iT}(x,\xi) < 0$ for all $(x,\xi) \in \operatorname{supp}\chi_1$, and
6. χ_0, χ_1 are positively homogeneous of degree zero in the sense that

$$\chi_0(x,\lambda\xi) = \chi_0(x,\xi), \quad \chi_1(x,\lambda\xi) = \chi_1(x,\xi) \quad \text{for all } \lambda \geq 1 \text{ and } |\xi| \geq 1.$$

Define

$$\begin{aligned} q(x,\xi) =& (1 - \chi_0(x,\xi) - \chi_1(x,\xi))\sqrt{\sigma_{\Box_b}(x,\xi)} \\ &+ \chi_0(x,\xi)\sigma_{iT}(x,\xi) - \chi_1(x,\xi)\sigma_{iT}(x,\xi). \end{aligned} \tag{8.1}$$

Note that $\sigma_{\Box_b}(x,\xi) > 0$ for all $(x,\xi) \notin \Sigma^- \cup \Sigma^+$. From this observation, it is easy to see that $q(x,\xi) \geq c\,|\xi|$ for all $(x,\xi) \in T^*M$ with $|\xi| \geq 1$, where $c > 0$ is a constant. Let $\widetilde{E}_1 \in L^1_{\mathrm{cl}}(M)$ with symbol $q(x,\xi) \in C^\infty(T^*M)$. Then $\widetilde{E}_1$ is a classical elliptic pseudodifferential operator. It is known that (see [20]) $\mathrm{WF}'(S) = \operatorname{diag}(\Sigma^- \times \Sigma^-)$ and $\mathrm{WF}'(\overline{S}) = \operatorname{diag}(\Sigma^+ \times \Sigma^+)$, where

$$\mathrm{WF}'(S) = \{(x,\xi,y,\eta) \in T^*M \times T^*M\colon\, (x,\xi,y,-\eta) \in \mathrm{WF}(S)\}$$

and $\mathrm{WF}(S)$ denotes the wave front set of S in the sense of Hörmander [18, Chapter 8]. Recall that S denotes the Szegő projection. We have $S(\widetilde{E} - iT) = SR$, where $R \in L^1_{\mathrm{cl}}(M)$ with symbol

$$r(x,\xi) = (1 - \chi_0(x,\xi) - \chi_1(x,\xi))\Big(\sqrt{\sigma_{\Box_b}(x,\xi)} - \sigma_{iT}(x,\xi)\Big) - 2\chi_1(x,\xi)\sigma_{iT}(x,\xi).$$

Since $r(x,\xi)$ vanishes in a neighborhood of Σ^- and $\mathrm{WF}'(S) \subseteq \operatorname{diag}(\Sigma^- \times \Sigma^-)$, we deduce that $S(\widetilde{E} - iT) = SR \equiv 0$. Similarly, we have $\widetilde{E}_1 S \equiv (iT)S$, $\overline{S}\widetilde{E}_1 \equiv \overline{S}(-iT)$,

$\widetilde{E}_1\overline{S} \equiv (-iT)\overline{S}$. Summing up, we have

$$S\widetilde{E}_1 \equiv S(iT),\quad \widetilde{E}_1 S \equiv (iT)S,\quad \overline{S}\widetilde{E}_1 \equiv \overline{S}(-iT),\quad \widetilde{E}_1\overline{S} \equiv (-iT)\overline{S}. \tag{8.2}$$

Alternatively, (8.2) can be checked directly from the fact that $d_x\varphi|_{x=y} = -\theta(x)$. Now, we can prove the following theorem.

Theorem 8.4. *With the notations above, there is an $\widetilde{E}_0 \in L^0_{\rm cl}(M)$ such that*

$$S\Delta_b S \equiv S(\widetilde{E}_1 + \widetilde{E}_0)S \quad \textit{and} \quad \overline{S}\Delta_b\overline{S} \equiv \overline{S}(\widetilde{E}_1 + \widetilde{E}_0)\overline{S}.$$

Proof. From Lemma 8.2, (8.2), and the observation that $\Box_b S = 0$, we have

$$S\Delta_b S = S(iT - L)S \equiv S\widetilde{E}_1 S + SLS. \tag{8.3}$$

We write $L = U + \overline{V}$ for $U, V \in C^\infty(M, T^{1,0}M)$. Since $\overline{\partial}_b S = 0$, we have

$$S\overline{V}S = 0. \tag{8.4}$$

Now,

$$(SUS)^* = SU^*S = S(-\overline{U} + r)S = SrS,$$

where $(SUS)^*$ and U^* are the adjoints of SUS and S respectively and $r \in C^\infty(M)$. Hence,

$$SUS = S\overline{r}S. \tag{8.5}$$

From (8.3), (8.4) and (8.5), we conclude that

$$S\Delta_b S \equiv S(\widetilde{E}_1 + g_0)S, \tag{8.6}$$

where $g_0 \in C^\infty(M)$. Similarly,

$$\overline{S}\Delta_b\overline{S} \equiv \overline{S}(\widetilde{E}_1 + g_1)\overline{S}, \tag{8.7}$$

where $g_1 \in C^\infty(M)$. Let $\widetilde{E}_0 \in L^0_{\rm cl}(M)$ with symbol

$$\chi_0(x,\xi)g_0 + \chi_1(x,\xi)g_1,$$

where χ_0, χ_1 are as in (8.1). As in the discussion before (8.2), we have

$$Sg_0S \equiv S\widetilde{E}_0S,\quad \overline{S}g_1\overline{S} \equiv \overline{S}\widetilde{E}_0\overline{S}. \tag{8.8}$$

The desired conclusion follows from (8.6), (8.7) and (8.8). □

Proof of Theorem 8.1. From Theorem 8.4 and (7.1), we have

$$\begin{aligned}
\tau\Delta_b\tau &\equiv (S + \overline{S})\Delta_b(S + \overline{S}) \\
&= S\Delta_b S + \overline{S}\Delta_b\overline{S} + S\Delta_b\overline{S} + \overline{S}\Delta_b S \\
&\equiv S(\widetilde{E}_1 + \widetilde{E}_0)S + \overline{S}(\widetilde{E}_1 + \widetilde{E}_0)\overline{S} + S\Delta_b\overline{S} + \overline{S}\Delta_b S \\
&= (S + \overline{S})(\widetilde{E}_1 + \widetilde{E}_0)(S + \overline{S}) - S(\widetilde{E}_1 + \widetilde{E}_0)\overline{S} - \overline{S}(\widetilde{E}_1 + \widetilde{E}_0)S \\
&\quad + S\Delta_b\overline{S} + \overline{S}\Delta_b S \\
&\equiv \tau(\widetilde{E}_1 + \widetilde{E}_0)\tau - S(\widetilde{E}_1 + \widetilde{E}_0)\overline{S} - \overline{S}(\widetilde{E}_1 + \widetilde{E}_0)S + S\Delta_b\overline{S} + \overline{S}\Delta_b S.
\end{aligned} \tag{8.9}$$

In view of Lemma 8.3 and Theorem 7.2, we see that $S(\widetilde{E}_1 + \widetilde{E}_0)\overline{S}$, $\overline{S}(\widetilde{E}_1 + \widetilde{E}_0)S$, $S\Delta_b\overline{S}$ and $\overline{S}\Delta_b S$ are smoothing. From this and (8.9), we get

$$\tau\Delta_b\tau = \tau(\widetilde{E}_1 + \widetilde{E}_0)\tau + G,$$

where G is smoothing. Hence,

$$\tau\Delta_b\tau = \tau^2\Delta_b\tau^2 = \tau^2(\widetilde{E}_1 + \widetilde{E}_0)\tau^2 + \tau G\tau = \tau(\widetilde{E}_1 + \widetilde{E}_0 + G)\tau. \tag{8.10}$$

Put $-E_1 = \widetilde{E}_1 + \widetilde{E}_0 + G \in L^1_{\mathrm{cl}}(M)$. From (8.10), we get $-\tau\Delta_b\tau = \tau E_1\tau$. The theorem follows. □

9. The operator $\left(\overline{P}'_4\right)^{-\frac{1}{2}}$

As explained in the Introduction, the proof of Theorem 1.3 begins by understanding some properties of the operator $\left(\overline{P}'_4\right)^{-1/2}$. To begin, we can repeat the proof of Theorem 8.1 with minor change to obtain the following result:

Theorem 9.1. *We have*

$$\overline{P}'_4 = \tau\big((2E_1)^2 + \hat{E}_1\big) \quad \text{on } \mathcal{P},$$

where $E_1 \in L^1_{\mathrm{cl}}(M)$ is as in Theorem 8.1 and $\hat{E}_1 \in L^1_{\mathrm{cl}}(M)$.

For a linear operator $F : \mathcal{P} \to \mathcal{P}$, we say that F is an elliptic pseudodifferential operator on $\mathcal{P}$ if we can find an elliptic pseudodifferential operator $E \in L^m_{\mathrm{cl}}(M)$, $m \in \mathbb{R}$, such that $F = \tau E$ on $\mathcal{P}$. From Theorem 9.1, we see that $\overline{P}'_4$ is an elliptic pseudodifferential operator on $\mathcal{P}$. Standard arguments for elliptic operators imply that the spectrum $\operatorname{Spec}\overline{P}'_4$ of $\overline{P}'_4$ is a discrete subset of $(-\infty,\infty)$ such that every $\lambda \in \operatorname{Spec}\overline{P}'_4$ is an eigenvalue of $\overline{P}'_4$ and the eigenspace

$$\mathcal{E}_\lambda(\overline{P}'_4) := \Big\{u \in \operatorname{Dom}\overline{P}'_4 \colon \overline{P}'_4 u = \lambda u\Big\}$$

is a finite dimensional subspace of $\mathcal{P}$.

Let

$$\pi \colon \hat{\mathcal{P}} \to \ker\overline{P}'_4$$

be the orthogonal projection. Let $\{g_1, g_2, \ldots, g_d\} \subset \mathcal{P}$ be an orthonormal frame for $\ker\overline{P}'_4$, where $d \in \mathbb{N}_0$. Then

$$\pi(x,y) = \sum_{j=1}^{d} g_j(x)\overline{g}_j(y) \in C^\infty(M \times M). \tag{9.1}$$

From (9.1), we can extend π to $\mathscr{D}'(M)$ as a smoothing operator on M.

Assume that $\overline{P}'_4$ is nonnegative. Then $\operatorname{Spec}\overline{P}'_4 \subset [0,\infty)$ and $\overline{P}'_4$ has a well-defined square root

$$\left(\overline{P}'_4\right)^{\frac{1}{2}} \colon \operatorname{Dom}\left(\overline{P}'_4\right)^{\frac{1}{2}} \subset \hat{\mathcal{P}} \to \hat{\mathcal{P}}.$$

Note that $\operatorname{Dom}\left(\overline{P}'_4\right)^{\frac{1}{2}} = \operatorname{Dom}\overline{P}'_4$. We write

$$\left(\overline{P}'_4\right)^{-\frac{1}{2}} \colon \hat{\mathcal{P}} \to \operatorname{Dom}\left(\overline{P}'_4\right)^{\frac{1}{2}}$$

to denote the Green function of $\left(\overline{P}'_4\right)^{\frac{1}{2}}$. That is,

$$\begin{aligned}
&\left(\overline{P}'_4\right)^{\frac{1}{2}}\left(\overline{P}'_4\right)^{-\frac{1}{2}} + \pi = I \quad \text{on } \hat{\mathcal{P}},\\
&\left(\overline{P}'_4\right)^{-\frac{1}{2}}\left(\overline{P}'_4\right)^{\frac{1}{2}} + \pi = I \quad \text{on } \operatorname{Dom}\left(\overline{P}'_4\right)^{\frac{1}{2}}.
\end{aligned}$$

For every $t > 0$, the operator

$$\overline{P}'_4 + t + \pi \colon \operatorname{Dom}\overline{P}'_4 \to \hat{\mathcal{P}}$$

has a continuous inverse

$$(\overline{P}'_4 + t + \pi)^{-1} \colon \hat{\mathcal{P}} \to \hat{\mathcal{P}}$$

and the operator $(\overline{P}'_4 + t + \pi)^{-1}$ depends continuously on t. Let $\lambda_1 > 0$ be the first non-zero eigenvalue of $\overline{P}'_4$. Then

$$\begin{aligned} \left\| (\overline{P}'_4 + t + \pi)^{-1} u \right\| &\leq \frac{1}{\lambda_1 + t} \left\| (I - \pi) u \right\| + \frac{1}{1+t} \left\| \pi u \right\| \\ &\leq \frac{1}{\min\{\lambda_1, 1\} + t} \left\| u \right\| \end{aligned} \tag{9.2}$$

for all $u \in \hat{\mathcal{P}}$. $\left(\overline{P}'_4\right)^{-1/2}$ can be understood as follows.

Lemma 9.2. *On $\hat{\mathcal{P}} \cap (\ker \overline{P}'_4)^{\perp}$, we have*

$$\left(\overline{P}'_4\right)^{-\frac{1}{2}} = c \int_0^\infty t^{-\frac{1}{2}} (\overline{P}'_4 + t + \pi)^{-1} dt,$$

where $c^{-1} = \int_0^\infty t^{-\frac{1}{2}} (1+t)^{-1} dt$.

Proof. Fix a positive eigenvalue $\lambda \in \operatorname{Spec} \overline{P}'_4$. Let $u \in \mathcal{E}_\lambda(\overline{P}'_4)$. Then,

$$\left(\overline{P}'_4\right)^{-\frac{1}{2}} u = \frac{1}{\sqrt{\lambda}} u.$$

We compute that

$$\Big(c \int_0^\infty t^{-\frac{1}{2}} (\mathrm{P}'_0 + t + \pi)^{-1} dt \Big) u = cu \int_0^\infty t^{-\frac{1}{2}} \frac{1}{\lambda + t} dt = \frac{1}{\sqrt{\lambda}} u.$$

Hence the conclusion is true on $\mathcal{E}_\lambda(\overline{P}'_4)$ for all $\lambda \in \operatorname{Spec} \overline{P}'_4$.

Let $u \in \hat{\mathcal{P}} \cap (\ker \overline{P}'_4)^{\perp}$. For each $N \in \mathbb{N}$, let u_N be the orthogonal projection of u onto $\bigoplus_{\lambda \leq N} \mathcal{E}_\lambda(\overline{P}'_4)$. It follows that $u_N \to u$ and that $\left(\overline{P}'_4\right)^{-\frac{1}{2}} u_N \to \left(\overline{P}'_4\right)^{-\frac{1}{2}} u$. From (9.2), we have

$$c \Big(\int_0^\infty t^{-\frac{1}{2}} (\overline{P}'_4 + t + \pi)^{-1} dt \Big) u_N \to c \Big(\int_0^\infty t^{-\frac{1}{2}} (P'_4 + t + \pi)^{-1} dt \Big) u$$

in $\hat{\mathcal{P}}$ as $N \to \infty$. Together these observations yield the result. □

To proceed, we require some additional symbol spaces.

Definition 9.3. Let m be a real number and let $d \in \mathbb{Z}$. The class $S^m_{1,0,d}(T^*M, \mathbb{R}_+)$ consists of all functions $a(x, \xi, t) \in C^\infty(T^*M \times \mathbb{R}_+)$ such that for arbitrary multi-indices $\alpha, \beta \in \mathbb{N}_0^3$, and for any compact set $K \subset M$ there exists $C_{\alpha,\beta,K} > 0$ such that $\left| \partial_x^\alpha \partial_\xi^\beta a(x, \xi, t) \right| \leq C_{\alpha,\beta,K} (1 + |\xi| + |t|^{\frac{1}{d}})^{m - |\beta|}$ for all $(x, \xi) \in T^*K$, $t \in \mathbb{R}_+$. Denote

$$S^{-\infty}(T^*M, \mathbb{R}_+) = \bigcap_{m \in \mathbb{R}} S^m_{1,0,d}(T^*M, \mathbb{R}_+).$$

Let $a_j \in S^{m_j}_{1,0,d}(T^*M, \mathbb{R}_+)$ for $j \in \{0, 1, 2, \dots\}$ with $m_j \to -\infty$ as $j \to \infty$. Then there exists $a \in S^{m_0}_{1,0,d}(T^*M, \mathbb{R}_+)$, unique modulo $S^{-\infty}(T^*M, \mathbb{R}_+)$, such that

$a - \sum_{j=1}^{k-1} a_j \in S^{m_k}_{1,0,d}(T^*M, \mathbb{R}_+)$ for $k \in \{0, 1, 2, \dots\}$. If a and a_j have the properties above, we write

$$a \sim \sum_{j=0}^{\infty} a_j \text{ in } S^{m_0}_{1,0,d}(T^*M, \mathbb{R}_+).$$

Let $S^m_{\mathrm{cl},d}(T^*M, \mathbb{R}_+)$ be the space of all symbols $a(x, \xi, t) \in S^m_{1,0,d}(T^*M, \mathbb{R}_+)$ with $a(x, \xi, t) \sim \sum_{j=0}^{\infty} a_{m-j}(x, \xi, t)$ in $S^m_{1,0,d}(T^*M, \mathbb{R}_+)$, where $a_{m-j}(x, \xi, t)$ is positively homogeneous of degree $m - j$ in $(\xi, t^{\frac{1}{d}})$; i.e.

$$a_{m-j}(x, \lambda\xi, \lambda^d t) = \lambda^{m-j} a_{m-j}(x, \xi, t), \quad \text{for } t \in \mathbb{R}_+,\ \lambda \geq 1,\ |\xi| \geq 1.$$

Let $a(x, \xi, t) \in S^m_{\mathrm{cl},d}(T^*M, \mathbb{R}_+)$. We construct a pseudodifferential operator P_t, depending smoothly on t, by

$$(P_t u)(x) = \frac{1}{(2\pi)^3} \int e^{i<x-y,\xi>} a(x, \xi, t) u(y) dy d\xi \quad \text{for all } u \in C^\infty(M).$$

We call $a(x, \xi, t)$ the symbol of P_t and $a_m(x, \xi, t)$ the principal symbol of P_t. In this case, we will write $P_t \in L^m_{\mathrm{cl},d}(M, \mathbb{R}_+)$.

Let $P_t \in L^{-2}_{\mathrm{cl},2}(M, \mathbb{R}_+)$. Then $P_t \colon H^s(M) \to H^{s+2}(M)$ is continuous for all $s \in \mathbb{Z}$ and all $t \in \mathbb{R}_+$. Let $f(t)$ be a strictly positive continuous function. We write

$$P_t = O(f(t)) \colon H^{s_1}(M) \to H^{s_2}(M), \quad s_1, s_2 \in \mathbb{Z},$$

if $\|P_t u\|_{s_2} \leq C f(t) \|u\|_{s_1}$ for all $u \in H^{s_1}(M)$ and all $t \in \mathbb{R}_+$, where $\|\cdot\|_s$ denotes the standard Sobolev norm of order s and $C > 0$ is a constant independent of t.

We return to our situation. Put

$$E_2 = (2E_1)^2 + \hat{E}_1, \tag{9.3}$$

where $E_1, \hat{E}_1 \in L^1_{\mathrm{cl}}(M)$ are as in Theorem 9.1. Let $e_2(x, \xi) \in S^2_{\mathrm{cl}}(T^*M)$ be the principal symbol of E_2. The following is well-known [28, Chapter 2].

Theorem 9.4. *There exists $G_t \in L^{-2}_{\mathrm{cl},2}(M, \mathbb{R}_+)$ depending continuously on t in $L^2(M)$ such that*

$$G_t = O\left(\frac{1}{1+t}\right) \colon H^s(M) \to H^s(M) \qquad \text{for all } s \in \mathbb{Z}, \tag{9.4}$$

$$G_t = O\left(\frac{1}{\sqrt{1+t}}\right) \colon H^s(M) \to H^{s+1}(M) \qquad \text{for all } s \in \mathbb{Z}, \tag{9.5}$$

$$G_t = O(1) \colon H^s(M) \to H^{s+2}(M) \qquad \text{for all } s \in \mathbb{Z}, \tag{9.6}$$

$$g_0(x, \xi, t) = \frac{1}{e_2(x, \xi) + t} \qquad \text{for all } |\xi| \geq 1, \tag{9.7}$$

$$(E_2 + t) G_t = I + F_t \qquad \text{for all } t > 0, \tag{9.8}$$

where $g_0(x, \xi, t)$ denotes the principal symbol of G_t and F_t is a smoothing operator on M depending smoothly on t with the property that for all $m \in \mathbb{N}_0$, there is a constant $C_m > 0$ such that for all $t \in \mathbb{R}_+$,

$$|F_t(x, y)|_{C^m(M \times M)} \leq C_m \frac{1}{1+t}.$$

Moreover, in local coordinates x, let $g(x,\xi,t)$ denote the full symbol of G_t. Then, for every $\alpha,\beta\in\mathbb{N}_0^3$, there is a constant $C_{\alpha,\beta}>0$, independent of t, such that

$$\left|\partial_x^\alpha\partial_\xi^\beta g(x,\xi,t)\right|\leq C_{\alpha,\beta}\frac{1}{\sqrt{1+t}}(1+|\xi|)^{-1-|\beta|}\quad \text{for all } |\xi|\geq 1,$$
$$\left|\partial_x^\alpha\partial_\xi^\beta g(x,\xi,t)\right|\leq C_{\alpha,\beta}\frac{1}{1+t}(1+|\xi|)^{-|\beta|}\quad \text{for all } |\xi|\geq 1.$$

10. Some smoothing properties for the Szegő projection

The next step towards the proof of Theorem 1.3 is to better understand the smooth properties of the Szegő projection S. Specifically, we need to understand the smooth properties of SP_t for a t-dependent family of pseudodifferential operators.

To begin, we recall the Carnot-Carathéodory metric on our CR manifold M. Fix $Z\in C^\infty(M,T^{1,0}M)$ with $\langle Z\,|\,Z\rangle=1$ on M. For $\delta>0$, let $C(\delta)$ be the class of all absolutely continuous mappings $\gamma\colon[0,1]\to M$ such that for almost every t,

$$\gamma'(t)=a_1(t)V_1(\gamma(t))+a_2(t)V_2(\gamma(t)),\quad |a_j(t)|<\delta,\quad j=1,2.$$

Here V_1 and V_2 are the real and imaginary parts of Z respectively. The Carnot-Carathéodory metric on X is then defined by

$$\vartheta(x,y)=\inf\{\delta>0\colon \text{ there exists } \gamma\in C(\delta) \text{ such that } \gamma(0)=x,\gamma(1)=y\}$$

for $x,y\in M$. Let (z,t) be CR normal coordinates defined in a neighborhood of $p\in M$ such that $(z(p),t(p))=(0,0)$. Define $\rho^4(z,t)=|z|^4+t^2$. It is easy to see (cf. [23, Section 3]) that there exist an open set U of p and a constant $C>1$ such that

$$\frac{1}{C}\vartheta(x,p)\leq\rho(x)\leq C\vartheta(x,p),\quad \text{for all } x\in U.$$

Denote by $B(x,r)$ the non-isotropic ball $\{y\in M\colon\vartheta(x,y)<r\}$ of radius r centered at x. Let $k\in\mathbb{N}$. We denote by ∇_b^k any differential operator of the form $L_1\dots L_k$, where $L_j\in C^\infty(M,H_{\mathbb{C}})$ satisfy $\langle L_j\,|\,L_j\rangle\leq 1$ for $j=1,\dots,k$.

Next, we define a class of (non-isotropic) smoothing operators of order j. For our purposes, it suffices to restrict to the case when $0\leq j<4$.

A r-dependent smooth function ϕ_r on M is said to be a *normalized bump function* if for every $r>0$, $\operatorname{supp}\phi_r\subset B(x,r)$ and

$$\left\|\nabla_b^k\phi_r\right\|_{L^\infty(B(x,r))}\leq C_k r^{-k}\tag{10.1}$$

for all $k\geq 0$; here $C_k>0$ are absolute constants independent of r. If (10.1) only holds for $0\leq k\leq N$ for some large integer N, we say that ϕ_r is a normalized bump function of order N.

Suppose that A is a continuous linear operator $A\colon C^\infty(M)\to C^\infty(M)$ and its adjoint A^* is also a continuous map $A^*\colon C^\infty(M)\to C^\infty(M)$. We say that A is a smoothing operator of order j, $j\geq 0$, if

(1) there exists a kernel $A(x,y)$, defined and smooth away from the diagonal in $M\times M$, such that

$$Af(x)=\int_M A(x,y)f(y)dv_M(y)\tag{10.2}$$

for any $f\in C^\infty(M)$, and every $x\notin\operatorname{supp}f$, where $dv_M=\theta\wedge d\theta$;

(2) for all $x \neq y$, the kernel $A(x,y)$ satisfies

$$|(\nabla_b)_x^{\alpha_1}(\nabla_b)_y^{\alpha_2} A(x,y)| \lesssim_\alpha \vartheta(x,y)^{-4+j-\alpha} \quad \text{for all } \alpha_1,\alpha_2 \in \mathbb{N}_0,\ \alpha=\alpha_1+\alpha_2;$$

(3) the operators A and A^* satisfy the following cancellation conditions of order j: if ϕ_r is a normalized bump function, then for every $r>0$

$$\|\nabla_b^\alpha A\phi\|_{L^\infty(B(x,r))} \leq C_\alpha r^{j-\alpha},$$
$$\|\nabla_b^\alpha A^*\phi\|_{L^\infty(B(x,r))} \leq C_\alpha r^{j-\alpha},$$

where $C_\alpha > 0$ is a constant independent of r.

Since M is embeddable, $\Box_b$ has L^2 closed range. Let

$$N\colon L^2(M) \to \operatorname{Dom}\Box_b$$

be the partial inverse of $\Box_b$ and let $N(x,y)$ be the distributional kernel of N. The following is well-known (see [23, Theorem 2.2])

Theorem 10.1. *The Szegő projection S and the partial inverse N of $\Box_b$ are smoothing operators of orders* 0 *and* 2*, respectively.*

We also need to study one-parameter families of smooth operators.

Definition 10.2. Let A_t be a t-dependent smoothing operator of order j, $0 \leq j < 4$, where $t \in \mathbb{R}_+$. Let $f(t)$ be a positive continuous function of $t \in \mathbb{R}_+$. We say that A_t is a smoothing operator of order j with size $f(t)$ if for every $m \in \mathbb{N}_0$, every $r>0$ and any normalized bump function ϕ, there are constants $C_m, C_{m,r} > 0$, independent of t, such that for all $t \in \mathbb{R}_+$,

$$|(\nabla_b)_x^{\alpha_1}(\nabla_b)_y^{\alpha_2} A_t(x,y)| \leq C_m f(t)\vartheta(x,y)^{-4+j-\alpha} \quad \text{for all } \alpha=\alpha_1+\alpha_2 \leq m,$$
$$\|\nabla_b^\alpha A_t\phi\|_{L^\infty(B(x,r))} \leq f(t) C_{m,r} r^{j-\alpha} \quad \text{for all } \alpha \leq m,$$
$$\|\nabla_b^\alpha A_t^*\phi\|_{L^\infty(B(x,r))} \leq f(t) C_{m,r} r^{j-\alpha} \quad \text{for all } \alpha \leq m.$$

We also need the following result [23, Theorem 2.2 and Theorem 2.3].

Theorem 10.3. *Let A_t and B_t be t-dependent smoothing operators of orders j_1 and j_2 with sizes $f(t)$ and $g(t)$, respectively, where $j_1, j_2 \geq 0$ and $j_1+j_2<4$. Then A_tB_t is a smoothing operator of order j_1+j_2 with size $f(t)g(t)$.*

Let $P_t^{(j)} \in L^{-j}_{\mathrm{cl},2}(M,\mathbb{R}_+)$ with symbol $p^{(j)}(x,\xi,t)$, $j=0,1,2$. It is easy to see that for every $\alpha,\beta \in \mathbb{N}_0^3$, there is a constant $C_{\alpha,\beta}>0$ independent of t such that

$$\left|\partial_x^\alpha \partial_\xi^\beta p^{(j)}(x,\xi,t)\right| \leq C_{\alpha,\beta}(1+t)^{-\frac{j}{2}}(1+|\xi|)^{-|\beta|} \quad \text{for all } |\xi| \geq 1, \quad j=0,1,2. \tag{10.3}$$

Using the following lemma, we establish an analogue of Theorem 10.1.

Lemma 10.4. *Consider $B(x,r)$, where $x \in M$ and $r>0$ is a small constant. Let $\chi_r \in C_0^\infty((B(x,2r))$ with $\chi_r \equiv 1$ on $B(x,r)$. Then, we can find ∇_b^j, $j=1,2,3$, and a constant $C>0$ independent of r such that*

$$\|f\|_{L^\infty(B(x,r))} \leq Cr\sum_{j=0}^{3}\left\|\nabla_b^j(\chi_r f)\right\| \quad \textit{for all } f \in C^\infty(M). \tag{10.4}$$

Proof. Consider $-\Delta_b + I\colon \mathrm{Dom}\,(-\Delta_b + I) \subset L^2(M) \to L^2(M)$, where

$$\mathrm{Dom}\,(-\Delta_b + I) = \left\{u \in L^2(M) \;\middle|\; (-\Delta_b + I)u \in L^2(M)\right\}.$$

It is clear that $-\Delta_b + I$ is injective, self-adjoint, has L^2 closed range and hence is surjective. Let $H\colon L^2(M) \to \mathrm{Dom}\,(-\Delta_b + I)$ be its inverse. Put $B := H^2$. We have

$$B(-\Delta_b + I)^2 = I \quad \text{on } C^\infty(M). \tag{10.5}$$

It is known that (see [23, Appendix A])

$$\begin{aligned} &B \text{ is a smoothing operator of order } 4 - \varepsilon \text{ for every } \varepsilon > 0,\\ &B\nabla_b \text{ is a smoothing operator of order } 3. \end{aligned} \tag{10.6}$$

Let $f \in C^\infty(M)$. From (10.5), we have

$$\chi_r f = B(-\Delta_b + I)^2 \chi_r f = \sum_{j=0}^{4} B\nabla_b^j \chi_r f. \tag{10.7}$$

Fix $x_0 \in B(x, r)$. From (10.7), we have

$$f(x_0) = (\chi_r f)(x_0) = (B\nabla_b^4 \chi_r f)(x_0) + \sum_{j=0}^{3} (B\nabla_b^j \chi_r f)(x_0). \tag{10.8}$$

We first estimate $\sum_{j=0}^{3}(B\nabla_b^j \chi_r f)(x_0)$. Let $0 < \delta < r$ and let ϕ_δ be a *normalized bump function* with $\mathrm{supp}\,\phi_\delta \subset B(x_0, \delta)$, $0 \le \phi_\delta \le 1$ and $\phi_\delta = 1$ near x_0. We have

$$\sum_{j=0}^{3} (B\nabla_b^j \chi_r f)(x_0) = \sum_{j=0}^{3} (B\phi_\delta \nabla_b^j \chi_r f)(x_0) + \sum_{j=0}^{3} (B(1 - \phi_\delta)\nabla_b^j \chi_r f)(x_0). \tag{10.9}$$

By (10.2), we have

$$\begin{aligned} &\left|\sum_{j=0}^{3} (B(1 - \phi_\delta)\nabla_b^j \chi_r f)(x_0)\right| \\ &= \left|\sum_{j=0}^{3} \int B(x_0, y)\big((1 - \phi_\delta)\nabla_b^j \chi_r f\big)(y) dv_M(y)\right| \\ &\le \sum_{j=0}^{3} \Big(\int_{y \in B(x_0, 2r), y \notin B(x_0, \delta)} |B(x_0, y)|^2 \, dv_M(y)\Big)^{\frac{1}{2}} \left\|\nabla_b^j (\chi_r f)\right\|. \end{aligned} \tag{10.10}$$

From (10.6), we can check that

$$\int_{y \in B(x_0, 2r), y \notin B(x_0, \delta)} |B(x_0, y)|^2 \, dv_M(y) \le C_2 \int_{B(x_0, 2r)} \vartheta(x_0, y)^{-2} dy \le C_3 r^2, \tag{10.11}$$

where C_2, C_3 are positive constants independent of r, δ and the point x_0. From (10.10) and (10.11), we deduce that

$$\left|\sum_{j=0}^{3} (B(1 - \phi_\delta)\nabla_b^j \chi_r f)(x_0)\right| \le Cr \left\|\nabla_b^j (\chi_r f)\right\|, \tag{10.12}$$

where $C > 0$ is a constant independent independent of r, δ and the point x_0. Note that $\phi_\delta \nabla_b^j \chi_r f$ is a *normalized bump function* with $\operatorname{supp}\phi_\delta \subset B(x_0, \delta)$. Fix $0 < \varepsilon_0 < 1$. Since B is a somoothing operator of order $4 - \varepsilon_0$, we have

$$\left|\sum_{j=0}^{3} (B\phi_\delta \nabla_b^j \chi_r f)(x_0)\right| \leq C_{j,f,r}\delta^{4-\varepsilon_0}, \tag{10.13}$$

where $C_{j,f,r} > 0$ is a constant independent of δ but depend on ∇_b^j, χ_r and f (possible depending on many derivatives of $\nabla_b^j \chi_r f$). From (10.9), (10.12) and (10.13), we deduce that

$$\left|\sum_{j=0}^{3} (B\nabla_b^j \chi_r f)(x_0)\right| \leq Cr \left\|\nabla_b^j(\chi_r f)\right\| + C_{j,f,r}\delta^{4-\varepsilon_0}. \tag{10.14}$$

Let $\delta \to 0$ in (10.14), we get

$$\left|\sum_{j=0}^{3} (B\nabla_b^j \chi_r f)(x_0)\right| \leq Cr \left\|\nabla_b^j(\chi_r f)\right\|. \tag{10.15}$$

We have $(B\nabla_b^4 \chi_r f)(x_0) = (B\nabla_b)(\nabla_b^3 \chi_r f)(x_0)$. We can repeat the proof of (10.15) with minor change and deduct that

$$\left|(B\nabla_b^4 \chi_r f)(x_0)\right| \leq \hat{C}r \left\|\nabla_b^3(\chi_r f)\right\|, \tag{10.16}$$

where $\hat{C} > 0$ is a constant independent independent of r and the point x_0. From (10.8), (10.15) and (10.16), the lemma follows. □

Lemma 10.5. *Fix $j \in \mathbb{N}$. For every $s \in \mathbb{Z}$ and any ∇_b^j, we have*

$$\nabla_b^j S : H^s(M) \to H^{s-\frac{j}{2}}(M).$$

Proof. It is known (see Proposition 5.18 in [20]) that S is a pseudodifferential operator of order 0 type $(\frac{1}{2}, \frac{1}{2})$; i.e. $S \in L^0_{\frac{1}{2},\frac{1}{2}}(M)$. Let $P \in C^\infty(M, \mathbb{C}TM)$ be any differential operator. We claim that

$$[P, S] = PS - SP \in L^{\frac{1}{2}}_{\frac{1}{2},\frac{1}{2}}(M). \tag{10.17}$$

Let $x = (x_1, x_2, x_3)$ be local coordinates of M defined on an open set Ω of M. Since $S \in L^0_{\frac{1}{2},\frac{1}{2}}(M)$, the distribution kernel of S satisfies $S(x, y) \equiv \int e^{i<x-y,\eta>} a(x, \eta) d\eta$ on Ω, where $a(x, \eta) \in S^0_{\frac{1}{2},\frac{1}{2}}(T^*\Omega)$. For simplicity, we may assume that $P = \frac{\partial}{\partial x_1}$. Then, is is easy to check that $[P, S] \equiv \int e^{i<x-y,\eta>} \frac{\partial}{\partial x_1} a(x, \eta)$. Since $\frac{\partial}{\partial x_1} a(x, \eta) \in S^{\frac{1}{2}}_{\frac{1}{2},\frac{1}{2}}(T^*\Omega)$, the claim (10.17) follows. Let $Z \in C^\infty(M, T^{1,0}M)$. We have $(SZ)^* = Z^*S = -\overline{Z}S + rS$, where $(SZ)^*$ and Z^* are adjoints of SZ and Z respective and r is a zero order differential operator. Since $\overline{Z}S = 0$, we deduce that $(SZ)^* \in L^0_{\frac{1}{2},\frac{1}{2}}(M)$ and hence $SZ \in L^0_{\frac{1}{2},\frac{1}{2}}(M)$. From this observation and (10.17), we have $ZS = [Z, S] + SZ \in L^{\frac{1}{2}}_{\frac{1}{2},\frac{1}{2}}(M)$. We have proved that for every $L \in C^\infty(M, H_{\mathbb{C}})$, we have

$$LS \in L^{\frac{1}{2}}_{\frac{1}{2},\frac{1}{2}}(M).$$

Now, assume that there is a $k_0 \in \mathbb{N}$ such that for any $\hat{L}_j \in C^\infty(M, H_{\mathbb{C}})$, $j = 1, \ldots, k_0$, we have $\hat{L}_1 \hat{L}_2 \cdots \hat{L}_{k_0} S \in L^{\frac{k_0}{2}}_{\frac{1}{2},\frac{1}{2}}(M)$. Take any $L_j \in C^\infty(M, H_{\mathbb{C}})$, $j = 1, \ldots, k_0 + 1$. We are going to prove that $L_1 L_2 \cdots L_{k_0+1} S \in L^{\frac{k_0+1}{2}}_{\frac{1}{2},\frac{1}{2}}(M)$. By reduction assumption and repeating the proof of (10.17), we have

$$[L_1, L_2 \cdots L_{k_0+1} S] = L_1 L_2 \cdots L_{k_0+1} S - L_2 \cdots L_{k_0+1} S L_1 \in L^{\frac{k_0+1}{2}}_{\frac{1}{2},\frac{1}{2}}(M). \tag{10.18}$$

Now, $L_2 \cdots L_{k_0+1} S L_1 = (L_2 \cdots L_{k_0+1} S)(S L_1)$. Since $L_2 \cdots L_{k_0+1} S \in L^{\frac{k_0}{2}}_{\frac{1}{2},\frac{1}{2}}(M)$ and $S L_1 \in L^{\frac{1}{2}}_{\frac{1}{2},\frac{1}{2}}(M)$, we deduce that

$$L_2 \cdots L_{k_0+1} S L_1 \in L^{\frac{k_0+1}{2}}_{\frac{1}{2},\frac{1}{2}}(M). \tag{10.19}$$

From (10.19) and (10.18), we get $L_1 L_2 \cdots L_{k_0+1} S \in L^{\frac{k_0+1}{2}}_{\frac{1}{2},\frac{1}{2}}(M)$. By induction assumption, we conclude that for any $j \in \mathbb{N}$ and any ∇_b^j, we have $\nabla_b^j S \in L^{\frac{j}{2}}_{\frac{1}{2},\frac{1}{2}}(M)$ and by classical result of Calderon-Vaillancourt (see Chapter VIII of [19]), we have

$$\nabla_b^j S : H^s(X) \to H^{s-\frac{j}{2}}(X), \quad \text{for every } s \in \mathbb{Z}.$$

The lemma follows. $\square$

Theorem 10.6. *For every $j = 0, 1, 2$, the operators $SP_t^{(j)}$ and $P_t^{(j)} S$ are smoothing operators of orders 0 with sizes $(1+t)^{-\frac{j}{2}}$.*

Proof. Let ϕ_r be a normalized bump function such that $\operatorname{supp} \phi_r \subset B(x, r)$, for every $r > 0$. From (10.4), we can find ∇_b^j, $j = 1, 2, 3$, and a constant $C > 0$ independent of r such that

$$\left\| SP_t^{(1)} \phi_r \right\|_{L^\infty(B(x,r))} \leq Cr \sum_{j=0}^{3} \left\| \nabla_b^j (\chi_r S P_t^{(1)} \phi_r) \right\|, \tag{10.20}$$

where χ_r is as in Lemma 10.4 and $C > 0$ is a constant independent of r, ϕ_r, x and t. We claim that for any ∇_b^j, $j = 0, 1, 2, 3, 4$, we have

$$\left\| \nabla_b^j S P_t^{(1)} \phi_r \right\| \leq c_j \frac{1}{\sqrt{1+t}} r^{2-j}, \tag{10.21}$$

where $c_j > 0$ is a constant independent of r, x and t. Fix $j \in \{0, 1, 2, 3, 4\}$. From Lemma 10.5, for any ∇_b^{2j}, we have

$$\nabla_b^{2j} S \colon H^s(M) \to H^{s-j}(M) \quad \text{for all } s \in \mathbb{Z}. \tag{10.22}$$

Moreover, from (10.3), we can check that

$$P_t^{(1)} = O(\frac{1}{\sqrt{1+t}}) \colon H^s(M) \to H^s(M) \quad \text{for all } s \in \mathbb{Z}. \tag{10.23}$$

From (10.22) and (10.23), we deduce that for any ∇_b^{2j}, we have

$$\nabla_b^{2j} S P_t^{(1)} = O(\frac{1}{\sqrt{1+t}}) \colon H^s(M) \to H^{s-j}(M) \quad \text{for all } s \in \mathbb{Z}. \tag{10.24}$$

Fix any ∇_b^j. From (10.24), for any we have

(10.25)
$$\begin{aligned}\left\|\nabla_b^j SP_t^{(1)}\phi_r\right\|^2 &= (\,\nabla_b^j SP_t^{(1)}\phi_r \,|\, \nabla_b^j SP_t^{(1)}\phi_r\,) = (\,(\nabla_b^j)^*\nabla_b^j SP_t^{(1)}\phi_r \,|\, SP_t^{(1)}\phi_r\,)\\ &\lesssim \frac{1}{1+t}\left\|\phi_r\right\|_j\left\|\phi_r\right\|\\ &\lesssim \frac{1}{1+t}\left\|\nabla_b^{2j}\phi_r\right\|\left\|\phi_r\right\|, \quad \text{for some } \nabla_b^{2j},\\ &\lesssim \frac{1}{1+t}r^{4-2j},\end{aligned}$$

where $\left\|\phi_r\right\|_j$ denotes the standard Sobolev norm of ϕ_r of order j. From (10.25), the claim (10.21) follows.

From (10.20) and (10.21) we can check that

$$\begin{aligned}\left\|SP_t^{(1)}\phi_r\right\|_{L^\infty(B(x,r))} &\lesssim r\sum_{j=0}^{3}\left\|\nabla_b^j(\chi_r SP_t^{(1)}\phi_r)\right\|\\ &\lesssim r\left\|\chi_r SP_t^{(1)}\phi_r\right\| + r\sum_{j=1}^{3}\sum_{s=0}^{j} r^{-j+s}\left\|\nabla_b^s(SP_t^{(1)}\phi_r)\right\|\\ &\lesssim r\frac{1}{\sqrt{1+t}} + r\sum_{j=1}^{3}\sum_{s=0}^{j} r^{-j+s}\frac{1}{\sqrt{1+t}}r^{2-s}\\ &\lesssim \frac{1}{\sqrt{1+t}}.\end{aligned}$$

We can repeat the method above with minor changes and get that for every $j\in\mathbb{N}_0$ and every ∇_b^j, $\left\|\nabla_b^j SP_t^{(1)}\phi_r\right\| \lesssim_j \frac{1}{\sqrt{1+t}}r^{-j}$. Thus, $SP_t^{(1)}$ satisfies the cancellation condition of order 0 with size $\frac{1}{\sqrt{1+t}}$. Similarly, we can repeat the procedure above with minor change and obtain that $(SP_t^{(1)})^*$ satisfies the cancellation condition of order 0 with size $\frac{1}{\sqrt{1+t}}$.

Now, we estimate the kernel $SP_t^{(1)}(x,y)$. Let $x=(x_1,x_2,x_3)$ be local coordinates for M defined in an open set $D\subset M$. From Theorem 7.2 and the complex stationary phase formula of Melin–Sjöstrand [27], it follows that

$$(SP_t^{(1)})(x,y) = \int_0^\infty e^{i\varphi(x,y)s}b(x,y,s,t)ds + F_t(x,y) \quad \text{on } D\times D,$$

where $b(x,y,s,t)\in C^\infty(D\times D\times\mathbb{R}_+\times\mathbb{R}_+)$, and for every $\alpha,\beta\in\mathbb{N}_0^3$, $\gamma\in\mathbb{N}_0$, there is a constant $C_{\alpha,\beta,\gamma}>0$, independent of t, such that on $D\times D$,

$$\begin{cases}\left|\partial_x^\alpha\partial_y^\beta\partial_s^\gamma b(x,y,s,t)\right| \le C_{\alpha,\beta,\gamma}(\sqrt{s^2+t})^{-\gamma}, & \text{if } \gamma\ge 1\\ \left|\partial_x^\alpha\partial_y^\beta b(x,y,s,t)\right| \le C_{\alpha,\beta,\gamma}(\frac{s}{\sqrt{s^2+t}}), & \text{if } \gamma=0,\end{cases} \tag{10.26}$$

and F_t is a smoothing operator on D depending smoothly on t with the property that for all $m\in\mathbb{N}_0$, there is a constant $C_m>0$ such that for all $t\in\mathbb{R}_+$,

$$\left|F_t(x,y)\right|_{C^m(M\times M)} \le C_m\frac{1}{\sqrt{1+t}}.$$

From (10.26), the formula

$$\int_0^\infty e^{i\varphi(x,y)s}b(x,y,s,t)ds=\int_0^\infty \frac{1}{(i\varphi(x,y))^2}\frac{\partial^2}{\partial s^2}(e^{i\varphi(x,y)s})b(x,y,s,t)ds,$$

and distribution theory (see Remark 10.7 below) one can check that

$$\begin{aligned}\int_0^\infty & e^{i\varphi(x,y)s}b(x,y,s,t)ds\\ &=\int_1^\infty \frac{1}{(i\varphi(x,y))^2}e^{i\varphi(x,y)s}\frac{\partial^2}{\partial s^2}b(x,y,s,t)ds+\frac{1}{(i\varphi(x,y))^2}H_t(x,y),\end{aligned}\tag{10.27}$$

where H_t is a smoothing operator on D depending smoothly on t with the property that for every compact set $K\subset D$, all $k\in\mathbb{N}_0$, there is a constant $\widetilde{C}_k>0$ such that for all $t\in\mathbb{R}_+$,

$$|H_t(x,y)|_{C^m(K\times K)}\leq \widetilde{C}_k\frac{1}{\sqrt{1+t}}.\tag{10.28}$$

Again, from (10.26), we have

$$\begin{aligned}\left|\int_1^\infty \frac{1}{(i\varphi(x,y))^2}e^{i\varphi(x,y)s}\frac{\partial^2}{\partial s^2}b(x,y,s,t)ds\right| &\leq \hat{C}\frac{1}{|\varphi(x,y)|^2}\int_1^\infty \frac{1}{s^2+t}ds\\ &\leq \hat{C}_1\frac{1}{\sqrt{1+t}}\frac{1}{|\varphi(x,y)|^2},\end{aligned}\tag{10.29}$$

for all $t\in\mathbb{R}_+$, where $\hat{C}>0$, $\hat{C}_1>0$ are constants independent of t. It is known that (see [20, Theorem 1.4]) $|\varphi(x,y)|\approx\vartheta(x,y)^2$. From this observation, (10.27) and (10.29), we conclude that

$$\left|(SP_t^{(1)})(x,y)\right|\leq C\frac{1}{\sqrt{1+t}}\vartheta(x,y)^{-4}$$

for all $x,y\in M$ with $x\neq y$, where $C>0$ is a constant independent of t.

For every $m\in\mathbb{N}$, we can repeat the procedure above with minor change and deduce that there is a constant $C_m>0$ independent of t such that

$$|(\nabla_b)_x^{\alpha_1}(\nabla_b)_y^{\alpha_2}(SP_t^{(1)})(x,y)|\leq C_m\frac{1}{\sqrt{1+t}}\vartheta(x,y)^{-4-\alpha}$$

for all $\alpha=\alpha_1+\alpha_2\leq m$. Thus, $SP_t^{(1)}$ is a smoothing operator of order 0 with size $\frac{1}{\sqrt{1+t}}$.

Arguing similarly yields that $SP_t^{(j)}$, $j=0,2$, are smoothing operators of order 0 with size $(1+t)^{-j/2}$. □

Remark 10.7. We explain (10.27). We have

$$\int_0^\infty e^{i\varphi(x,y)s}b(x,y,s,t)ds=\int_0^1 e^{i\varphi(x,y)s}b(x,y,s,t)ds+\int_1^\infty e^{i\varphi(x,y)s}b(x,y,s,t)ds.$$

The kernel $\mathcal{R}_t(x,y):=\int_0^1 e^{i\varphi(x,y)s}b(x,y,s,t)ds$ is smooth and from (10.26), we have that for every compact subset $K\Subset D$ and every $k\in\mathbb{N}_0$, there is a constant $C_k>0$ independent of t such that

$$|\mathcal{R}_t(x,y)|_{C^k(K\times K)}\leq C_k\sqrt{1+t},\quad\text{for all } t\in\mathbb{R}_+.$$

We only need to study the kernel $\int_1^\infty e^{i\varphi(x,y)s}b(x,y,s,t)ds$. From distribution theory and by using integration by parts, we have

$$\begin{aligned}
&\int_1^\infty e^{i\varphi(x,y)s}b(x,y,s,t)ds \\
&= \lim_{\varepsilon\to 0^+}\int_1^\infty e^{i(\varphi(x,y)+i\varepsilon)s}b(x,y,s,t)ds \\
&= \lim_{\varepsilon\to 0^+}\int_1^\infty \frac{1}{(i(\varphi(x,y)+i\varepsilon))^2}\frac{\partial^2}{\partial s^2}(e^{i(\varphi(x,y)+i\varepsilon)s})b(x,y,s,t)ds \\
&= \lim_{\varepsilon\to 0^+}\Big(-\frac{1}{(i(\varphi(x,y)+i\varepsilon))}e^{i(\varphi(x,y)+i\varepsilon)}b(x,y,1,t) \\
&\quad + \frac{1}{(i(\varphi(x,y)+i\varepsilon))^2}e^{i(\varphi(x,y)+i\varepsilon)}\frac{\partial b}{\partial s}(x,y,1,t) \\
&\quad + \int_1^\infty e^{i(\varphi(x,y)+i\varepsilon)s}\frac{\partial^2}{\partial s^2}b(x,y,s,t)ds\Big)
\end{aligned} \tag{10.30}$$

From (10.30) and (10.27), we deduce that

$$H_t(x,y) = -(i\varphi(x,y))e^{i\varphi(x,y)}b(x,y,1,t) + e^{i\varphi(x,y)}\frac{\partial b}{\partial s}(x,y,1,t) + (i\varphi(x,y))^2\mathcal{R}(x,y). \tag{10.31}$$

From (10.26) and (10.31), it is easy to see that $H_t(x,y)$ satisfies (10.28).

We need two results about the smoothing properties of the operators G_t from Theorem 9.4.

Lemma 10.8. *Let $G_t \in L^{-2}_{\mathrm{cl},2}(M,\mathbb{R}_+)$ be as in Theorem 9.4. Then, $\tau G_t\tau$ is a smoothing operator of order 2 with size $\frac{1}{\sqrt{1+t}}$. Moreover, $\tau G_t\tau$ is also a smoothing operators of order 0 with size $\frac{1}{1+t}$.*

Proof. From Theorem 7.1, Lemma 8.3 and (9.4), it is straightforward to see that

$$\begin{aligned}
\tau G_t\tau &= SG_tS + \overline{S}G_t\overline{S} + F_t \\
&= S\overline{N}\,\overline{\Box}_bG_tS + \overline{S}N\Box_bG_t\overline{S} + H_t,
\end{aligned} \tag{10.32}$$

where F_t and H_t are smoothing operators on M depending smoothly on t with the property that for all $m \in \mathbb{N}_0$, there is a constant $C_m > 0$ such that for all $t \in \mathbb{R}_+$,

$$\begin{aligned}
|F_t(x,y)|_{C^m(M\times M)} &\le C_m\frac{1}{1+t}, \\
|H_t(x,y)|_{C^m(M\times M)} &\le C_m\frac{1}{1+t}.
\end{aligned}$$

Note that $\Box_bG_t, \overline{\Box}_bG_t \in L^0_{\mathrm{cl},2}(M,\mathbb{R}_+)$. From this observation, Theorem 10.3, Theorem 10.6 and (10.32), we conclude that $\tau G_t\tau$ is a smoothing operator of order 0 with size $\frac{1}{1+t}$.

From Lemma 8.2, we have

$$\begin{aligned}
S\overline{N}\,\overline{\Box}_bG_tS &= S\overline{N}\Box_bG_tS + S\overline{N}EG_tS \\
&= S\overline{N}[\Box_b, G_t]S + S\overline{N}EG_tS,
\end{aligned}$$

where E is a first order partial differential operator. Note that $[\Box_b, G_t], EG_t \in L^{-1}_{\mathrm{cl},2}(M,\mathbb{R}_+)$. From this observation, Theorem 10.3 and Theorem 10.6, we conclude that $S\overline{N}[\Box_b, G_t]S + S\overline{N}EG_tS$ is a smoothing operator of order 2 with size $\frac{1}{\sqrt{1+t}}$. Similarly, $\overline{S}N\Box_bG_t\overline{S}$ is a smoothing operator of order 2 with size $\frac{1}{\sqrt{1+t}}$. From (10.32), we conclude that $\tau G_t\tau$ is a smoothing operator of order 2 with size $\frac{1}{\sqrt{1+t}}$. The lemma follows. $\Box$

Lemma 10.9. *Let $E_2 \in L^2_{\mathrm{cl}}(M)$ be as in* (9.3). *Then $\tau E_2(I-\tau)G_t\tau$ is a smoothing operator of order* 1 *with size* 1.

Proof. From Theorem 7.1, Lemma 8.3 and (9.4), we check that

$$\begin{aligned}\tau E_2(I-\tau)G_t\tau &= SE_2(I-S)G_tS + \overline{S}E_2(I-\overline{S})G_t\overline{S} + F_t\\ &= SE_2\Box_bNG_tS + \overline{S}E_2\overline{\Box}_b\overline{N}G_t\overline{S} + F_t,\end{aligned} \tag{10.33}$$

where F_t is a smoothing operators on M depending smoothly on t with the property that for all $m \in \mathbb{N}_0$, there is a constant $C_m > 0$ such that for all $t \in \mathbb{R}_+$,

$$|F_t(x,y)|_{C^m(M\times M)} \leq C_m\frac{1}{1+t}.$$

Again, from Theorem 7.1, Lemma 8.3 and (9.4), we check that

$$\begin{aligned}SE_2\Box_bNG_tS &= S[E_2, \overline{\partial}^*_b]\overline{\partial}_bNG_tS\\ &= S[E_2, \overline{\partial}^*_b]\overline{\partial}_bN\overline{N}^2\,\overline{\Box}^2_bG_tS + H_t,\end{aligned} \tag{10.34}$$

where H_t is a smoothing operator on M depending smoothly on t with the property that for all $m \in \mathbb{N}_0$, there is a constant $C_m > 0$ such that for all $t \in \mathbb{R}_+$,

$$|H_t(x,y)|_{C^m(M\times M)} \leq C_m\frac{1}{1+t}.$$

From Lemma 8.2, we have

$$\begin{aligned}&S[E_2, \overline{\partial}^*_b]\overline{\partial}_bN\overline{N}^2\,\overline{\Box}^2_bG_tS\\ &= S[E_2, \overline{\partial}^*_b]\overline{\partial}_bN\overline{N}^2\overline{\Box}_b[\Box_b, G_t]S + S[E_2, \overline{\partial}^*_b]\overline{\partial}_bN\overline{N}^2\overline{\Box}_bZ_0S\\ &= S[E_2, \overline{\partial}^*_b]\overline{\partial}_bN\overline{N}^2[\Box_b, [\Box_b, G_t]]S + S[E_2, \overline{\partial}^*_b]\overline{\partial}_bN\overline{N}^2Z_1[\Box_b, G_t]S\\ &\quad + S[E_2, \overline{\partial}^*_b]\overline{\partial}_bN\overline{N}^2[\Box_b, Z_0]G_tS + S[E_2, \overline{\partial}^*_b]\overline{\partial}_bN\overline{N}^2Z_2Z_0G_tS,\end{aligned} \tag{10.35}$$

where Z_0, Z_1, Z_2 are first order partial differential operators. Note that

$$[\Box_b, [\Box_b, G_t]], Z_1[\Box_b, G_t], [\Box_b, Z_0]G_t, Z_2Z_0G_t \in L^0_{\mathrm{cl},2}(M, \mathbb{R}_+).$$

From this observation and Theorem 10.6, we deduce that $[\Box_b, [\Box_b, G_t]]S$, $Z_1[\Box_b, G_t]S$, $[\Box_b, Z_0]G_tS$ and $Z_2Z_0G_tS$ are smoothing operators of order 0 with sizes 1. Moreover, from the symbolic calculus of Stein–Yung [29], we check that $S[E_2, \overline{\partial}^*_b]\overline{\partial}_bN\overline{N}^2$ is a smoothing operator of order 1.

From the discussion above and (10.35), we conclude that $S[E_2, \overline{\partial}^*_b]\overline{\partial}_bN\overline{N}^2\,\overline{\Box}^2_bG_tS$ is a smoothing operator of order 1 with size 1. Similarly, we can repeat the procedure above and conclude that $\overline{S}E_2(I-\overline{S})G_t\overline{S}$ is a smoothing operator of order 1 with size 1. The lemma now follows from (10.33). $\Box$

11. Leading term for $\left(\overline{P}_4'\right)^{-\frac{1}{2}}$

In order to identify the leading term for $\left(\overline{P}_4'\right)^{-1/2}$, we must invert $\overline{P}_4' + t + \pi$. We begin by constructing a parametrix.

Proposition 11.1. *For every $N > 0$, there are continuous operators*

$$A_{N,t} = O(\frac{1}{1+t})\colon H^s(M) \to H^{s+\frac{1}{2}}(M) \quad \textit{for all } s \in \mathbb{Z},$$
$$R_{N,t} = O(\frac{1}{1+t})\colon H^s(M) \to H^{s+N}(M) \quad \textit{for all } s \in \mathbb{Z}$$

depending continuously on t such that

1. *$A_{K,t}$ is a smoothing operator of order 3 with size $\frac{1}{\sqrt{1+t}}$;*
2. *$A_{K,t}$ is a smoothing operator of order 1 with size $\frac{1}{1+t}$;*
3. *$(\overline{P}_4' + t + \pi)(\tau G_t \tau + \tau A_{K,t}\tau) = \tau + \tau R_{K,t}\tau$ on $\mathcal{P}$.*

Proof. From Theorem 9.1 and Theorem 9.4, we have

$$\begin{aligned}(\overline{P}_4' + t + \pi)(\tau G_t \tau) &= \tau(E_2 + t)\tau G_t \tau + \pi\tau G_t\tau \\ &= \tau(E_2+t)G_t\tau - \tau E_2(I-\tau)G_t\tau + \pi\tau G_t\tau \\ &= I + \tau A_t \tau \quad \text{on } \mathcal{P},\end{aligned} \tag{11.1}$$

where

$$A_t = -\tau E_2(I-\tau)G_t\tau + \tau\widetilde{F}_t\tau. \tag{11.2}$$

Here $\widetilde{F}_t$ is a smoothing operator on M depending smoothly on t with the property that for all $m \in \mathbb{N}_0$, there is a constant $C_m > 0$ such that for all $t \in \mathbb{R}_+$,

$$\left|\widetilde{F}_t(x,y)\right|_{C^m(M\times M)} \le C_m \frac{1}{1+t}.$$

By Lemma 10.9, we have that A_t is a smoothing operator of order 1 with size 1. We claim that

$$A_t = O(1) : H^s(M) \to H^{s+\frac{1}{2}}(M) \quad \text{for all } s \in \mathbb{Z}. \tag{11.3}$$

From (10.34) and (10.35) we see that

$$\begin{aligned}&SE_2\Box_b N G_t S \\ &= S[E_2, \overline{\partial}_b^*]\overline{\partial}_b N\overline{N}^2[\Box_b,[\Box_b,G_t]]S + S[E_2,\overline{\partial}_b^*]\overline{\partial}_b N\overline{N}^2 Z_1[\Box_b, G_t]S \\ &\quad + S[E_2,\overline{\partial}_b^*]\overline{\partial}_b N\overline{N}^2[\Box_b, Z_0]G_tS + S[E_2,\overline{\partial}_b^*]\overline{\partial}_b N\overline{N}^2 Z_2Z_0G_tS + H_t,\end{aligned} \tag{11.4}$$

where Z_0, Z_1, Z_2 are first order partial differential operators and H_t is a smoothing operator on M depending smoothly on t with the property that for all $m \in \mathbb{N}_0$, there is a constant $C_m > 0$ such that for all $t \in \mathbb{R}_+$,

$$|H_t(x,y)|_{C^m(M\times M)} \le C_m \frac{1}{1+t}.$$

It is known that (see [20, 21])

$$N, \overline{N}\colon H^s(M) \to H^{s+1}(M) \quad \text{for all } s \in \mathbb{Z},$$
$$\overline{\partial}_b N\colon H^s(M) \to H^{s+\frac{1}{2}}(M, T^{*0,1}M) \quad \text{for all } s \in \mathbb{Z}.$$

From this observation, (9.6) and (11.4), we deduce that

$$SE_2\Box_b NG_tS = O(1)\colon H^s(M) \to H^{s+\frac{1}{2}}(M) \quad \text{for all } s \in \mathbb{Z}.$$

Similarly, we have $\overline{S}E_2\overline{\Box}_b\overline{N}G_t\overline{S} = O(1) : H^s(M) \to H^{s+\frac{1}{2}}(M)$ for all $s \in \mathbb{Z}$. Inserting this into (10.33) yields the claim (11.3).

Now put

$$A_{K,t} = \tau G_t\tau(I - (\tau A_t\tau) + (\tau A_t\tau)^2 - (\tau A_t\tau)^3 + \cdots + (\tau A_t\tau)^{2K+4}) - \tau G_t\tau.$$

From Theorem 10.3 and Lemma 10.8 we observe that $A_{K,t}$ is a smoothing operator of order 3 with size $\frac{1}{\sqrt{1+t}}$, and also $A_{K,t}$ is a smooth operator of order 1 with size $\frac{1}{1+t}$. Moreover, from (9.4) and (11.3) we conclude that

$$A_{K,t} = O(\frac{1}{1+t})\colon H^s(M) \to H^{s+\frac{1}{2}}(M)$$

for all $s \in \mathbb{Z}$. Furthermore, from (11.1), we observe that

$$(\overline{P}'_4 + t + \pi)(\tau G_t\tau + \tau A_{K,t}\tau) = \tau + (\tau A_t\tau)^{2K+5}. \tag{11.5}$$

From (11.3), we see that

$$(\tau A_t\tau)^{2K+4} = O(1)\colon H^s(M) \to H^{s+K+2}(M)$$

for all $s \in \mathbb{Z}$. Moreover, from (9.4) and (11.2), we observe that

$$\tau A_t\tau = O(\frac{1}{1+t})\colon H^s(M) \to H^{s-2}(M)$$

for all $s \in \mathbb{Z}$. Thus, $(\tau A_t\tau)^{2K+5} = O(\frac{1}{1+t})\colon H^s(M) \to H^{s+K}(M)$ for all $s \in \mathbb{Z}$. Combining this with (11.5) yields the result. □

Remark 11.2. It is easy to see that $A_{K,t}$ depends continuously on t in $L^2(M)$.

From now on, we identify the operator $(\overline{P}'_4 + t + \pi)^{-1}\colon \hat{\mathcal{P}} \to \hat{\mathcal{P}}$ with $\tau(\overline{P}'_4 + t + \pi)^{-1}\tau$. Thus $(\overline{P}'_4 + t + \pi)^{-1}\colon L^2(M) \to L^2(M)$. We can extend and identify this operator as follows.

Proposition 11.3. *$(\overline{P}'_4 + t + \pi)^{-1}$ can be continuously extended to $(\overline{P}'_4 + t + \pi)^{-1}\colon H^s(M) \to H^s(M)$ for every $s \in \mathbb{Z}$. Moreover, for every $K \in \mathbb{N}_0$ we have*

$$(\overline{P}'_4 + t + \pi)^{-1} - (\tau G_t\tau + \tau A_{2K,t}\tau) = O(\frac{1}{1+t})\colon H^{-K}(M) \to H^K(M),$$

where $A_{2K,t}$ is as in Proposition 11.1.

Proof. Fix $K \in \mathbb{N}_0$ and let $A_{2K,t}$ and $R_{2K,t}$ be as in Proposition 11.1. Then

$$\tau G_t\tau + \tau A_{2K,t}\tau = (\overline{P}'_4 + t + \pi)^{-1} + (\overline{P}'_4 + t + \pi)^{-1}\tau R_{2K,t}\tau. \tag{11.6}$$

Note that $\tau R_{2K,t}\tau = O(\frac{1}{1+t})\colon H^{-s}(M) \to L^2(M)$ for all $s \in \mathbb{Z}$ with $|s| \leq 2K$. By (9.4), $\tau G_t\tau + \tau A_{2K,t}\tau = O(\frac{1}{1+t})\colon H^s(M) \to H^s(M)$ for all $s \in \mathbb{Z}$. By (9.2), we observe that $(\overline{P}'_4 + t + \pi)^{-1} = O(\frac{1}{1+t})\colon L^2(M) \to L^2(M)$. From these observations we conclude that we can extend to $(\overline{P}'_4 + t + \pi)^{-1}$ to $H^{-s}(M)$ for all $s \in \mathbb{N}_0$ with $s \leq 2K$; indeed

$$(\overline{P}'_4 + t + \pi)^{-1} = O(\frac{1}{1+t})\colon H^{-s}(M) \to H^{-s}(M) \tag{11.7}$$

for all $s \in \mathbb{N}_0$ with $s \leq 2K$. By taking the adjoint in (11.7), we conclude that we can extend to $(\overline{P}_4' + t + \pi)^{-1}$ to

$$(\overline{P}_4' + t + \pi)^{-1} = O(\frac{1}{1+t}) \colon H^s(M) \to H^s(M) \tag{11.8}$$

for all $s \in \mathbb{N}_0$ with $s \leq 2K$. From (11.6) and (11.8) we conclude that

$$(\overline{P}_4' + t + \pi)^{-1} - (\tau G_t \tau + \tau A_{2K,t}\tau) = O(\frac{1}{1+t}) \colon H^{-K}(M) \to H^K(M). \qquad \square$$

Proposition 11.3 allows us to prove the following theorem.

Theorem 11.4. *There is a $G \in L^{-1}_{\rm cl}(M)$ such that $2GE_1 - I \in L_{\rm cl}(M)$ for $E_1 \in L^1_{\rm cl}(M)$ as in Theorem 9.1 and for every $\ell \in \mathbb{N}_0$,*

$$(\overline{P}_4')^{-\frac{1}{2}} = \tau G \tau + \tau A_\ell \tau + \tau R_\ell \tau$$

on $\hat{\mathcal{P}}$, where $A_\ell, R_\ell \colon C^\infty(M) \to \mathscr{D}'(M)$ are continuous operators, $R_\ell(x,y) \in C^\ell(M \times M)$, and A_ℓ is a smooth operator of order $3 - \varepsilon$ for every $0 < \varepsilon < 1$.

Proof. Fix $\ell \in \mathbb{N}_0$ and take $K \gg \ell$. Put

$$\Xi_{2K,t} = (\overline{P}_4' + t + \pi)^{-1} - (\tau G_t \tau + \tau A_{2K,t}\tau),$$

where $A_{2K,t}$ is as in Proposition 11.1. By Proposition 11.3, $\Xi_{2K,t}$ is well-defined as a continuous operator $H^s(M) \to H^s(M)$ for every $s \in \mathbb{Z}$. Observe that $\Xi_{2K,t} = \tau \Xi_{2K,t} \tau$. From Lemma 9.2 we see that

$$(\overline{P}_4')^{-\frac{1}{2}} = c\int_0^\infty t^{-\frac{1}{2}} \tau G_t \tau dt + c\int_0^\infty t^{-\frac{1}{2}} \tau A_{2K,t} \tau dt + c\int_0^\infty t^{-\frac{1}{2}} \tau \Xi_{2K,t} \tau dt.$$

It is known that (see Section 11.2 in [28])

$$c\int_0^\infty t^{-\frac{1}{2}} \tau G_t \tau dt = \tau G \tau,$$

where $G \in L^{-1}_{\rm cl}(M)$ with $2GE_1 - I \in L^{-1}_{\rm cl}(M)$.

We claim that

$$\Xi(x,y) := (c\int_0^\infty t^{-\frac{1}{2}} \Xi_{2K,t} dt)(x,y) \in C^\ell(M \times M)$$

if K is large enough. Fix $k \in \mathbb{N}_0$. For every $m \in \mathbb{N}$, consider

$$\hat{\Xi}_{k,m} := c\sum_{j=1}^m \frac{1}{m} \Xi_{2K,k+\frac{j}{m}} \frac{1}{\sqrt{k + \frac{j}{m}}}.$$

It is clear that, in $L^2(M)$,

$$\lim_{m\to\infty} \hat{\Xi}_{k,m} = c\int_k^{k+1} t^{-\frac{1}{2}} \Xi_{2K,t} dt. \tag{11.9}$$

By Proposition 11.3, we see that

(11.10)

$$\left\|\hat{\Xi}_{k,m}\right\|_{\mathscr{L}(H^{-K}(M), H^K(M))} \leq c_1 \sum_{j=1}^m \frac{1}{m} \frac{1}{1+k+\frac{j}{m}} \frac{1}{\sqrt{k+\frac{j}{m}}} \leq c_1 \int_k^{k+1} \frac{1}{(1+t)\sqrt{t}} dt,$$

where $c_1 > 0$ is a constant and $\left\|\hat{\Xi}_{k,m}\right\|_{\mathscr{L}(H^{-K}(M),H^K(M))}$ denotes the standard operator norm of $\hat{\Xi}_{k,m}$ in $\mathscr{L}(H^{-K}(M),H^K(M))$. From (11.10) and the Sobolev embedding theorem, if $K \gg \ell$, there is a subsequence (m_s) such that $m_s \to \infty$ as $s \to \infty$,

$$\lim_{s\to\infty} \hat{\Xi}_{k,m_s}(x,y) = \Xi_k(x,y) \tag{11.11}$$

in $C^\ell(M \times M)$, and

$$\|\Xi_k(x,y)\|_{C^\ell(M\times M)} \leq \widetilde{c}_1 \int_k^{k+1} \frac{1}{(1+t)\sqrt{t}}dt, \tag{11.12}$$

where $\widetilde{c}_1 > 0$ is a constant independent of k. From (11.9), (11.11) and (11.12), we conclude that

$$\begin{aligned}
&\Xi_k(x,y) = (c\int_k^{k+1} t^{-\frac{1}{2}}\Xi_{2K,t}dt)(x,y) \in C^\ell(M\times M),\\
&\left\|c\int_k^{k+1} t^{-\frac{1}{2}}\Xi_{2K,t}dt\right\|_{C^\ell(M\times M)} \leq \widetilde{c}_1 \int_k^{k+1} \frac{1}{(1+t)\sqrt{t}}dt.
\end{aligned}$$

Since $\sum_{k=0}^\infty \int_k^{k+1} \frac{1}{(1+t)\sqrt{t}}dt = \int_0^\infty \frac{1}{(1+t)\sqrt{t}}dt < \infty$, we deduce that

$$\Xi(x,y) = (c\int_0^\infty t^{-\frac{1}{2}}\Xi_{2K,t}dt)(x,y) = \sum_{k=0}^\infty \Xi_k(x,y) \in C^\ell(M\times M),$$

as claimed.

From now on, we take K large enough so that $\Xi(x,y) \in C^\ell(M\times M)$. Put $A := c\int_0^\infty t^{-\frac{1}{2}}A_{2K,t}dt$. We now study the kernel of A. Fix $x_0, y_0 \in M$ and set $\vartheta(x_0,y_0) = r$. Take $\chi \in C_0^\infty(B_{x_0}(\frac{r}{4}))$ and $\chi_1 \in C_0^\infty(B_{y_0}(\frac{r}{4}))$ such that $\chi = 1$ near x_0 and $\chi_1 = 1$ near y_0. Consider $\widetilde{A} := c\int_0^\infty t^{-\frac{1}{2}}\chi A_{2K,t}\chi_1 dt$. Then,

$$\widetilde{A} = c\int_0^{r^{-4}} t^{-\frac{1}{2}}\chi A_{2K,t}\chi_1 dt + c\int_{r^{-4}}^\infty t^{-\frac{1}{2}}\chi A_{2K,t}\chi_1 dt. \tag{11.13}$$

For every $m \in \mathbb{N}$, consider

$$B_m = c\sum_{j=1}^m \frac{r^{-4}}{m}(\chi A_{2K,\frac{j}{m}r^{-4}}\chi_1)(\frac{j}{m}r^{-4})^{-\frac{1}{2}}.$$

It is easy to see that, in L^2,

$$\lim_{m\to\infty} B_m = c\int_0^{r^{-4}} t^{-\frac{1}{2}}\chi A_{2K,t}\chi_1 dt. \tag{11.14}$$

Recall from Proposition 11.1 that $A_{2K,t}$ is a smoothing operator of order 3 with size $\frac{1}{\sqrt{1+t}}$. From this and (11.14), we have that, for any $x \in B_{x_0}(\frac{r}{4})$, $y \in B_{y_0}(\frac{r}{4})$,

$$\begin{aligned} |B_m(x,y)| &\le c\sum_{j=1}^{m} \frac{r^{-4}}{m}\left|(\chi A_{2K,\frac{r^{-4}j}{m}}\chi_1)(x,y)\right|(\frac{r^{-4}j}{m})^{-\frac{1}{2}} \\ &\le c\sum_{j=1}^{m} \frac{r^{-4}}{m}\frac{1}{\sqrt{1+\frac{r^{-4}j}{m}}}\vartheta(x,y)^{-1}(\frac{r^{-4}j}{m})^{-\frac{1}{2}} \\ &\le c_2\vartheta(x,y)^{-1}\int_0^{r^{-4}}\frac{1}{\sqrt{1+t}}t^{-\frac{1}{2}}dt \\ &\le c_3\vartheta(x,y)^{-1}\left|\log\vartheta(x,y)\right|, \end{aligned}$$

where $c_2 > 0$, $c_3 > 0$ are constants independent of m, r, χ, χ_1, x_0, y_0. Similarly, for every $\alpha_1, \alpha_2 \in \mathbb{N}_0$ and $\varepsilon > 0$, there is a constant $C_{\alpha_1,\alpha_2,\varepsilon}$, independent of m, r, χ, χ_1, x_0, y_0, such that

$$\left|(\nabla_b)_x^{\alpha_1}(\nabla_b)_y^{\alpha_1}B_m(x,y)\right| \le C_{\alpha_1,\alpha_2,\varepsilon}\vartheta(x,y)^{-1-|\alpha|-\varepsilon}. \tag{11.15}$$

From (11.15), we deduce that there is a subsequence (m_s) such that $m_s \to \infty$ as $s \to \infty$ for which $B_{m_s}(x,y)$ converges to some $B(x,y)$ in the $C^\infty(M\times M)$ topology with the property that for every $\alpha_1, \alpha_2 \in \mathbb{N}_0$ and every $\varepsilon > 0$, there is a constant $C_{\alpha_1,\alpha_2,\varepsilon}$, independent of $m, r, \chi, \chi_1, x_0, y_0$, such that

$$\left|(\nabla_b)_x^{\alpha_1}(\nabla_b)_y^{\alpha_2}B(x,y)\right| \le C_{\alpha_1,\alpha_2,\varepsilon}\vartheta(x,y)^{-1-|\alpha|-\varepsilon}. \tag{11.16}$$

In particular, from (11.14) we have that

$$(c\int_0^{r^{-4}} t^{-\frac{1}{2}}\chi A_{2K,t}\chi_1 dt)(x,y) = B(x,y). \tag{11.17}$$

Fix $k \in \mathbb{N}_0$. For every $m \in \mathbb{N}$, consider

$$D_{k,m} := c\sum_{j=1}^{m}\frac{r^{-4}}{m}\chi A_{2K,r^{-4}k+\frac{j}{m}r^{-4}}\chi_1\frac{1}{\sqrt{r^{-4}k+\frac{j}{m}r^{-4}}}.$$

It is clear that

$$\lim_{m\to\infty} D_{k,m} = c\int_{r^{-4}k}^{r^{-4}(k+1)} t^{-\frac{1}{2}}\chi A_{2K,t}\chi_1 dt \tag{11.18}$$

in $L^2(M)$. Recall from Proposition 11.1 that $A_{2K,t}$ is a smoothing operator of order 1 with size $\frac{1}{1+t}$. From this observation, we find that for every $x \in B_{x_0}(\frac{r}{4})$, $y \in B_{y_0}(\frac{r}{4})$, we have that

$$\begin{aligned} |D_{k,m}(x,y)| &\le \widetilde{c}_1\sum_{j=1}^{m}\frac{r^{-4}}{m}\left|(\chi A_{2K,r^{-4}k+\frac{j}{m}r^{-4}}\chi_1)(x,y)\right|(r^{-4}k+\frac{j}{m}r^{-4})^{-\frac{1}{2}} \\ &\le \widetilde{c}_2\sum_{j=1}^{m}\frac{r^{-4}}{m}\vartheta(x,y)^{-3}\frac{1}{1+r^{-4}k+\frac{j}{m}r^{-4}}(r^{-4}k+\frac{j}{m}r^{-4})^{-\frac{1}{2}} \\ &\le \widetilde{c}_2\int_{r^{-4}k}^{r^{-4}(k+1)}\vartheta(x,y)^{-3}\frac{1}{1+t}\frac{1}{\sqrt{t}}dt, \end{aligned}$$

where $\widetilde{c}_1 > 0$, $\widetilde{c}_2 > 0$ are constants independent of k, m, r, χ, χ_1, x_0, y_0. Similarly, for every $\alpha_1, \alpha_2 \in \mathbb{N}_0$, there is a constant C_{α_1,α_2}, independent of $m, k, r, \chi, \chi_1, x_0, y_0$, such that

$$\left|(\nabla_b)_x^{\alpha_1}(\nabla_b)_y^{\alpha_1} D_{k,m}(x,y)\right| \leq C_{\alpha_1,\alpha_2}\int_{r^{-4}k}^{r^{-4}(k+1)} \vartheta(x,y)^{-3-|\alpha|}\frac{1}{1+t}\frac{1}{\sqrt{t}}dt.$$

Therefore there is a subsequence (m_s) such that $m_s \to \infty$ as $s \to \infty$ for which $D_{k,m_s}(x,y)$ converges to some $D_k(x,y)$ in the $C^\infty(M\times M)$ topology with the property that for every $\alpha_1, \alpha_2 \in \mathbb{N}_0$ and every $\varepsilon > 0$, there is a constant $\widetilde{C}_{\alpha_1,\alpha_2,\varepsilon}$ such that

$$\left|(\nabla_b)_x^{\alpha_1}(\nabla_b)_y^{\alpha_2} D_k(x,y)\right| \leq \widetilde{C}_{\alpha_1,\alpha_2,\varepsilon}\int_{r^{-4}k}^{r^{-4}(k+1)} \vartheta(x,y)^{-3-|\alpha|-\varepsilon}\frac{1}{1+t}\frac{1}{\sqrt{t}}dt. \tag{11.19}$$

In particular, from (11.18) we find that

$$\Big(c\int_{r^{-4}k}^{r^{-4}(k+1)} t^{-\frac{1}{2}}\chi A_{2K,t}\chi_1 dt\Big)(x,y) = D_k(x,y). \tag{11.20}$$

Note that for $x \in B_{x_0}(\frac{r}{4})$ and $y \in B_{y_0}(\frac{r}{4})$,

$$\sum_{k=1}^{\infty}\int_{r^{-4}k}^{r^{-4}(k+1)} \vartheta(x,y)^{-3-|\alpha|-\varepsilon}\frac{1}{1+t}\frac{1}{\sqrt{t}}dt \leq \hat{c}_0\vartheta(x,y)^{-1-|\alpha|-\varepsilon}, \tag{11.21}$$

where $\hat{c}_0 > 0$ is a constant. From (11.19), (11.20), and (11.21) we deduce that $(c\int_{r^{-4}}^{\infty} t^{-\frac{1}{2}}\chi A_{2K,t}\chi_1 dt)(x,y) \in C^\infty(M\times M)$ and for every $\alpha_1,\alpha_2 \in \mathbb{N}_0$ and $\varepsilon > 0$, there is a constant $\hat{C}_{\alpha_1,\alpha_2,\varepsilon}$, independent of r, χ, χ_1, x_0, y_0, such that

$$\left|(\nabla_b)_x^{\alpha_1}(\nabla_b)_y^{\alpha_2}\Big(c\int_{r^{-4}}^{\infty} t^{-\frac{1}{2}}\chi A_{2K,t}\chi_1 dt\Big)(x,y)\right| \leq \hat{C}_{\alpha_1,\alpha_2,\varepsilon}\vartheta(x,y)^{-1-|\alpha|-\varepsilon}. \tag{11.22}$$

From (11.13), (11.16), (11.17) and (11.22), we deduce that $A(x,y)$ satisfies the following differential inequalities when $x \neq y$: For every $\varepsilon > 0$ and every $\alpha_1, \alpha_2 \in \mathbb{N}_0$, there is a constant $C_{\alpha_1,\alpha_2,\varepsilon} > 0$ independent of x and y such that

$$|(\nabla_b)_x^{\alpha_1}(\nabla_b)_y^{\alpha_2} A(x,y)| \leq C_{\alpha_1,\alpha_2,\varepsilon}\vartheta(x,y)^{-1-|\alpha|-\varepsilon}. \tag{11.23}$$

Now, we prove that A satisfies the cancellation condition of order $3-\varepsilon$ for every $0 < \varepsilon < 1$. Let ϕ_r be a normalized bump function with $\operatorname{supp}\phi_r \in B(x,r)$, for every $r > 0$. Then

$$\begin{aligned}&\|\nabla_b^\alpha A\phi_r\|_{L^\infty(B(x,r))}\\ &\leq c\int_0^{r^{-4}} t^{-\frac{1}{2}}\left\|\nabla_b^\alpha A_{2K,t}\phi_r\right\|_{L^\infty(B(x,r))} + c\int_{r^{-4}}^{\infty} t^{-\frac{1}{2}}\left\|\nabla_b^\alpha A_{2K,t}\phi_r\right\|_{L^\infty(B(x,r))}.\end{aligned} \tag{11.24}$$

Since $A_{2K,t}$ is a smoothing operator of order 3 with size $\frac{1}{\sqrt{1+t}}$, we have that

$$\int_0^{r^{-4}} t^{-\frac{1}{2}}\left\|\nabla_b^\alpha A_{2K,t}\phi_r\right\|_{L^\infty(B(x,r))} \leq c_2 r^{3-\alpha}\left|\log r\right|, \tag{11.25}$$

where $c_2 > 0$ is a constant independent of r. Since $A_{2K,t}$ is also a smoothing operator of order 1 with size $\frac{1}{1+t}$, we have

$$\int_{r^{-4}}^{\infty} t^{-\frac{1}{2}}\left\|\nabla_b^\alpha A_{2K,t}\phi_r\right\|_{L^\infty(B(x,r))} \leq \hat{c}_1 r^{1-|\alpha|}\int_{r^{-4}}^{\infty} t^{-\frac{1}{2}}\frac{1}{1+t}dt \leq \hat{c}_2 r^{3-\alpha}, \tag{11.26}$$

where $\hat{c}_1 > 0$ and $\hat{c}_2 > 0$ are constants independent of r. From (11.24), (11.25) and (11.26), we deduce that A satisfies the cancellation condition of order $3-\varepsilon$ for every $0<\varepsilon<1$. Similarly, A^* satisfies the cancellation condition of order $3-\varepsilon$ for every $0<\varepsilon<1$. The conclusion follows from (11.23). □

12. The proof of Theorem 1.3

Since the leading order term of P_4' is Δ_b^2, we begin our study of the asymptotics of the Green function of $\left(\overline{P}_4'\right)^{1/2}$ by first considering the operator $2\Delta_b + \frac{1}{2}R$ extended to $L^2(M)$ in the standard way. As $-2\Delta_b + \frac{1}{2}R$ is hypoelliptic with loss of one derivative,

$$-2\Delta_b + \frac{1}{2}R \colon \mathrm{Dom}\,(-2\Delta_b + \frac{1}{2}R) \to L^2(M)$$

has closed range, is self-adjoint, and $\ker(-2\Delta_b+\frac{1}{2}R)$ is a finite-dimensional subspace of $C^\infty(M)$. Let $\hat{N}\colon L^2(M) \to \mathrm{Dom}\,(-2\Delta_b + \frac{1}{2}R)$ be the partial inverse and let $p\colon L^2(M) \to \ker(-2\Delta_b + \frac{1}{2}R)$ be the orthogonal projection. Then p is a smoothing operator on M and we have

$$\begin{aligned}
&\hat{N}(-2\Delta_b + \frac{1}{2}R) + p = I \quad \text{on } \mathrm{Dom}\,(-2\Delta_b + \tfrac{1}{2}R),\\
&(-2\Delta_b + \frac{1}{2}R)\hat{N} + p = I \quad \text{on } L^2(M).
\end{aligned}$$

Note that $\hat{N}\colon H^s(M) \to H^{s+1}(M)$ for all $z \in \mathbb{Z}$. Moreover, $\hat{N}$ is a smoothing operator of order 2 (see [23, Section 10] and [29]).

Proposition 12.1. *With the notations above, $\tau G \tau - \tau\hat{N}$ is a smoothing operator of order 3, where $G \in L^{-1}_{\mathrm{cl}}(M)$ is as in Theorem 11.4.*

Proof. From Theorem 8.1 and Theorem 11.4, we have that

$$(\tau G\tau)(\tau(-2\Delta_b + \frac{R}{2})\tau) = \tau + \tau P_{-1}\tau - \tau G(I-\tau)(2E_1 + \frac{R}{2})\tau, \tag{12.1}$$

where $P_{-1} \in L^{-1}_{\mathrm{cl}}(M)$.

We claim that

(12.2) $\tau P_{-1}\tau$ is a smoothing operator of order 2,

(12.3) $\tau G(I-\tau)(2E_1 + \frac{R}{2})\tau$ is a smoothing operator of order 1.

From Theorem 7.1 and Lemma 8.3, we have that

$$\tau P_{-1}\tau \equiv SP_{-1}S + \overline{S}P_{-1}\overline{S}. \tag{12.4}$$

From Lemma 8.2 and Lemma 8.3 we have that

$$\begin{aligned}
SP_{-1}S \equiv S\overline{N}\,\overline{\Box}_b P_{-1}S &= S\overline{N}\Box_b P_{-1}S + S\overline{N}L_1P_{-1}S\\
&= S\overline{N}[\Box_b, P_{-1}]S + S\overline{N}L_1P_{-1}S,
\end{aligned} \tag{12.5}$$

where L_1 is a first order partial differential operator. From the symbolic calculus of Stein–Yung [29], we check that $[\Box_b, P_{-1}]S$ and $L_1P_{-1}S$ are smoothing operators of order 0. From this observation, (12.5) and Theorem 10.3, we conclude that $SP_{-1}S$ is a smoothing operator of order 2. Similarly, $\overline{S}P_{-1}\overline{S}$ is a smoothing operator of order 2. From (12.4), we obtain (12.2).

Again, from Theorem 7.1, Lemma 8.2 and Lemma 8.3, we have that

$$\begin{aligned}
&\tau G(I-\tau)(2E_1+\frac{R}{2})\tau \\
&\equiv SG(I-S)(2E_1+\frac{R}{2})S+\overline{S}G(I-\overline{S})(2E_1+\frac{R}{2})\overline{S} \\
&\equiv SG\overline{\Box}_b\,\overline{N}N\Box_b(2E_1+\frac{R}{2})S+\overline{S}G\Box_bN\overline{N}\,\overline{\Box}_b(2E_1+\frac{R}{2})\overline{S} \qquad (12.6)\\
&= S[G,\Box_b]\overline{N}N\overline{\partial}_b^*[\overline{\partial}_b,2E_1+\frac{R}{2}]S+SGL_1\overline{N}N\overline{\partial}_b^*[\overline{\partial}_b,2E_1+\frac{R}{2}]S \\
&\quad+\overline{S}[G,\overline{\Box}_b]N\overline{N}\partial_b^*[\partial_b,2E_1+\frac{R}{2}]\overline{S}+\overline{S}G\overline{L}_1N\overline{N}\partial_b^*[\partial_b,2E_1+\frac{R}{2}]\overline{S},
\end{aligned}$$

where L_1 is a first order partial differential operator. Since $\overline{N}N\overline{\partial}_b^*[\overline{\partial}_b,2E_1+\frac{R}{2}]S$, $N\overline{N}\partial_b^*[\partial_b,2E_1+\frac{R}{2}]\overline{S}$ are smoothing operators of order 1 and $S[G,\Box_b]$, SGL_1, $\overline{S}[G,\overline{\Box}_b]$, $\overline{S}G\overline{L}_1$ are smoothing operators of order 0 (see [29]), we may combine (12.6) and Theorem 10.3 to deduce (12.3).

Recalling that $-\Delta_b=\Box_b+\overline{\Box}_b$, we conclude from Theorem 7.1, Lemma 8.2, and Lemma 8.3 that

(12.7)

$$\begin{aligned}
(\tau(-2\Delta_b+\frac{R}{2})\tau)\hat{N} &\equiv \tau-\tau(-2\Delta_b+\frac{R}{2})(I-\tau)\hat{N} \\
&\equiv \tau-S(-2\Delta_b+\frac{R}{2})(I-S)\hat{N}-\overline{S}(-2\Delta_b+\frac{R}{2})(I-\overline{S})\hat{N} \\
&= \tau-S(\overline{\Box}_b+\frac{R}{2})\Box_bN\hat{N}-\overline{S}(\Box_b+\frac{R}{2})\overline{\Box}_b\,\overline{N}\hat{N} \\
&\equiv \tau-S[L_1+\frac{R}{2},\overline{\partial}_b^*]\overline{\partial}_bN\hat{N}-\overline{S}[\overline{L}_1+\frac{R}{2},\partial_b^*]\partial_b\overline{N}\hat{N},
\end{aligned}$$

where L_1 is a first order partial differential operator. Since $[L_1+\frac{R}{2},\overline{\partial}_b^*]\overline{\partial}_bN\hat{N}$ and $[\overline{L}_1+\frac{R}{2},\partial_b^*]\partial_b\overline{N}\hat{N}$ are smoothing operators of order 1 (see [29]), we may combine (12.7) and Theorem 10.3 to deduce that

$$(\tau(-2\Delta_b+\frac{R}{2})\tau)\hat{N}=\tau+H, \qquad (12.8)$$

where H is a smoothing operator of order 1. From (12.1) and (12.8), we find that

$$\tau G\tau+(\tau G\tau)H=\tau\hat{N}+(\tau P_{-1}\tau)\hat{N}-\tau G(I-\tau)(2E_1+\frac{R}{2})\tau\hat{N}. \qquad (12.9)$$

We can repeat the proof of (12.2) and deduce that $\tau G\tau$ is a smoothing operator of order 2 and hence

(12.10) $(\tau G\tau)H$ is a smoothing operator of order 3.

From (12.2), (12.3), (12.9) and (12.10) we deduce that $\tau G\tau-\tau\hat{N}$ is a smoothing operator of order 3. □

Fix a point $\zeta\in X$. The Green function of $(\overline{P}_4')^{\frac{1}{2}}$ at ζ is given by

$$G_\zeta:=(\overline{P}_4')^{-\frac{1}{2}}\tau\delta_\zeta\tau\in\mathscr{D}'(M).$$

It is easy to see that

$$(\overline{P}_4')^{\frac{1}{2}}G_\zeta=\delta_\zeta-\pi(x,\zeta)\text{ on }\mathcal{P}.$$

Note that $\pi(x,\zeta) \in C^\infty(M) \cap \ker(\overline{P}'_4)^{-\frac{1}{2}}$.

Proof of Theorem 1.3. Fix $\zeta \in M$ and let (z,t) be CR normal coordinates defined in a neighborhood of ζ such that $(z(\zeta), t(\zeta)) = (0,0)$. For $m \in \mathbb{R}$, let $\mathcal{E}(\rho^m)$ be as in the discussion before Theorem 1.3. Let $\ell_0 \in \mathbb{N}_0$ and fix $\ell \gg \ell_0$. From Theorem 11.4 and Proposition 12.1, we have

$$\begin{aligned} G_\zeta &= \tau G \tau \delta_\zeta \tau + \tau A_\ell \tau \delta_\zeta \tau + \tau R_\ell \tau \delta_\zeta \tau \\ &= \tau \hat{N} \delta_\zeta \tau + \tau K \delta_\zeta \tau + \tau A_\ell \tau \delta_\zeta \tau + \tau R_\ell \tau \delta_\zeta \tau, \end{aligned} \tag{12.11}$$

where K is a smoothing operator of order 3. Since $R_\ell(x,y) \in C^\ell(M \times M)$, we can take ℓ large enough so that

$$R_\ell \tau \delta_\zeta \in C^{\ell_0}(M). \tag{12.12}$$

Since K is a smoothing operator of order 3,

$$K\delta_\zeta \in \mathcal{E}(\rho^{-1}). \tag{12.13}$$

From Theorem 10.3 and Theorem 11.4 we see that $A_\ell \tau$ is a smoothing operator of order $3-\varepsilon$, for every $0 < \varepsilon < 1$. Hence,

$$A_\ell \tau \delta_\zeta \in \mathcal{E}(\rho^{-1-\varepsilon}) \tag{12.14}$$

for all $0 < \varepsilon < 1$.

Finally, we consider $\hat{N}\delta_\zeta$. It is clear that $\hat{N}\delta_\zeta$ is the Green function of $2\Delta_b + \frac{1}{2}R$. It was shown in [10, Section 5] that, near ζ, $\hat{N}\delta_\zeta$ has the form

$$\hat{N}\delta_\zeta(z,t) = \rho(z,t)^{-2} + \omega_0 \tag{12.15}$$

for some $\omega_0 \in C^1(M)$. Moreover, repeating the method in [23, Section 10], we conclude that

$$\omega_0 \in \mathcal{E}(\rho^{-\varepsilon}) \tag{12.16}$$

for all $\varepsilon > 0$. The conclusion follows from (12.11), (12.12), (12.13), (12.14), (12.15) and (12.16). ☐

Now, we can prove Theorem 4.2:

Proof of Theorem 4.2. In view of (2.2), we see that $\overline{P}'_4 = \tau(4\Delta_b^2 + L_2)\tau$, where $L_2 = \nabla_b^2 + \nabla_b + r$, $r \in C^\infty(X)$. Let H be a parametrix of $4\Delta_b^2 + L_2$. Then $H\colon H^s(M) \to H^{s+2}(M)$ for every $s \in \mathbb{Z}$ and H is a smoothing operator of order $4-\varepsilon$ for every $0 < \varepsilon < 1$. From Theorem 7.1 and Lemma 8.3, we have that

$$\begin{aligned} \tau H \tau \overline{P}'_4 &= (\tau H \tau)(\tau(4\Delta_b^2 + L_2)\tau) \\ &= \tau - \tau H(I-\tau)(4\Delta_b^2 + L_2)\tau - F_0 \\ &= \tau - SH(I-S)(4\Delta_b^2 + L_2)S - \overline{S}H(I-\overline{S})(4\Delta_b^2 + L_2)\overline{S} - F_1, \end{aligned} \tag{12.17}$$

where F_0 and F_1 are smoothing operators on M. Put

$$\Upsilon = SH(I-S)(4\Delta_b^2 + L_2)S + \overline{S}H(I-\overline{S})(4\Delta_b^2 + L_2)\overline{S} + F_1. \tag{12.18}$$

Note that $\Upsilon = \tau\Upsilon\tau$. Repeating the procedure in (12.7), we conclude that

$$\begin{aligned} SH(I-S)(4\Delta_b^2 + L_2)S &= SHN\overline{\partial}_b^* Q_2 S, \\ \overline{S}H(I-\overline{S})(4\Delta_b^2 + L_2)S &= \overline{S}H\overline{N}\partial_b^* \widetilde{Q}_2 \overline{S}, \end{aligned} \tag{12.19}$$

where $Q_2, \widetilde{Q}_2 \in L^2_{\mathrm{cl}}(M)$. From (12.18) and (12.19), we conclude that $\Upsilon\colon H^s(M) \to H^{s+\frac{1}{2}}(M)$ for all $s \in \mathbb{Z}$ and Υ is a smoothing operator of order 1. Fix $K \in \mathbb{N}$. Put

$$B_K := (\tau H \tau)(\tau + \Upsilon + \Upsilon^2 + \cdots + \Upsilon^K).$$

Then, B_K is a smoothing operator of order $4 - \varepsilon$ for all $0 < \varepsilon < 1$. From (12.17), we have that

$$B_k \overline{P}'_4 = \tau - \Upsilon^{K+1}.$$

Since $\Upsilon^{K+1}\colon H^s(M) \to H^{s+\frac{K+1}{2}}(M)$ for every $s \in \mathbb{Z}$, given $\ell \in \mathbb{N}_0$, we can take K large enough so that $\Upsilon^{K+1}(x,y) \in C^\ell(M \times M)$. The theorem follows. ☐

To prove Theorem 4.3, we need the following Adams-type theorem of Fontana and Morpurgo [12].

Theorem 12.2. *Let $A\colon L^2(M) \to L^2(M)$ be a continuous operator with distribution kernel $A(x,y) \in C^\infty(M \times M \setminus \operatorname{diag}(M \times M))$. Suppose that the kernel $A(x,y)$ satisfies*

$$\sup_{x\in M} \left|\{y \in M : \, |A(x,y)| > s\}\right| \leq K s^{-2},$$
$$\sup_{y\in M} \left|\{x \in M : \, |A(x,y)| > s\}\right| \leq K s^{-2}$$

as $s \to \infty$, where $K > 0$ is a constant and

$$\left|\{y \in M : \, |A(x,y)| > s\}\right|, \quad \left|\{x \in M : \, |A(x,y)| > s\}\right|$$

denote the volumes of the sets $\{y \in M \colon |A(x,y)| > s\}$ and $\{x \in M\colon |A(x,y)| > s\}$, respectively with respect to the given volume form on M. Then, for any $f \in L^2(M)$ with $Tf \in L^2(M)$, there is a constant $c > 0$ such that $e^{c|f|^2} \in L^1(M)$.

Proof of Theorem 4.3. Put $g := (-\Delta_b + I)w \in L^2(M)$. Let Q be the inverse of $-\Delta_b + I$. Then, $w = Qg$. It is known that (see [10, Section 2] and [23, Section 10])

$$|Q(x,y)| \lesssim \vartheta(x,y)^{-2}. \tag{12.20}$$

From (12.20), one readily checks that

$$\begin{aligned} &\sup{}_{x\in M} \left|\{y \in M : \, |Q(x,y)| > s\}\right| \lesssim s^{-2}, \\ &\sup{}_{y\in M} \left|\{x \in M : \, |Q(x,y)| > s\}\right| \lesssim s^{-2}, \end{aligned} \tag{12.21}$$

as $s \to \infty$. The conclusion follows from (12.21) and Theorem 12.2. ☐

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